JOURNAL OF THE MYANMAR ACADEMY OF ARTS AND SCIENCE



Physics

Vol. XVII, No.2B, August 2019

Myanmar Academy of Arts and Science

Journal of the Myanmar Academy of Arts and Science Vol. XVII, No. 2B

Contents

Physics

<u>Sr. No.</u>	<u>Title</u>	Page
1	Moe Moe Aung. Radionuclide Levels in Coal Ash Sample Discharged from Cement Factory	1
2	Min Maung Maung , Structural Characterization and Magnetic Properties of Rubber Ferrite Composites	9
3	Sint Ohnmar Preparation and Characterization of Chitosan-Based Solid Polymer Electrolyte Films with Zinc Acetate	23
4	Thant Thant Zin, Study on Characterization of Chitosan-ZnO Film	35
5	Aye Thandar, Feasibility Study of Bamboo Ash on Concrete Members	49
6	Kyauk Khe Sein, Estimate of Uncertainty of Measurement in the Determination of Cu, Zn, Fe in Proficiency Test (PT) Drinking Water Sample	65
7	Nyunt Win, Synergic Synthesis Route for the Fabrication of Organic-Inorganic Composite Film	77
8	Ei Shwe Sin Oo, Acoustic Property of Polyurethane-TiO ₂ Composite Foams	89
9	Khin Win Mu, Fast and Facile Synthesis of Copper Nanowires and Their Application as Conductive Ink	105
10	Mi Mu Mu Khaing, Synthesis of Copper Nanoparticles for Application of Conductive Ink	115
11	Saw Thiri, Synthesis of Silver Nanowires Using NaCl Assisted Ethylene Glycol Mediated Polyol Method	123
12	Su Myat Aung, Chemical Bath Deposition of Zinc Oxide Nanoflower Film on Silver Nanoparticle Seed Layer	137
13	Aung Zaw Oo, GPS-GSM Based Location and Position Tracking System	149
14	Zin Bo Htut , Characterization of Perovskite-Type $XSnO_3$ (where $X = Ca$, Sr and Ba) Ceramics	163

<u>Sr. No.</u>	<u>Title</u>	Page
15	Wai Khaing Moe , Synthesis and Characterization of Magnesium-Zinc Ferrite Prepared by Flash-Combustion Technique	179
16	Tin Tin Htay Phantom Scalar Fields and Its Physical Implications	197
17	Hla Hla Maw, Dynamical Systems Approach to FRW Models	215
18	Nyein Thida, Theoretical and Numerical Aspects of Gravitational Waves	223
19	Yee May Thwin, An Analysis of Numerical Hydrodynamics for Spherically Symmetric Spacetimes	235
20	Naing Naing Wint Htoon, Simple Simulations of Massless Scalar Field Minimally Coupled to Gravitational Field	243
21	Zaw Shin , Simple Astrophysical Simulations for Collisionless Stellar Systems	251
22	Htwe Nwe Oo [•] Gravitational Collapse in Self- Similar Spacetimes	265
23	Han Win Than, Axion Dark Matter, CP Violation Problem in QCD	277
24	San San Maw , Simple Simulations of Magnetohydrodynamics in Star Formations	283
25	Zin Min Myat, Synthesis and Characterization of Dye-Sensitized Solar Cell Based on Silver Oxide Nanowires	293
26	Nway Han Myat Thin, Characterization and Dielectric Properties of Zinc Titanate (ZnTiO ₃) Ceramics	307
27	Thin Thin Kyu, Structural, Morphological and Optical Studies of Zinc Oxide (ZnO) Thin Films Prepared by Chemical Bath Deposition Technique	321
28	Kyaw Thu , Analysis of Time of Flight of ⁸ He Nuclei in Nuclear Emulsion using Range-Energy Relation Program	333
29	Cho Cho San., Comparison Between Single particle Energy States of ${}^{12}_{A}C$ And ${}^{12}_{C}C$	343
30	Khin Su Su Han, Investigation of Nickel Contained from Sulfide Ore Deposit Samples in Namtu Mine Area By Measuring Half-Life of Cobalt-58	353

<u>Sr. No.</u>	<u>Title</u>	Page 1
31	Ei Ei Minn , Real-Time Audio Transmission System Based on Visible Light Communication	365
32	No No Htike , Coupled-Channels Analysis for Heavy-Ion Fusion Reactions of ${}^{16}O + {}^{A}X$ systems	375
33	Su Mon Myat, Improtance of Transfer Channels in Sub-barrier Fusion Reactions	383
34	Khin Sandar Khaing, Investigation of Environmental Pollution Impacts on Radon Levels and Elemental Contents in Agricultural Soil Samples from Myingyan Township	391
35	Zar Zar Myint Aung , Study on Structural and Magnetic Properties of Ytterbium doped Zinc Ferrite Prepared by Solid State Method	407
36	Myat Shwe Wah , Structure and Magnetic Properties of Nanocrystalline NiZnFe ₂ O ₄ Prepared via Conventional Ceramic Method	415
37	Mar Mar Htay, Theoretical Investigation on Λ (1405) Resonance Within $\overline{K}N$ Frame Work of $\overline{K}N - \Sigma^+\pi^-$ Coupled Channel	425
38	Thet Thet Naing, Photovoltaic Performance of MEH-PPV:PCBM Polymer Solar Cells with an Integration of Zinc Oxide (ZnO) Nanoparticles	437
39	Yin Mar Aung , Single-Particle Energy Levels of Even-Even Silicon Isotope	447
40	Khaing Pwint Wai, Calculation of Potential Energy Surfaces for Light Nuclei in $\beta - \gamma$ Plane	457
41	Hnin Nu Aye , Constructing a Coupled Channel $\overline{K}N-\pi\Sigma$ Separable Potential	465
42	MayThawdaPhoo,SynthesisandCharacterizationofCopperZincSulphide(CuZnS2)Thin FilmsFilmsFilmsFilms	477

RADIONUCLIDE LEVELS IN COAL ASH SAMPLE DISCHARGED FROM CEMENT FACTORY

Moe Moe Aung¹, Ni Ni Lwin²

Abstract

This research work was to analyze the content of radionuclide in coal ash sample which collected from Myanmar Elephant cement factory, Pathein Gyi Township, Mandalay division. The HPGe detector was used for the study of radionuclide in coal ash sample and analyzed by using Gamma Vision-32 software. The radionuclide present in coal ash sample such as Bi-207, U-235, Ac-228, Pb-212, Pb-214, Tl-208, Bi-214 and K-40 were observed. But Bi-207 and K-40 do not exactly present in coal ash sample. The radionuclide (Ac-228, Pb-212, Pb-214, Tl-208 and Bi-214) found in the measured sample was the daughter nuclei of Actinium, Uranium and Thorium series. U-235 is the parent nucleus of Actinium series. It is expected that Actinium, Uranium and Thorium are concentrated in coal ash sample.

Introduction to Coal and Coal Ash

1.1 Coal

Coal is a fossil fuel created from the remains of plants that lived and died millions of years ago. Coal is the most carbon-rich of all fossil fuels and generates 70% more carbon dioxide (CO_2) than natural gas for every unit of energy produced. This carbon dioxide is dangerous to human health and greatly contributes to global warming.

Coal forms when dead plant matter is converted into peat, which in turn is converted into lignite, then sub-bituminous coal, after that bituminous coal, and lastly anthracite. Coal is located worldwide – it can be found on every continent in over 70 countries, with the biggest reserves in the United States, Russia, China and India.

Coal is used to make electricity. The steel and iron industries use coal for smelting metals. Other industries use coal, too. Paper, brick, limestone, and cement industries all use coal to make products.

^{1.} Demonstrator, Department of Physics, University of Magway

² Head and Professor (Rtd.), Department of Physics, Yadanabon University

1.2 Coal Ash

Coal ash is the waste left over from burning coal. Coal ash can be breathed into a person' s lungs and can cause serious respiratory problems. Coal ash can carry heavy metals into water sources, poisoning ground water and drinking water nearby coal dump storage sites.

1.3 Health Effects and Environmental Effects of Coal

Burning coal releases enormous amounts of harmful pollutants into the air and water, with serious health consequences. In the United States, power plant pollution is responsible for 38,200 nonfatal heart attacks and 554,000 asthma attacks each year.

Burning coal can pollute the air. It also produces carbon dioxide and pollutes the air with sulfur dioxide, and nitrogen oxides, all of which can cause respiratory problems.

Burning coal can pollute the water. A single large power plant may require several hundred acres of landfill space to dispose of its coal ash, which causes the destruction of green areas. The pollutants in the coal ash can get into the soil and contaminate ground water and drinking water nearby coal dump storage sites, endangering marine life, poisoning the fish we eat.

Experimental Procedure

2.1 Sample Collection and Preparation for Gamma Ray Detection Method

Coal ash sample was collected from Myanmar Elephant cement factory, Pathein Gyi Township, Mandalay division. 500g of coal ash sample was transferred to plastic container for gamma activity analysis.

2.2 Experimental Set-Up for Gamma Emission Measurement

In gamma ray spectroscopy system, the follow equipment's were included. They were HPGe detector ORTEC (model GMX 10P4- 70- RB-SMN), cooler (model CFG- X- COOL-III- 230), preamplifier (model A257N), fast spectroscopy amplifier ORTEC (Model- 671), high voltage power supply, photomultiplier tube, digital signal processor (DSPEC-LF), a pulse stored

multi-channel analyzer (MCA) together with Gamma Vision-32 software installed in PC and data readout devices. The operation voltage for HPGe detector is negative 1500 V dc. The experimental setup is as shown in Figure (3.1).

To reduce a possible background radiation that comes from the environment, lead (Pb) shielding (thickness is 7 cm) was used in this measurement. For present measurement, the sample (500g) was placed in container and measured for about 3 hours. The background spectrum was measured with the same condition. At the end of the counting period, the spectrum that was recorded may be displayed on the screen. The spectra stored in MCA were analyzed by the application of Gamma Vision-32 software. Using the displayed energy information, an unknown radioisotope can be identified radionuclide with activity concentration and a picture of the spectrum and then determined by gross and net area of full energy peak.

2.3 Calculation of Activity

The activity of the coal ash sample was calculated by following equation

$$A = \frac{N_A}{m \epsilon P_{\gamma} T}$$
(2.1)

Where, N_A = net count rate for sample

m = mass of sample

 P_{γ} = gamma ray intensity

T = counting time (in second)

 ϵ = efficiency of the interest gamma energy



Figure 2.1: Coal Ash Sample



Figure 2.2: The photo of the experimental set up of HPGe detection system

Results and Discussions

3.1 Results

The presence of radionuclide in coal ash sample was investigated with HPGe detector and analyzed using Gamma Vision-32 Software. The radionuclide present in coal ash sample are²⁰⁷Bi, ²³⁵U, ²²⁸Ac, ²¹²Pb, ²¹⁴Pb, ²⁰⁸Tl, ²¹⁴Bi and ⁴⁰K. They were found at different energies. The energy spectra of the background and coal ash sample are shown in Figure (3.1) and (3.2). The activity of radionuclide in this sample is also shown in Table (3.1).

3.2 Discussions

The radionuclide present in coal ash sample was collected by the HPGe detector. ²⁰⁷Bi, ²¹⁴Pb, ²³⁵U, ²²⁸Ac, ²¹²Pb, ²⁰⁸Tl, ²¹⁴Bi and ⁴⁰K were found in the spectrum. But ²⁰⁷Bi and ⁴⁰K do not exactly present in coal ash sample. They were found at different energies. Also, they have different activities.

 $(^{214}\text{Pb} \text{ and } ^{214}\text{Bi})$ are the daughter nuclei of ^{238}U and $(^{212}\text{Pb}, ^{208}\text{Tl})$ and ^{228}Ac are the daughter nuclei of ^{232}Th decay series. ^{235}U is the parent nucleus of Actinium decay series.

It was found in the amount of 500g of coal ash sample that high levels of radionuclide and the activity of each radionuclide, is also very much higher than the world standard of average activity. The average specific activity of ²³²Th and ²³⁸U at standard deviations was found to be 39.8 \pm 18.8 and 34.4 \pm 22.0 Bqkg⁻¹ in the typical coal ash sample.



Figure 3.1: The energy spectrum of the background



Figure 3.2: The energy spectrum of the Coal ash sample

Sr.No	Radionuclides	Energy(keV)	Activity(Bq/kg)
1	²⁰⁷ Bi	74.97	218.59
2	²⁰⁷ Bi	87.30	487.29
3	²³⁵ U	143.76	39.53
4	²³⁵ U	185.71	61.73
5	²²⁸ Ac	209.40	112.43
6	²¹² Pb	238.63	113.25
7	²¹⁴ Pb	295.21	486.07
8	²²⁸ Ac	338.40	117.62
9	²¹⁴ Pb	351.92	501.32
10	²⁰⁸ Tl	510.72	119.06
11	²⁰⁸ Tl	583.14	38.36
12	²¹⁴ Bi	609.31	478.24
13	²¹⁴ Bi	768.36	716.24
14	²⁰⁸ Tl	860.47	160.14
15	²²⁸ Ac	911.07	68.11
16	214 Bi	934.06	599.59

 Table 3.1: The activity of radionuclide in coal ash sample

Sr.No	Radionuclides	Energy(keV)	Activity(Bq/kg)
17	²²⁸ Ac	968.90	143.56
18	²¹⁴ Bi	1120.29	407.41
19	²¹⁴ Bi	1155.19	484.16
20	²¹⁴ Bi	1238.11	478.33
21	²¹⁴ Bi	1377.67	543.27
22	⁴⁰ K	1460.75	849.78

Acknowledgements

Author gratefully acknowledges to Dr Ni Ni Lwin, Head and Professor (Retd.), Department of Physics, Yadanabon University, for her patience, kindness, excellent advice and continuous guidance throughout this research work.

References

- A.K. Sam et al., "Radiological Evaluation of Gold Mining Activities in Ariab" Eastern Sudan, (2000).
- Bickel L., "The story of uranium: The deadly element", Stein and Day, New York, (1979).
- Cox P.A., "The elements, their origin, abundance and distribution", Oxford University Press, (1989).
- http:// www.nucleide.org/ DDEP WG/ DDEP data.htm.

IAEA-368.

- IAEA, Preparation and certification of IAEA gamma spectrometry reference materials RGU-1, RGTh-1 and RGK-1. Report No. IAEA/RL/148, International Atomic Energy Agency, Vienna (1987).
- IAEA, Measurement of radionuclides in food and the environment: A guide book. Technical Reports Series No. STI/DOC/10/295, International Atomic Energy Agency, Vienna (1989).
- M.Tzortzis et al., "Gamma ray measurement of naturally occurring radioactive samples from Cyprus characteristic geological rocks", Medical Physics Department, Nicosia (2000).
- ORTEC Application Note, "AN-34", Second Edition, USA (1976).
- UNSCEAR (United Nations Scientific Committee on the Effects of Atomic Radiation) Report to the general assembly. Annex B: exposures from natural radiation sources (2000).

STRUCTURAL CHARACTERIZATION AND MAGNETIC PROPERTIES OF RUBBER FERRITE COMPOSITES

Min Maung Maung¹, Thein Tun Linn², and Aung Min³

Abstract

Rubber ferrite composites (RFCs) were prepared by incorporating ferrites in rubber matrixes has the advantage of easy flexibility. The loading of barium ferrite and nickel ferritein natural rubber matrices(120 phr) have been prepared with rubber accelerator chemical agents and using the processes of mixing, stirring and milling. The dielectric constant of the composite as well as the ferrite filler and natural rubber vulcanization was analyzed by Instek GW 821 LCR meter. The dielectric constant decreased with increase of frequency for ceramic samples of NFO and BFO, natural rubber vulcanisate and for the RFC samples. Magnetic hysteresis was measured by using a Permagraph L apparatus at room temperature. The remanence (B_r) and coercivity (H_c) were derived from the hysteresis loops. From the magnetic behaviour results, a rather low density, high coercivity, large stored energy and high flexibility rubber ferrite composites was successfully obtained.

Keywords: Hysteresis; magnetic properties; natural rubber; remanence; coercivity; Permagraph L; XRD; Grain size; composites.

Introduction

Ferrites represent an important category of materials, which are largely used, due to their numerous practical applications, as for example magnetic devices in electronic, optical and microwave installations. The M-type of ferrites with general formula MeO.6Fe₂O₃, where Me is divalent metal such as Ba, Sr or Pb, have been extensively used as permanents magnets due to their low cost, high coercivity and remanent magnetic induction.

Ferrospinel compounds are a very important group of magnetic materials due to their extensive use in a wide range of applications from low to high permeability devices including electronics, ferrofluid, magnetic drug delivery microwave devices and high density information storage devices.

¹ Dr, Associate Professor, Department of Physics, Dawei University

² Assistant Lecturer, Department of Physics, Hpaan University

³ Assistant Lecturer, Department of Physics, Mawlamyine University

Polymers and polymer based composites are playing a crucial role in the day to day life of human beings. With the advent of nanotechnology aided by the capacity to modify the electrical, mechanical and magnetic properties of polymers, polymer composites are increasingly playing a lead role in everyday life. The magnetic polymer composites especially rubber ferrite composites is one of the many composite materials in which the scientist and engineers are interested and find scope for possible exploitation of commercial applications. High flexibility, chemical resistance and easy moudability are the main attributes of rubber magnetic composites.

The main focus of this research work was to synthesis, characterize and investigate the magnetic, dielectric properties of Nickel ferrite, Barium ferrite and rubber-Ni/Ba ferrite composites. The natural rubber is chosen as one of the polymer matrixes because of its easy availability and low cost.

Materials and Experimental Methods

Natural Rubber

Natural rubber (NR) is obtained from the sap of a tree caned 'caoutchou' or 'weeping wood' and is botanicalty known as 'Hevea Brasiliensis', named after the large forest tree, which is its outstanding source. The chemical name of natural rubber is polyisoprene, since it is a polymer of isoprene. Rubber is a poor conductor of electricity and hence it is very valuable as an electrical insulator. Some of the applications include the manufacture of automobile tyres, mechanical goods, footwear, hoses, beltings, adhesives and latex based products like gloves, foam rubber and thread. Rubber in this research work was collected from Mawlamyine district, Mon state (Myanmar).

Preparation of Nickel ferrite

Nickel nitrate Ni(NO₃)₂·7H₂O, ferric nitrate Fe(NO₃)₃·9H₂O, citric acid and liquor ammonia have been used as starting materials. The polycrystalline nickel ferrites were prepared by the sol-gel combustion method. Stoichiometricamounts of cationic salts were weighed separately and dissolved in minimum amount of deionised water to make clear solution; they are mixed and stirred for 1 hr to get ahomogenous solution. Citric acid

solution is prepared in deionised water and 1 : 1 molarratio of metal nitrates to citric acid solutions were mixed and stirred. A small amount of liquor NH_3 was added to the solution to adjust the pH value at 7.0. The solution was heated, stirred continuously to transform into a highly viscous gel. The gel was heated gradually up to 90°C, to evolve reddish brown color gases and finally the dried gel was finally burnt-out completely to form loose powders. These particles are further purified by acetone and toluene to get dark brown precipitate or black precipitate. Finely powdered materials were annealed at 800°C for 2 h for further crystallization. The sizes of particles were calculated by X-ray diffraction patterns.

Preparation of Barium ferrite

Barium ferrite (BaFe₁₂ O_{19}) is a magnetic material, in the form of nanoparticles, having a hexagonal crystal structure, resistance to high temperature. resistance to corrosive and oxidative environments. Nanostructured barium hexaferrite powders were synthesized using the solgel combustion method. The starting materials were iron nitrate, barium nitrate, citric acid and ammonia, all of analytic purity. Appropriate amount of $Fe(NO_3)_3 \cdot 9H_2O$ and $Ba(NO_3)_2$, in a molar ratio of 12:1, were dissolved in a minimum amount of deionized water. Citric acid was then added into the prepared aqueous solution to chelate Ba2+ and Fe3+ in the solution, thensonicated for 20 min. The mixed solution was neutralized to pH 7 by adding liquor ammonia. The neutralized solution was evaporated to dryness by heating at 100 °C on a hot plate with continuous stirring. As water evaporated, the solution became viscous and finally formed a very viscous brown gel. Increasing the temperature up to about 300 °C led to the ignition of the gel. The dried gel burnt in a self-propagating combustion manner until all gels are completely burnt out to form a loose powder. Finally, the as-burnt powders were calcined in air at 1000 °C for 2 h to obtain barium hexaferrite nanoparticles. The flow diagram of sol-gel combustion method for ferrites was shown in figure 1. The photo graph of preparation of ferrite powder samples were shown in figure 2.

Preparation of rubber ferrite composites

Rubber ferrite composites are magnetic polymer composites consisting of ferrite fillers and natural rubber matrix. Nickel ferrite and Barium ferrite prepared by sol-gel auto-combustion method wereincorporated in a natural rubber matrix at loadings of 120 phr to obtain rubber ferrite composites (RFCs). The incorporation of ferrite in a natural rubber matrix was performed by appropriate amounts of ZnO, Stearic acid, cyclohexyl-2-benothiazole sulphonamide (CBS) and sulphur. The mixing was carried out in a ceramic. The temperature of the mixing cup is controlled by magnetic stirred can bevaried up to 300°C. Sulphur plays the role of a cross linking agent, while zinc oxide is added for activation. Stearic acid, CBS act as accelerators. The mixing was performed at around 50°C and the mixing operation went on for around 7 minutes at a frequency of rotation of 50rpm was maintained throughout the course of mixing. The mixing is rolled by roller and compressed with hydraulic press of 20 tons for 30 min. The photo graph of preparation rubber ferrite samples were shown in figure 3.

Results and Discussion

Characterization of ferrite powders

Powder X-ray diffraction studies (XRD) for nickel ferrite and barium ferrite have been carried out on the powder sample sintered at 800°C and 1000°C temperatures for 2 hrs, respectively and these patterns were shown in figure 4(a) and (b). The XRD pattern of the NFO and BFO samples were recorded by using a powder X-ray diffractometer {Schimadzu model: XRD 6100 using CuK α ($\lambda = 1.54$ Å) radiation}, with a diffraction angle between 10° and 70° respectively. The figure 4(a) showed that the as prepared sample consisted entirely of nano-crystalline NiFe₂O₄ particles and it showed the formation of single phase cubic spinal crystal structure. Then the lattice parameter of NFO compound, a = 8.33Å was calculated assuming cubic symmetry by using the relation, d = $\frac{a}{h^2+k^2+l^2}$. The XRD patterns of BFO compound indicated that it was mono-phase and highly crystalline in nature, without any detectable impurities.XRD pattern indicates that all the crystal planes of the BaFe₁₂O₁₉ correspond to the 00-007-0276 standard cart related

to the crystal structure of barium hexaferrite. The lattice parameter was observed a = b = 5.895 Å and c = 23.199 Å. According to the XRD pattern the nanoparticles were fully calcined and no carbonic phase, relating to the citric acid and cotton template, was found in the pattern.From the XRD data, the average particle sizes of particles were calculated by using Debye Scherrer

formula t = $\frac{0.9\lambda}{\beta\cos\theta}$ where t is the particle size λ is the wavelength of X-ray

radiation, β is the full width half maximum(FWHM = 0.299)of X-ray peak broadening peak (311) and θ is the Bragg angle35.5° in NFO compound and FWHM = 0.228 of X-ray peak (110), angle 31.31° in BFO compound. The particle size was estimated to be about56.99 nm and 71.17 nm respectively. This shows that the synthesized powder has nano-size crystalinity.

Thermal Gravimetric Analysis (TGA)

Thermal Gravimetric Analysis (TGA) was done to determine the calcinations temperature of the as prepared powders and has been carried out to study the mass changes the increase temperature. The mass loss of sample was due to the vaporization process occurred when the temperature increased until a certain high temperature. TGA was performed from 37.97°C to 601.28°C. Figure 5 presents TGA curves and the weight loss as a function of temperature of the as prepared of Nickel ferrite and Barium ferrite. The results of weight loss at 3% are important to understand the thermal behaviour at initial stage and to determine the thermal stability of nanoparticle. From this analysis, 474.23°C is chosen as the minimum calcinations temperature for these barium ferrite powders. Four distinct regions (70.57°C, 125.98°C to 195.12°C and 474.23°C) of weight loss are observed. The weight loss around 474.23°C is observed to saturate compared to other regions. It was observed that the weight loss of Barium ferrite sample was 5.812 mg (7.774%). The weight loss of this sample was due to the vaporization process occurred when the temperature increased until a certain high temperature.

SEM analysis

The morphology and the size distribution of the NFO, BFO and their rubber based composites were determined using SEM. Typical SEM images of these compounds are shown in Figure 6. SEM micrograph depicts that the samples contain micrometrical aggregation of tiny particles. The existence of high dense agglomeration indicates that pore free crystallites are present on the surface. The SEM images show the agglomerated form of $NiFe_2O_4$ compound. As the nanoparticles possess high surface energies, they tend to agglomerate and grow into larger assemblies.

Dielectric behaviour of rubber ferrite composites

A study of the dielectric nature of NFO and BFO compound could furnish useful information about the electric field allocation within these compounds. The dielectric studies of both ceramic and rubber ferrite composites were carried out using LCR meter of model Instek GW 821. Disc shaped samples were used to evaluate the dielectric constant. The capacitance and dielectric loss in the frequency range 1 kHz to 200 kHz were determined. Dielectric constant or relative permittivity were calculated using formula

 $\varepsilon_r = \frac{C \times d}{\epsilon_0 A}$ where d is the thickness of the sample, C is the capacitance, A is

the area of cross section of the sample and ε_0 is the permittivity of the free space. ε_r is the relative permittivity of the material which is a dimensionless quantity. It was noticed that the value of the dielectric constant decreased with increase in the frequency. In ferrite materials, it is very high dielectric constant at very low frequencies and fall in the order of tens around frequency 100kHz. From the dielectric studies it became evident that the frequency negatively impacted both the dielectric constant and the dielectric loss as decreased with increase in the frequency. The frequency dependence dielectric constant value of Rubber, NFO, BFO and their rubber ferrites are shown in figure 6. A decrease in dielectric constant with increase in temperature was observed for natural rubber. Almost similar behavior as that of the ceramic component present in the matrix was obtained in the case of rubber ferrite were found to be greater than that of the natural rubber, but less than that of the ceramic NFO and BFO.

FTIR Analysis of rubber ferrite composites

Chemical functional groups of rubber ferrite composites were characterized by FT-IR spectroscopy and shown in the figure 7. There have similarly the same peak was observed in all of rubber ferrite samples. The absorbing bands at 1076.22 cm⁻¹ is assigned to the hexagonal positions of metal-oxide stretching vibrations. The peaks at 1374.95, 1447.82, and 1637.29 cm⁻¹ are related to the O-H vibrations related to the adsorbed water. The peak at 3331.20 cm⁻¹ is attributed to the adsorbed CO₂ on the surface of these samples. FT-IR result showed that all the carbonic functional groups related to the precursors were eliminated.

Magnetic properties of rubber ferrite composites

The magnetic measurement of all samples was measured by using PERMAGRAPH L apparatus and which shows that samples exhibited magnetic behavior. The high coercivity values account for the slower rate of growth of crystallite size that takes place during the heating process. It is not only the temperature but also the morphology that seems to significantly influence the magnetic properties. The increased value of the coercivity could be attributed to the magnetic spin orientation along the axis that eases magnetization. On account of the grain boundaries and free surface, the magnetic properties improved. Figure 6 showed the magnetic hysteresis loops of the Natural Rubber, NFO, BFO and their runbber ferrites at room temperature. The magnetic parameters, namely retentivity (or) remanence, coercivity, and saturation magnetization of the samples were measured are shown in table 1 and their B-H loops were shown in figure 8.

Conclusion

Nickel ferrite and barium ferrite powders having the particle size of 56.99 and 71.17nm were incorporated into a natural rubber with loading levels 120 phr to obtain RFCs. It was successfully produced the RFCs having a rather low density, high coercivity, large stored energy and high flexibility even at relatively low mass fraction of the filler. The dielectric constant decreased with increase of frequency for ceramic samples of NFO and BFO, natural rubber vulcanisate and for the RFC samples. Useful magnets can be

made by bonding ferrite powders in various resins, natural rubber. If no special steps are taken, the material is isotropic and energy product is unlikely to exceed 5.5 kJ/m³. If good flexibility is required the proportion of ferrite powder must not be too large and $(B-H)_{max}$ becomes considerably lower. These magnetic composites have a variety of applications as flexible magnets, pressure/photo sensors and microwave absorbers. One of the familiar applications of rubber magnets is the refrigerator door seal. They are lightweight, soft, elastic, stable, flexible, easy to be processed, energy saving and low cost.



Figure 1: The flow chart of preparation of ferrites powder.



Figure 2 : The photograph of preparation of ferrites powder.



Figure 3 : The photograph of preparation of rubber ferrite matrices.



Figure 4:(a) The XRD pattern of Nickel ferrite compound and(b) : The XRD pattern of Barium ferrite compound



Figure 5: (a) TGA-DTA result of Nickel ferrite compound and

(b) TGA-DTA result of Barium ferrite compound



Figure 5: The SEM image of NFO, BFO and their rubber composites (120phr)





Figure 6 : The frequency dependence of dielectric constant of NFO. BFO and



Figure 7: The FTIR results of pure rubber, Ni rubber ferrite and Ba rubber ferrite composites.



Figure 8: The B-H measurement of NFO, BFO and rubber ferrite composites with PERMAGRAPH L apparatus.

Materials	Remanence, B _r (T)	Intrinsic coercivity, H _{c1} (kAm ⁻¹)	Energy Product, (B-H) _{max} kJ/m ³
Nickel ferrite	0.03060	31.8	0.120
Barium ferrite	0.00359	43.7	0.019
Rubber Ni ferrite	0.00543	76.2	0.028
Rubber Ba ferrite	0.00311	92.3	0.038

Table 1 : The magnetic parameters of RFC samples

Acknowledgements

I would like to express appreciation to Rector Dr Theingi Shwe, and Pro-rector Dr Khin May Aung and Dr Cho Cho Myint, Dawei University for their encouragement and kind permission to undertake the present research. I also would like to express my profound thanks to Professor Dr San San Aye, Head of Department of Physics, and Professor Dr Kyaw Myint Htoo, Department of Physics, Dawei University, for their kind permission to carry out this work, their encouragement and help during this work.

References:

- Ahmad S et al, (2004), Ferroelectric Ceramics Processing Properties and Applications, Department of Ceramic Science and Engineering, Rutgers University: USA
- Dr. Steingroever GmbH (2010), Computer controlled permagraph® L" Cologne-Germany.

"Instruction Manual LCR meter GW 820", USA

JCM 6000 Plus, Scanning Electron Microscope.

Moulson A J & Herbert J M, (1997), Electroceramic Materials Properties Applications, New Delhi: Thomson Press

Rajagopal K. (2009) Textbook of engineering physics part II.New Delhi-110001.

- Suryanarayana C. and Norton M. G. (1998), X-ray Diffraction A Practical Approach, (New York: Plenum)
- Tyagi M S, (1991), Introduction to Semiconductor Materials and Devices, New York: Wiley
- Xu Y, (1991), Ferroelectric Materials and their Applications, New York: Elsevier Science Publishing Co. Inc.

PREPARATION AND CHARACTERIZATION OF CHITOSAN-BASED SOLID POLYMER ELECTROLYTE FILMS WITH ZINC ACETATE

Sint Ohnmar^{*}

Abstract

Solid polymer electrolytes based on chitosan with different weight percent ratios of zinc acetate have been prepared by the solution cast technique and then the flexible polymer electrolyte film were made. The conductivity and dielectric response of the solid polymer electrolyte systems were studied within the frequency range of 120Hz and 1kHz at room temperature. The conductivity of an electrolyte depends on the ability of the polymer host to solvate the zinc acetate. Polymers with higher dielectric constant will serve the purpose better. The dielectric constant and ionic conductivity follow the same trend with zinc acetate concentration. The dielectric constant is frequency dependent, so that the values of dielectric constant were decreased with increasing frequency. The sample containing 30 wt.% exhibited the highest room temperature conductivity of $2.44 \times 10^{-9} \text{ S cm}^{-1}$ 1 , dielectric constant of 2.87×10^{-6} at 120Hz and 4.84×10^{-7} at 1kHz. Structural changes and complex formations of the polymer-salt systems were ascertained from x-ray diffraction (XRD). In order to check the suitability of the solid polymer electrolyte for its application in energy storage devices, polymer capacitor has been fabricated by sandwiching a separator sheet containing the electrolyte between two electrodes. The overall capacitance has been found to be of the order of 19.8 mF at the operating voltage 0.63 V.

Keywords: Chitosan, Zinc acetate, Polymer electrolytes, Polymer capacitor.

Introduction

Ion conducting polymers are an active area of study in materials research. They are prepared by complexing polymers containing polar groups with alkali metal salts . Being light weight and flexible, attempts have been made to use solid polymer electrolytes in solid-state electrochemical devices such as batteries, fuel cells, electrochromic displays, and smart windows . Polymer electrolytes usually contain both crystalline and amorphous phases. It has been reported that the ion conduction takes place primarily in the

^{*} Dr, Lecturer, Department of Physics, Dawei University

amorphous phase .Chitosan is a derivative of chitin which can be obtained from crab and shrimp shells. Chitosan is produced from deacetylation of chitin to overcome the solubility limitation of chitin in common solvents . Due to the NH2 and OH functional groups that can serve as conjunction sites, chitosan is a good sorbent with high affinity for transition metal ions. Chitosan has good film forming ability, porous scaffolds, and hydrogels. Ion-conducting polymer electrolytes based on chitosan have also been reported. From the fundamental point of view, ionic conduction in polymer electrolysis still poorly understood. Ion transport is complex and depends on factors such as salt concentration, dielectric constant of host polymer, degree of salt dissociation and ion aggregation, and mobility of polymer chains. Dielectric analysis of ion conducting polymer electrolytes can provide information on ion transport behavior and ionic/molecular interaction in solid polymer electrolytes. This is due to the fact that dielectric constant is both frequency and temperature dependent. Recently Petrowsky and Frech hypothesized that the DC conductivity is not only a function of temperature, but also is dependent on the dielectric constant in organic liquid electrolytes. The main objective of the present work is to investigate the Petrowsky and Frech postulate for solid polymer electrolyte based onchitosan:CH3COONa, as well as to investigate the physics behind the relationship between ionic conductivity and dielectric constant. The X-ray diffraction (XRD) has been used to characterize the chitosan-based solid electrolytes prepared in this study. This paper offers a concise review on the renaissance of a conventional capacitor to electrochemical double layer capacitor or polymer capacitor. Capacitors are fundamental electrical circuit elements that store electrical energy in the order of microfarads and assist in filtering. Capacitors have two main applications; one of which is a function to charge or discharge electricity. This function is applied to smoothing circuits of power supplies, backup circuits of microcomputers, and timer circuits that make use of the periods to charge or discharge electricity. The other is a function to block the flow of DC. This function is applied to filters that extract or eliminate particular frequencies. This is indispensable to circuits where excellent frequency characteristics are required. Electrolytic capacitors are next generation capacitors which are commercialized in full scale. They are similar to batteries in cell construction but the anode and cathode materials remain the same. They are aluminum,

tantalum and ceramic capacitors where they use solid/liquid electrolytes with a separator between two symmetrical electrodes. The third generation evolution is the electric double layer capacitor, where the electrical charge stored at a metal/electrolyte interface is exploited to construct a storage device. The interface can store electrical charge in the order of ~106 Farad. The main component in the electrode construction is activated carbon. Though this concept was initialized and industrialized some 40 years ago, there was a stagnancy in research until recent times; the need for this revival of interest arises due to the increasing demands for electrical energy storage in certain current applications like digital electronic devices, implantable medical devices and stop/start operation in vehicle traction which need very short high power pulses that could be fulfilled by electric double layer capacitors (EDLCs). They are complementary to batteries as they deliver high power density and low energy density. They also have longer cycle life than batteries and possess higher energy density as compared to conventional capacitors. This has led to new concepts of the so-called hybrid charge storage devices in which electrochemical capacitor is interfaced with a fuel cell or a battery. These capacitors using carbon as the main electrode material for both anode and cathode with organic and aqueous electrolytes are commercialized and used in day to-day applications.

Experimental Materials and Methods

Preparation of Samples

Solid polymer electrolyte films were used as host polymer electrolytes and were prepared by standard solution casting techniques. All samples were prepared at room temperature and stored under dry conditions. A 6 g of prepared chitosan flake was dissolved in 600 mL of 1 % (w/v) acetic acid solution. The solution was stirred by hotplate stirrer, for 90 hours at an ambient temperature and then the chitosan acetate host polymer solution was kept on overnight. The solution was maintained at 80 °C in water bath for one hour. The degassed and well-mixed solutions (30 mL) were casted onto petri dish, and dried in air for 3 days at room temperature until constant weight. The dried transparent chitosan films (0% doping salt) were detached from the petri dish. A 1 g of zinc acetate was dissolved in 100 mL with distill water to make 1 % (w/v) doping salt solution by using magnetic stirrer. A 3 mL of 1 % (w/v) doping salt solution was mixed with 27 mL of 1 % (w/v) chitosan acetate solution by using hotplate stirrer. The 30 mL of polymer salt solution was obtained as 10wt % doping salt solution. It was prepared to more 10wt % in each still to still 50wt% dopant . The degassed and well-mixed solution was cast onto petri dish, and dried in air for 3 days at room temperature until constant weight.

The dried transparent chitosan films (10wt% doping salt) were detached from the petri dish. Finally, chitosan film compound of 10 wt% was obtained. The same procedure were carried out for the preparation of chitosan films compound of 20, 30, 40 and 50wt% were prepared. The various compositions of zinc acetate used in preparing the polymer electrolytes are depicted in Table 1.

Characterization of Samples

The ionic conductivities of the samples were measured at within at room temperature using EXTECH 380193 LCR meter with a frequency range of 120 Hz and 1 kHz. The conductivity (σ) was determined using the equation below:

$$\sigma = \frac{1}{\rho(0)/2S/W * \log(e)2} \tag{1}$$

From equation 1, $\rho(0) = 2\pi SR$, 'S' represents the distance between the two contact probe, 'W' represents the thickness of sample and R is the resistance of the sample. The dielectric constant ε_r can be defined as:

$$\boldsymbol{\varepsilon}_{r} = C_{p} t / \boldsymbol{\varepsilon}_{o} A \tag{2}$$

From equation 2, 't' represents the thickness of sample, 'A' is the area of the surface of the sample, C_p is the capacitance of the specimen in Farad and ε_o is the permittivity of free space.

X-ray diffraction (XRD): In this work, X-ray diffraction were carried out using a Rigaku x-ray powder diffractometer which employs $Cu-K_{\alpha}$

x- radiation of wavelength $\lambda = 1.54056\dot{A}$ between a 2 θ angle of 5° to 70°. X-ray diffraction was carried out to determine the nature of the materials whether a material is amorphous or crystalline.

Results and Discussion

The structural, conductivity and dielectric properties of the polymer electrolytes based on zinc acetate were investigated. The samples were prepared by solution cast method by taking different concentration of different ratio (i.e., Cs0%, 10%, 20%, 30%, 40% and 50%). The compatibility between the polymer matrix and the inorganic dopants has great influence on the properties ionic conductivity of the polymer electrolytes.

X-ray Diffraction Studies

In order to investigate the effect of zinc acetate on the structure of chitosan-based polymer electrolyte, x-ray diffraction of pure chitosan film, and their complexes have been performed. These crystalline structures contribute to the peaks in the XRD pattern of Cs0%, 10%, 20%, 30%, 40% and 50% are shown in Fig. 1. As seen in the XRD pattern of the pure chitosan Cs0%, the high intensity peak at around $2\theta = 27^{\circ}$, $2\theta = 40^{\circ}$ and $2\theta=56^{\circ}$. However, upon the addition of the zinc acetate liquid as seen in Cs30% , the intensity of the peak at $2\theta = 27^{\circ}$ was found to be decreased and the peak at $2\theta = 40^{\circ}$ and $2\theta = 56^{\circ}$ was found to be disappeared from the XRD pattern. This shows that the addition of the zinc acetate liquid decreased the crystallinity of the backbone of the chitosan and increased the amorphous region of the Cs30wt% sample. This is in agreement with what has been found that in ionic conductivity studies. Furthermore, the changes in the intensity and the disappearance of peaks show that there is some complexation occurring in the polymer matrix of the Cs30 wt% sample.





Electrical Conductivity Studies of Solid Polymer Electrolytes

Table.1 shows the various composition of zinc acetate and chitosan solution. The value of ionic conductivity for solid polymer electrolytes samples with different weight percentages of zinc acetate is plotted in Fig.2 and shown in Table.2. The highest value of conductivity was observed 2.44 $\times 10^{-11}$ Sm⁻¹ from 30 wt % at room temperature. The increase of the ionic conductivity up to 30wt % of the zinc acetate added is due to increasing number of mobile ions. However, there is a decrease in ionic conductivity that could be observed when 40 wt % and 50 wt % of zinc acetate added into the system. This is due to the agglomeration of the excess ions from the zinc acetate which causes the mobile ions to form neutral pairs, and this could lead to a decrease in ionic mobility of the solid polymer electrolytes.

Sample	Volume of 1 % (w/v) Zinc Acetate (mL)	Volume of 1 % (w/v) Chitosan (mL)	Weight percent of Zinc Acetate (%)
Cs0	0	30	0
Cs1	3	27	10
Cs2	6	24	20
Cs3	9	21	30
Cs4	12	18	40
Cs5	15	15	50

 Table 1: Various composition of zinc acetate and chitosan solution.

Table 2:	Conductivity	measurement for	r vario	ous composition of	zinc
	acetate solid p	olymer electroly	te film	at room temperature).

Name of Sample	Weight percent of Salt (%)	Conductivity(Sm ⁻¹)
Cs0	0	1.32E-11
Cs1	10	1.56E-11
Cs2	20	1.91E-11
Cs3	30	2.44E-11
Cs4	40	1.67E-11
Cs5	50	1.41E-11



Figure 2: Conductivity measurement for various weight ratio zinc acetate polymer electrolyte films

Dielectric Studies of Solid Polymer Electrolytes

The value of dielectric value for solid polymer electrolytes samples with different weight percentages of zinc acetate is plotted in Fig.3 and shown in Table.3. The dielectric constant was found to increase upon the addition of zinc acetate and these parameters are significantly influenced by the frequency. Higher values of the dielectric constant observed at 30 wt % with frequencies 120 Hz have been also explained on the basis of interfacial/space polarization due to nonhomogeneous dielectric structure.

Name of Sample	Weight percent of Salt (%)	Dielectric (Farad) (120Hz)	Dielectric (Farad) (1kHz)
Cs0	0	6.24E-08	2.30E-08
Cs1	10	8.89E-08	4.48E-08
Cs2	20	9.66E-07	2.76E-07
Cs3	30	2.87E-06	4.84E-07
Cs4	40	1.58E-08	3.79E-09
Cs5	50	9.85E-09	3.09E-09

Table 3: Dielectric measurement for various composition of zinc acetatesolid polymer electrolyte film at room temperature.



Figure 3: Dielectric measurement for various weight ratio zinc acetate polymer electrolyte films at 120Hz and 1kHz

Capacitance Studies of Double Layer Polymer Capacitor

The primary test platform was a electronics project board, and additional multimeter, variable DC power supply and EXTECH 380193 LCR meter. It is further notable that the capacitance of different weight ratio of double polymer capacitors were measured by silver electrode using the above described instruments and protocol as shown in Table.4. In order to check the suitability of the solid polymer electrolyte for its application in energy storage devices, polymer capacitor has been fabricated by sandwiching a separator sheet containing the electrolyte between two electrodes. The overall capacitance has been found to be of the order of 19.8 mF at the operating voltage 0.63 V. The increasing capacitance with decreasing the sample thickness, but the maximum effective operating voltage of about 0.64 V.

 Table 4: Capacitance measurement with silver electrode for various composition of zinc acetate solid polymer electrolyte film.

Sample (wt %)	Sample Thickness (mm)	Operating Voltage (V)	Capacitance Value (mF)
0 %	1.1	0.64	11.7
10%	1.08	0.64	12.6
20%	1	0.64	16.0
30%	0.88	0.63	19.8
40%	1.04	0.64	15.8
50%	0.91	0.64	16.3

Conclusion

The ionic conducting solid polymer electrolytes based on zinc acetate and various concentrations of sodium acetate were prepared using the solution casting method. XRD analyses reveal increase in amorphous nature of the polymer-salt electrolyte films and confirm interaction and complexation between the polymer and the salt. An increase in conductivity is observed with the increase in zinc acetate concentration up to a certain salt content. The ionic conductivity is found to be 2.44×10^{-11} Sm⁻¹ at 30 wt.% and also the dielectric constant was found to increase upon the addition of zinc acetate and these parameters are significantly influenced by the frequency. Higher values of the dielectric constant observed 2.87×10^{-6} at 30 wt %. The capacitance of different weight ratio of double polymer capacitors employed zinc acetate based solid polymer electrolyte is 19.8 mF at 30 wt %. Thus, these present the sold polymer electrolyte has potential in energy storage for flexible and lightweight devices.

Acknowledgements

I would like to express appreciation to Acting Rector Dr Theingi Shwe, Pro-rector Dr Khin May Aung and Dr Cho Cho Myint, Dawei University for their encouragement and kind permission to undertake the present research. I also would like to express my profound thanks to Professor Dr San San Aye, Head of Department of Physics, and Professor Dr Kyaw Myint Htoo, Department of Physics, Dawei University, for their kind permission to carry out this work, their encouragement and help during this work.
References

- David Liu, Michael J. Sampson, (2010), "Physical and Electrical Characterization of Polymer Aluminum Capacitors", MEI Technologies, Inc. and NASA Goddard Space Flight Center.
- Jin Hee Kang, (2015), "Fabrication and characterization of nano carbon-based electrochemical double-layer capacitors", Mechanical Engineering (Nanotechnology), Canada.
- M Jayalakshmi M, Balasubramanian K, (2008), "Simple Capacitors to Supercapacitors An Overview", Non-Ferrous Materials Technology Development Centre (NFTDC), Kanchanbagh Post, Hyderabad-500058, India.
- Meryl D. Stoller and Rodney S. Ruoff*, "Review of Best Practice Methods for Determining an Electrode Material's Performance for Ultracapacitors", Department of Mechanical Engineering and the Texas Materials Institute, The University of Texas at Austin, One University Station C2200, Austin, Texas, 78712-0292 USA.
- Nur Hamizah Mohd Zaki, Zaidatul Salwa Mahmud, Oskar Hasdinor Hassan, Muhd Zu Azhan Yahya, Ab Malik Marwan Ali1, (2016), "A Symmetric Supercapacitor Based On 30% Poly (Methyl Methacrylate) Grafted Natural Rubber (MG30) Polymer and Activated Carbon Electrodes", Universiti Teknologi Mara, 40450 Shah Alam, Selangor, Malaysia.
- Pandey G P, Yogesh Kumar & Hashmi SH, (2010), "Ionic Liquid Incoporated Polymer Electrolytes For Super Capacitor Application", Department of Physics and Astrophysics, University of Dehili, India.
- Samuel Fromille and Jonathan Phillips*, "Super Dielectric Materials", Physics Department, Naval Postgraduate School.
- Stevic Z, Rajcic-Vujasinovic M, Bugarinovicb S and Dekanskic A, (2010), "Construction and Characterisation of Double Layer Capacitors", University of Belgrade, Technical Faculty in Bor, Serbia.

STUDY ON CHARACTERIZATION OF CHITOSAN-ZnO FILM

Thant Thant Zin¹, Than Than Win², Yin Maung Maung²

Abstract

The chitosan, the naturally abundant and renewable polymers, have excellent properties such as biodegradability, bio-compatibility, nontoxicity and absorption. The polymer sample consisting of the purified chitosan powder was firstly prepared by the slow evaporation of aqueous solution. Demineralization and deproteinization processes were done to obtain purified chitosan powder. The molecular vibration spectrum of the purified chitosan powder was recorded by using Fourier Transform Infrared (FTIR) Spectroscopy. Chitosan, zinc acetate and chitosan-ZnO films were deposited onto the glass slide by using the spin-coating method. The crystalline state of chitosan powder, the chitosan-ZnO powder and the film were characterized by X-ray diffraction (XRD) and Scanning electron microscopy (SEM). The lattice microstrain of as-grown chitosan powder was calculated to be about 0.9 and it was consistent with the theoretical value of orthorhombic crystal. The crystallite size was calculated to be about 33.2 nm for the chitosan-ZnO powder. According to the XRD results, the chitosan-ZnO film has smaller crystallite size than the chitosan-ZnO powder and it was about 25.6 nm.

Keywords: Chitosan, demineralization, deproteinization, characterization,

spin-coated film

Introduction

Chitin is a long-chain polymer of N-acetylglucosamine and a derivative of glucose. It is a primary component of cell walls in fungi, the exoskeletons of arthropods, such as crustaceans(e.g., crabs, lobsters and shrimps). The structure of chitin is comparable to another polysaccharide-cellulose, forming crystalline nanofibers or whiskers.

Chitosan is a natural biopolymer that can be retrived from alkaline deacetylation of chitin. Chitosan can dissolve in dilute acetic acid at room temperature. Chitosan has a amine group in which the nitrogen atom has lone

^{1.} Dr, Demonstrator, Physics Department, Hpa-an University

^{2.} Dr, Associate Professor, Department of Physics, Mandalay University of Distance Education

^{3.} Dr, Associate Professor, Department of Physics, University of Yangon

pair electron. This lone pair electron can interact with the cation from the salt to form a polymer which is a criterion that must be fulfilled for polymer electrolytes.

Zinc acetate is the chemical compound with the formula $(O_2CCH_3)_2$ Zn but more commonly refers to the dehydrate $(O_2CCH_3)_2$ Zn $(H_2O)_2$. Both the hydrate and the anhydrous forms are colourless solids that are commonly used in chemical synthesis and as dietary supplements. Zinc acetates are prepared by the action of acetic acid on zinc carbonate or zinc metal.

If the sample is a mixture, XRD data can be analyzed to determine the proportion of the different minerals present. Thin film diffraction methods are used as important process development and control tools, as hard X-rays can penetrate through the epitaxial layers and measure the properties of both the film and the substrate.X-ray powder diffraction is most widely used for the identification of unknown crystalline materials (e.g. minerals, inorganic compounds).

A Scanning Electron Microscope (SEM) is a tool for seeing otherwise invisible worlds of microspace and nanospace. IR spectroscopy utilizes a special light source to pass infrared radiation through the substance being analyzed and then measures how much of the infrared light is absorbed at each frequency. The absorbance bands that appear at various wavelengths indicate the presence of certain types of bonds in the molecular structure of the sample[6]. In this paper, structural, microstructural, vibrational and optical characteristics of the as-prepared chitosan-ZnO powder and film are studied by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) spectroscopy.

Experimental Procedure

Preparation of Chitosan Powder

Purified chitosan powder was obtained by slow evaporation of aqueous solution. The choice of raw material was chitin shown in Fig 1. Firstly, the raw material of chitin was weighed by digital balance. A purification step was introduced and recommended optimum condition for the two stages of demineralization and deproteinisation. Demineralization was performed the following steps.

- Weight out the desired quantity of chitin.
- Added the ratio of 2ml of acetic acid to 1g of chitin.
- Left mixing for 1h to allow any minerals present to dissolve.
- Filtered by passing through filter paper.
- Washed with de-ionized water to remove any excess acid and prevent an acid.

Illustration of demineralization processes were demonstrated in Fig 2(a & b).

Deproteinisation process was as follow.

- Added 1M sodium carbonate to mixture solution drop by drop and mixing for 1h at room temperature to dissolve any unwanted proteins by p^H control shown in Fig 3.
- Filtered to remove the sodium carbonate and washed with de-ionized water sample in 50°C oven to dry.

Final product yield purified chitosan powder. The experimental procedure of chitosan powder was shown in Fig 4.

Preparation of Chitosan-ZnO Powder

Chitosan-ZnO powder was prepared using in precipitation method. The precipitation was prepared using a 2% chitosan solution of degree of deacetylation> 85%. Fig 5 showed the schematic overview of the preparation of chitosan-ZnO powder. The zinc acetate salt was added to a solution of chitosan in acetic acid and was kept for 24h. Then sodium hydroxide solution was added drop wise and kept for 12h. The precipitate formed was filtered, washed several times with water and dried at 100°C. Chitosan-ZnO obtained was dried and calcined temperature. The chitosan-ZnO powder formed was calcined at 600°C.

Preparation of Chitosan-ZnO Film

To get the chitosan-ZnO film, the substrate in this experiment was used as glass substrate. Before the deposition, glass substrate was cleaned with standard cleaning process. After the cleaning process chitosan-ZnO powder was dissolved in acetic acid. This mixture was continuously stirred with a magnetic stirrer to be homogeneous for 1 h. The solution was deposited onto glass substrate by spin-coating technique and heat treated at 600°C for 1h. Finally chitosan-ZnO film was successfully formed. The experimental procedure of chitosan-ZnO film was shown in Fig 6.

In this paper, as-prepared chitosan-ZnO powder and film are studied by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) spectroscopy.



Figure 1: Raw chitin



Figure 2: (a) Chitin + Acetic solution



Figure 2:(b). Filtering process



Figure 3: p^H control process



Figure 5: Schematic overview for precipitation of chitosan-ZnO powder.



Figure 6: Experimental procedure of the chitosan-ZnO film

Results and Discussion

Structural Characterization of Chitosan Powder

X-ray diffraction, XRD is a non-destructive technique for the qualitative and quantitative analysis of the crystalline materials, in form of powder or solid. The information about the crystallographic properties such as crystallite size and lattice parameters of over all the samples has been obtained from the XRD profiles. The XRD spectrum of chitosan powder, the upper site of the graph was represented the observed peaks and the lower site of the graph was represented the standard peaks. Fig 7 gave the observed XRD spectrum of as grown chitosan. On the spectrum, 20 reflection of observed peaks were scanned within diffraction angle (2θ) .

The chitosan powder annealed at 200°C was shown in Fig 8. From the figure appeared 8 reflections. They were (042), (007), (081), (161), (202),

(033), (0,0,10) and (1,10,1). The corresponding Bragg angles were 20.855°, 27.265°, 27.570°, 31.613°, 32.724°, 37.520°, 39.344° and 41.30°. The XRD profile of chistosan at 300°C was shown in Fig 9. On the spectrum, 18 reflections were formed between diffraction angle (2θ) of some scanned range (10° to 70°). The (hkl) planes were successfully formed in Fig 7 & 9.

Lattice Parameter Determination

Some crystallographic parameter such as crystallite size and bond length were calculated and collected in Table 1. Comparison of lattice parameters of chitosan powder and lattice parameters of chitosan presented by Mazeau K et al (1994)was shown in Table 2.Concerning with the above Table2 the observed lattice parameters were found to be little different in those of Mazeau K.

Microstructural Properties of Purified Chitosan

A microstructural property of purified chitosan powder was studied by SEM. The magnification of scanning electron image was 2700. Fig 10 showed scanning electron image of purified chitosan powder. In this Fig, it could be clearly seen that polymer like nature of microstructure was uniformly distributed.

Molecular Vibration of Purified Chitosan

Chitins were major constituents of exo-skeleton of crustaceans such as crab, shrimp and lobster. They were biopolymer composed of glucosamine and N-acetylated glucosamine linked by glycosidic bonds. Chitosan has an amine group in which nitrogen atom has a lone pair electron. Molecular vibrational spectrum of purified chitosan powder was shown in Fig 11. Vibrational frequency and mode assignment of chitosan powder was tabulated in Table 3.

XRD Analysis of Chitosan-ZnO Powder and Film

Fig 12 gave the observed XRD spectrum of chitosan-ZnO powder at 600°C. On the spectrum, 9 reflections of observed peaks were scanned within diffraction angle (2 θ) of some scanned range(10°to 70°).The chitosan-ZnO

film annealed at 600°C was shown in Fig 13. From the figure, 5 reflections were appeared. The (hkl) planes were successfully formed in Fig 12&13. From the figures that the major reflection between 30° and 40° (20 value) indicate higher crystalline region in the chitosan-ZnO samples. Also the less intense peaks 47.5°,57°,68° (20's) indicate the high crystallinty of chitosan-ZnO samples.

Lattice parameters, lattice distortions and Bond length were given in Table 4. Bond Length (BL) was calculated by the following equation (1)

BL =
$$\sqrt{\frac{a^2}{3} + (\frac{1}{2} - u)^2 c^2}$$
 (1)

Where $u = position parameters = \frac{a^2}{3c^2} + 0.25$

The crystallite size was calculated by Debye Scherer formula in equation (2)

 $= \frac{\beta \times \lambda(\text{Å})}{\text{FWHM(deg)} \times \cos\theta_{\text{B}}}$ G (2)Where β Scherer constant ≈ 0.899 =G = Crystallite size wavelength of CuK_{α} = 1.54056 Å $\lambda_{CuK_{\alpha}}$ =FWHM Full Width at Half Maximum = $\theta_{\rm B}$ Bragg angle =

Table 5 showed crystallite size of chitosan-ZnO powder and film at 600°C. The full width at half maximum of an (hkl) peak at (θ value) and crystallite size of all the chitosan-ZnO samples show that chitosan-ZnO film has smaller crystallite size compared to the chitosan-ZnO powder. It is also seen that chitosan-ZnO film shows lower particle size but higher FWHM value.

Table 6 showed crystallite size and FWHM value of chitosan-ZnO powder presented by Sousa V C et al (1998). Concerning with the Table 5 & 6

the observed crystallite size were found to be little difference in those of Sousa V C.

SEM Analysis of Chitosan-ZnO Powder and Film

A microstructural property of chitosan-ZnO powder and film at 600°C were studied by SEM. The magnification of scanning electron image was 2700. Fig14(a-b) showed scanning electron image of chitosan-ZnO powder and film. Grain growth patterns were observed all samples. The grain size were (0.35 μ m) and (1.31 μ m) respectively. From the Fig 14(a), it is clear that the chitosan-ZnO powder is formed uniform and honey comb like shape. It is also found that the photograph of chitosan-ZnO powder is formed crystalline as its shape is changed from the cauli flower structure of chitosan-ZnO film was shown in Fig 14(b).

Condition	G (nm)	BL(Å)
as-grown	5.797	7.06
200 °C	2.183	3.16
300 °C	2.173	3.14

Table 1: Crystallite size and bond length of chitosan powder

Table 2: Comparison	of	lattice	parameters	of	chitosan	powderand
Mazeau Kchi	tosa	npowde	r (1994)			

Lattice parameters										
Condition	a (nm)	b (nm)	c (nm)	c/a						
as-grown	1.190	0.901	1.095	0.92						
200 °C	0.384	2.716	1.092	2.84						
300 °C	0.392	2.702	1.084	2.75						
Mazeau K - chitosan	0.807	0.844	1.032	1.27						

No	Wave No(cm ⁻¹)	Vibrational Mode Assignment
1	538.1	C-H Stretching
2	621.0	C-H Stretching
3	700.1	C-C Bending
4	779.2	C-H Bending
5	862.1	C-H Bending
6	906.5	O-H Bending
7	1035.7	C-O-C Symmetric Stretching
8	1072.3	C-O Bending
9	1155.3	C-O Bending
10	1257.5	C-O-C Asymmetric Stretching
11	1375.2	CH Stretching for CH ₃
12	1419.5	CH Stretching for CH ₃ and CH ₂
13	1483.2	CH Stretching for CH ₃ and CH ₂
14	1585.4	NH ₂ Bending
15	1656.7	NH ₂ Bending
16	3401.2	NH ₂ Group Stretching

Table 3: Vibrational mode assignment of purified chitosan powder

Table 4: Lattice parameters, lattice distortion and bond length.

Sampla	Lattice Para	ımeter (Å)	С	DI (Å)
Sample	a-axis	c-axis	\overline{a}	DL(A)
Powder (600°C)	3.2229	5.1796	1.606	1.962
Film (600°C)	3.2095	5.1569	1.610	1.9551

Table 5: Crystallite size and FWHM value of chitosan-ZnO powder and film

Sample	Crystallite size (nm)	d spacing (101)	FWHM (deg)
Powder (600°C)	33.2	2.4571	0.252
Film (600°C)	25.6	2.4467	0.326

Table 6: Crystallite size and FWHM value of chitosan-ZnO powder presented bySousa V C(1998)

Sample	Crystallite size (nm)	FWHM (deg)
Powder (550°C)	33.59	0.25982



Figure 7: XRD profile of as-grown chitosan powder



Figure 8: XRD profile of chitosan powder at 200°C



Figure 9: XRD profile of chitosan powder at 300°C



Figure10: Scanning Electron Image of purified chitosan powder



Figure 12: XRD spectrum of chitosan-ZnO powder at 600°C



Figure 11: IR transmission spectrum for purified chitosan powder



Figure 13: XRD spectrum of chitosan-ZnO film at 600°C



Figure 14: (a). SEM image of chitosan-ZnO powder at 600°C



Figure 14: (b).SEM image of chitosan-ZnO film at 600°C

Conclusion

According to the XRD results, it was obvious that all chitosan powders were clearly formal with orthorhombic symmetry. The as-grown chitosan was also appeared and gave the low temperature condition. The lattice microstrain of as-grown powder was calculated to be about 0.9 and consistent with the theorectical value of orthorhombic crystal. Mazerau K et al (1994) reported that the c/a value was 1.27. Concerning with that report, the as-grown powder was better than Mazeau K et al (1994) (chitosan at 180°C).

From SEM image, polymer like nature of microstructure was uniformly distributed on purified chitosan powder. Our measurement of FTIR spectrum was good agreement with reported values. IR transmission spectrum has characteristics of alcohol, N-H containing amine.

Characterization and crystalline state of ZnO powder and film with chitosan medium have been successfully implemented. According to the XRD results, it was obvious that, chitosan-ZnO film has smaller crystallite size than that of chitosan-ZnO powder. The chitosan-ZnO powder and film were also appeared and gave the temperature at 600°C. The crystallite size was calculated to be about 33.2 nm for chitosan-ZnO powder and corresponding FWHM was 0.252 deg. Sousa V C et al (1998)reported that the crystallite size was 33.59 nm and corresponding FWHM was 0.259 deg. Concerning with this report, the observed chitosan-ZnO powder was smaller than Sousa V C et al (1998) (chitosan-ZnO at 550°C) in crystallite size. Micro grain of chitosan-ZnO powder and film were uniformly distributed and high dense.

Acknowledgement

The authors would like to express my profound gratitude to Dr Mya Mya Aye, Rector, Hpa-an University who gives us permission to present this paper. We would to acknowledge our deep gratitude to Professor Dr. Khin Yu Mon, Head of Department of Physics, Hpa-an University, for allowing and encouraging us to present this paper. We like to thank Materials Lab, Department of Physics, University of Yangon for their apparatus support of our research.

References

- Ardel G et al (1996) Solid State Ionics 85
- Barnes P R F et al (2002) Journal of Microscopy205 (2) 118
- Danilatos G D (1988) "Foundations of environmental scanning electron microscopy". Advances in Electronics and Electron Physics <u>71</u> 109
- Ogawa K et al (2004) J Biological Macromolecules 341
- Suryanarayana C & Grant Norton M (1998)" X-ray Diffraction" (New York : Plenum)
- Tiwari A et al (2007) Express Polymer Letters 1 (5) 308

FEASIBILITY STUDY OF BAMBOO ASH ON CONCRETE MEMBERS

Aye Thandar ¹, Marlar Wai ², Aye Thandar Oo³ and Yin Maung Maung ⁴

Abstract

This study investigates the strength performance of concrete using partial blends of cement and bamboo ash. The bamboos were dried under sunlight and burnt in air. Bamboo ash was obtained after passing the residual through 200µm sieve. Elemental analysis was conducted on bamboo ash and ordinary portland cement, OPC by EDXRF (Energy Dispersive X-ray Fluorescence) technique to evaluate its percentage composition. Bamboo ash shows pozzolanic activity and it was used as supplementary cementitious material. Bamboo ash was then used to replace OPC by weight in ratio of 0%, 5%, 10%, 15%, 20% and 25% in concrete (M-15 & M-20). Base upon the quantities of ingredients of the mixes (1:2:4), M-15 grade and mixes (1:1.5:3), M-20 grade concretes were prepared. Twelve pieces of 150 mm concrete cubes were prepared. These cubes were tested at 28 days of curing ages and then maximum load and compressive strength of cubes were determined respectively. To investigate the pozzolanic behavior of bambo ash, (95% OPC+5% bamboo ash) and (90% OPC+10% bamboo ash) concrete crushes were analyzed by XRD analysis.

Keywords: – bamboo waste ash, EDXRF, pozzolanic, compressive strength, concrete

Introduction

Agricultural wastes are widely available, renewable and virtually free and it is important resource. Researchers all over the world today are focusing on ways of utilizing either industrial or agricultural waste, as a source of raw materials for industry. Agricultural wastes are converted into heat, steam, charcoal, methanol ethanol, bio diesel as well as raw materials (animal's feed, composting, energy and biogas construction etc.). The production of energy from agricultural waste has been utilized to varying degrees in different parts of the world. This waste, utilization would not only be economical, foreign exchange earnings and environmental pollution control. Industrial wastes, such as blast furnace slag, fly ash and silica fume are being used as supplementary cement replacement materials. Natural pozzolans by

^{1.} Demonstrator, Physics Department, Dawei University

² Dr, Lecturer, Physics Department, University of Yangon

^{3.} Dr, Associate Professor, Physics Department, Myeik University

⁴ Dr, Associate Professor, Physics Department, University of Yangon

themselves possess little or no cementing value, but finely ground in the presence of moisture, they will chemically react with calcium hydroxide at ordinary temperature to form hydrated phases possessing cementing properties. Nowadays, some industrial by-products and wastes are attracting much research because of their high silica and/or alumina content for the use as additives in commercial Portland cements. It is well known that hydrated phases formed during pozzolanic reaction commonly improve the performance of concrete.

Pozzolan is a siliceous or siliceous and aluminous material, which in itself possesses little or no cementitious value but will, in finely divided form and in the presence of moisture, chemically react with calcium hydroxide Ca(OH)2 to form compounds possessing hydraulic cementitious properties. Ordinary Portland Cement is the most extensively used construction material in the world. Since the early 1980's, there has been an enormous demand for the mineral admixture and in future this demand is expected to increase even more. If some of raw material having similar composition can be replaced by weight of cement in concrete then cost could be reduced without affecting its quality. For this reason bamboo ash is one of the main byproduct can be used as mineral admixture due to its high content in silica (SiO2). Also in this modern age every structure has its own intended purpose and hence to meet this purpose modification in traditional cement concrete has become essential. This situation has led to the extensive research on concrete resulting in mineral admixture to be partly used as cement replacement to increase workability in most structural application. We found that ash obtained from bamboo is amorphous in nature and has pozzolanic properties. The annual production of bamboos all over the world is about 20 million tonnes but about 10 million tonnes are produced in India, China and Japan. Bamboo is one of the fastest-growing plants on Earth, with reported growth rates of 250 cm (98 in) in 24 hours. However, the growth rate is dependent on local soil and climatic conditions, as well as species, and a more typical growth rate for many commonly cultivated bamboos in temperate climates is in the range of 3-10 centimeters (1.2-3.9 in) per day during the growing period. Primarily growing in regions of warmer climates during the late Cretaceous period, vast fields existed in what is now Asia. Bamboo is the fastest growing, renewable natural resource known to us. It is a small wonder, therefore, that this material

was used for building extensively by our ancestors. It has a long and well established tradition as a building material throughout the tropical and subtropical regions. It is used in many forms of construction, particularly. It has also been found that bamboo acts very well in buckling but due to low stresses than compared to steel and due to it not being straight it may not be very good. Further, it has been established that in seismic zones the failure of bamboo is very less as the maximum absorption of the energy is at the joints. Cellulose is the main component present in bamboo which is the main source of mechanical properties of bamboo. Concrete is a composite material composed of coarse aggregate bonded together with a fluid cement that hardens over time. Most concrete used are lime-based concretes such as Portland cement concrete or concretes made with other hydraulic cements. When aggregate is mixed together with dry Portland cement and water, the mixture forms a fluid mass that is easily moulded into shape. The cement reacts chemically with the water and other ingredients to form a hard matrix that binds the material together into a durable stone-like material that has many uses.

Experimental

Materials and Methods

Preparation of Samples

The bamboo wastes were collected from Tanintharyi region of Dawei, Myanmar. They were dried under sunlight to reduce the moisture content in wastes. The dry bamboo wastes were burnt in air and the gray bamboo ash was obtained. Bamboo ash was then sieved with a 200 µm standard sieve and purified bamboo ash was obtained. Bamboo ash and ordinary portland cement OPC were analyzed by (Energy Dispersive X-ray Fluorescence) EDXRF technique, to evaluate their chemical composition. By observing the EDXRF results, the chemical composition of bamboo ash and OPC were determined. For concrete cubes sample preparation, the main ingredients are Ordinary Portland Cement (OPC), bamboo ash, sand, coarse aggregates and water. In this experimental work, twelve 150mm concrete cubes, grade M-15 (1:2:4) and grade M-20 (1:1.5:3) were designed. Based upon the quantities of ingredient of the mixes, OPC (replacing cement by 0% bamboo ash) concrete cube, which is regarded as "sample 1" and the bamboo ash was used for 5%, 10%, 15%, 20% and 25% replacing cement concrete cubes which were marked out as sample 2,3,4,5,6 were prepared for concrete grade M-15 and M-20 respectively. The ingredients of concrete were thoroughly mixed in pan and during mixing the ingredients of concrete, water were used to form concrete paste. Water to cement ratio (w/c) was different for different specimens and then uniform thoroughly consistency concrete paste was achieved and concrete specimens were casted by using the plastic mould as shown in figure 1. These concrete cubes were produced for 28 days curing age. These were tested by compression machine, the maximum load and compressive strength of concrete cubes were determined. To investigate the pozzolanic behavior of bamboo ash, (95% OPC+5% bamboo ash) and (90% OPC+10% bamboo ash) concrete crushes were analyzed by XRD analysis. For sample preparation, bamboo ash, cement, sand and coarse aggregates weight ratio for concrete cubes were shown in table (1&2).

EDXRF Analysis of the (5% & 10% bamboo ash) admixture cement paste

The chemical composition of bamboo ash determined by EDXRF analysis was shown in table 3. The chemical composition of bamboo ash illustrates that it contains high amount of silicon (Si) as dominant element and the second dominant elements are potassium (K), calcium (Ca), Iron (Fe) and in addition to small amount of sulfur (S), manganese (Mn), titanium (Ti), zinc (Zn), rubidium (Rb), copper (Cu), strontium (Sr) and yttrium (Y).

The chemical composition of OPC by EDXRF analysis was shown in table 4. The chemical composition of OPC illustrates that it contains high amount of calcium (Ca) as dominant element and the second dominant elements are silicon (Si), Iron (Fe), potassium (K), sulfur (S), titanium (Ti) manganese (Mn), strontium (Sr) and zirconium (Zr).

XRD analysis of the (5% & 10% bamboo ash) admixture cement paste

In this research, an XRD analysis is used to investigate the pozzolanic behavior of bamboo ash and to identify the hydration products formed during the hydration of OPC in concrete making is shown in Fig 2 (a & b). By

observing the XRD patterns of (5% and 10% bamboo ash) admixture cement paste at curing age 28 days (concrete crushes), it was found that calcium silicate hydrate, C-S-H, calcite, CaCo₃ and calcium hydroxide, Ca (OH)₂ peaks were observed in both patterns. The most intense C-S-H peaks were observed on both observed file and the XRD pattern of (5% bamboo ash) has more intense peaks than (10% bamboo ash). This C-S-H peaks indicate the pozzolanic reaction between Ca(OH)₂ and amorphous silica present in bamboo ash. This additional hydration product C-S-H has the cementitious properties and it improves the compressive strength of concrete.

Maximum load and Compressive Strength

The maximum load and compressive strength of all concrete cubes were measured and tested at Myanmar Engineering Society, MES Quality Control Laboratory, Compression Test of Concrete Specimens room, Hlaing University Campus, Hlaing Township, Yangon Myanmar. The compressive strength of 5, 10, 15, 20 & 25% (bamboo ash concretes) grade M-15 did not exceed than that of OPC and it had nearly equal value of OPC. The maximum load and compressive strength were tested by 2000kN compression machine and the results were shown in Table 5&6. The maximum load and compressive strength of MES results were shown in Figure 3 and bar graphs were shown in Figure4(a, b)&5(a, b).

Target Strength of Concrete

According to IS, the target strength of the compressive strength of the concrete mixture is defined as:

Target Strength = $f_{ck} + 1.65\sigma$,

Where σ is the standard deviation and f_{ck} is the characteristic strength [Quantity Control Issue].

The results were shown in Table 7&8.

Target Strength of Concrete Grade M-15 (1:2:4) and M-20 (1:1.5:3)

For Grade M-15 (1:2:4)

Target Strength,

 $f_t = f_{ck} + 1.65 \sigma$ $f_t = 15 + 1.65 \times 3.5$ (Standard Deviation for grade M-15 is 3.5) $f_t = 20.775 \text{ MPa}$

For Grade -20 (1:1.5:3)

Target Strength,

 $f_t = f_{ck} + 1.65 \sigma$

 $f_t = 15 + 1.65 \times 4$ (Standard Deviation for grade M-20 is 4)

 $f_t = 26 MPa$



Figure 1: The photograph of concrete paste pour in plastic mould



Figure 2: (a) The XRD pattern of 5 % bamboo ash admixture cement paste



Figure 2: (b) The XRD pattern of 10 % bamboo ash admixture cement paste

Company i Project :	Ma Aye That	Myanmar F ndar Oo ຊົດຈ້ະ ລຸດດາວນຊາ	MES Compress ingineering Soc Yangon, My	Quality Cont ion Test of C iety, Hlaing Ur anmar. Phone :	rol Laborator oncrete Spec tiversity Camp 01-519673 – 76,	y imens as, Hlaing Town Ext-115 -	nship,	MES CONCOL TERNATI CONCOL MES CONCOL CON	ADIA IONAL CONAL
Method of Test : Specimen no:	BS 1610, 1881	Without Bamboo Ash	Bamboo Ash- 5%	Bamboo Ash- 10%	Bamboo Ash- 15%	Bamboo Ash- 20%	Bamboo Ash- 25%	the mine at	and a local design of the
Making on Specimen		17-11-2017	17-11-2017	17-11-2017	17-11-2017	17-11-2017	17-11-3017		- /
Date of Test		15-12-2017	15-12-2017	15-12-2017	15-12-2017	15-12-2017	15-12-2017		- /-
Age (days)		25	28	28	28	25	216		1
Weight (Kg)	23	7.68	7.86	7.76	7.8	7,86	7.74 -		1
Length (mm)	<u> </u>	150.35	150.34	150.36	150.52	150.42	150.61		1
Width (mm)	1	150.42	150.29	150,39	150.28	150.51	150.34	1	
Height (mm)		150.62	150.25	150.45	150.38	150.21	150.36	1	
Density (Ib/ft	3	143.01	146.86	144.68	145.45	146.60	144.18	1	
Maoiimum Load	(k:N)	725.73	789.52	685.49	504s.81	485.39	518.91	1	
Contraction data and	(N/mm ²)	32.09	34.27	30.31	25.06	21.44	22.92	1/	
compossive surridro	(lb/in ²)	4654.62	5042.78	4397.11	3634.63	3109.54	3324.16	1	
temarks: This certificate If any) Tested b	MES	for the receipt of th Const Lateratory	e test sample.	Арри	(In Accurancy 1)	(22%) Dumage befor Out of Shape	Condition when retest	unseined Uneven sutfa Normal Lab Consultant Ato	N#
Lynn Lynn F Lab Techni MUS QC L	tttke fon ab	555555400 4/7 15-1-510872 - 5106	Sed of the	Myii MEE (Per (CEO) I	nt Soe nv-Engg.) (M-MES		ILE (S M.ASCE, AER,	San Kyu Svil), M.Engg (Su FM-MES, PE, ACI	ucture) E.(Constructio

Figure 3: The photograph of MES's certificate



Figure 4: (a) Maximum load bar graph of M-15 concrete cubes



Figure 4: (b) Compressive Strength bar graph of M-15 concrete cubes



Figure 5: (a) Maximum load bar graph of M-20 concrete cubes



Figure 5: (b) Compressive Strength bar graph of M-20 concrete cubes

Table	1:	Cement,	bamboo	ash,	sand,	coarse	aggregates	and	water	to
		cement r	atio for g	grade	M-15	concrete	e			

Sample No.	Cement (%) (1)	Sand (2)	Coarse Aggregates (4)	Bamboo ash (%)	Total Weight	Water to Cement ratio (w/c)
Sample (1)	1.071kg (100%)	2.142kg	4.284kg	0kg (0%)	7.5 kg	0.5 (0.53) kg
Sample (2)	0.97 kg(95%)	2.142 kg	4.284 kg	0.05 kg (5%)	7.5 kg	0.35 (0.38)kg
Sample (3)	0.9639 kg (90%)	2.142 kg	4.284kg	0.1071kg (10%)	7.5kg	0.35 (0.38)kg
Sample (4)	0.9103kg (85%)	2.142kg	4.284kg	0.1606kg (15%)	7.5kg	0.35 (0.38kg)
Sample (5)	0.8568kg (20%)	2.142kg	4.284kg	0.2142kg (20%)	7.5kg	0.35 (0.38kg)
Sample (6)	0.803kg (25%)	2.142kg	4.28kg	0.268kg (25%)	7.5kg	0.4 (0.43kg)

Sample No.	Cement (%) (1)	Sand (1.5)	Coarse Aggregates (3)	Bamboo ash (%)	Total Weight	Water to Cement ratio (w/c)
(1)	1.3636 kg (100%)	2.045kg	4.09 kg	0kg (0%)	7.5 kg	0.6 (0.82) kg
Sample (2)	1.295 kg(95%)	2.045 kg	4.09 kg	0.0686 kg (5%)	7.5 kg	0.5 (0.68)kg
Sample (3)	1.227 kg (90%)	2.045 kg	4.09 kg	0.1366 kg (10%)	7.5kg	0.57 (0.78)kg
Sample (4)	1.159kg (85%)	2.045 kg	4.09 kg	0.2046 kg (15%)	7.5kg	0.55 (0.75)kg
Sample (5)	1.091 kg (20%)	2.045kg	4.09 kg	0.2726 kg (20%)	7.5kg	0.56 (0.76)kg
Sample (6)	1.023 kg (25%)	2.045kg	4.09 kg	0.3406 kg (25%)	7.5kg	0.56 (0.76)kg

 Table 2: Cement, bamboo ash, sand, coarse aggregates and water to cement ratio for grade M-20 concrete

Table 3: Chemical composition of bamboo ash by EDXRF analysis

Component	Si	K	Ca	Fe	S	Mn	Ti	Zn	Rb	Cu	Sr	Y
	%	%	%	%	%	%	%	%	%	%	%	%
Bamboo Ash	51.47	14.98	14.44	9.12	1.47	1.11	0.59	0.59	0.09	0.08	0.07	0.07

Component	Ca%	Si%	Fe%	K %	S %	Ti %	Mn %	Sr%	Zr%
OPC	83.87	6.55	6.37	1.58	1.02	0.41	0.1	0.8	0.23

Table 4: Chemical composition of ordinary portland cement, OPC byEDXRF analysis

Table 5:	Maximum Load and Compressive Strength of specimens (grade
	M -15, 1:2:4 cement replacement by bamboo wastes ash)

G	Sample (1)	Sample (2)	Sample (3)	Sample (4)	Sample (5)	Sample (6)
Specimen No.	0% Bamboo	5% Bamboo	10% Bamboo	15% Bamboo	20% Bamboo	25% Bamboo
	ash	Ash	Ash	Ash	Ash	Ash
Making on Specimen	10.10.17	10.10.17	14.10.17	12.10.17	12.10.17	14.10,17
Date of Test	7.11.17	7.11.17	11.11.17	9.11.17	9.11.17	11.11.17
Age(days)	28	28	28	28	28	28
Weight (kg)	7.58	7.4	7.65	7.5	7.66	7.7
Length (mm)	150.12	150.26	150.13	150.21	150.27	150.12
Width (mm)	150.5	150.84	150.47	150.3	150.42	150.51
Height (mm)	150.39	150.3	150.58	150.42	150.5	150.85
Density (kg/m ³)	141.50	137.79	142.65	140.09	142.83	143.30
Maximum Load(kN)	897.26	836.95	622.91	472.6	531.01	366.66
Compressive Strength (N/mm ²)	39.71	36.93	27.57	20.93	23.49	16.23
(lb/in^2)	5760.51	5356.21	3999.96	3036.36	3407.55	2353.84

Table 6: Maximum Load and Compressive Strength of sp	pecimens (grade
M -20, 1:1.5:3 cement replacement by bamboo wa	astes ash)

Specimen No.	Sample(1) 0% Bamboo ash	Sample(2) 5% Bamboo Ash	Sample(3) 10% Bamboo Ash	Sample(4) 15% Bamboo Ash	Sample(5) 20% Bamboo Ash	Sample(6) 25% Bamboo Ash
Making on Specimen	17.11.17	17.11.17	17.11.17	17.11.17	17.11.17	17.11.17
Date of Test	15.12.17	15.12.17	15.12.17	15.12.17	15.12.17	15.12.17
Age(days)	28	28	28	28	28	28
Weight (kg)	7.68	7.86	7.76	7.8	7.86	7.74
Length(mm)	150.35	150.34	150.36	150.52	150.42	150.61
width(mm)	150.42	150.29	150.39	150.28	150.51	150.34
Height (mm)	150.62	150.25	150.45	150.38	150.21	150.38
Density (kg/m ³)	143.01	146.86	144.68	145.45	146.60	144.18
Maximum Load(kN)	725.73	785.52	685.49	566.81	485.39	518.91
Compressive Strength (N/mm ²)	32.09	34.77	30.31	25.06	21.44	22.92
(lb/in^2)	4654.62	5042.78	4397.11	3634.63	3109.84	3324.16

Sample No	Concrete Grade	Measurable Compressive Strength (MPa)	Target Strength (MPa)	Curing Age (Days)	Remark
1(0%)	M-15	39.71	20.775	28	MCS>TS
2(5%)	M-15	36.93	20.775	28	MCS>TS
3(10%)	M-15	27.57	20.775	28	MCS>TS
4(15%)	M-15	20.93	20.775	28	MCS>TS
5(20%)	M-15	23.49	20.775	28	MCS>TS
6(25%)	M-15	16.23	20.775	28	MCS <ts< td=""></ts<>

Table 7:	Comparison	of Measurable	Compressive	Strength	and	Target
	Strength for	grade M-15 (ba)	mboo Ash)			

Table 8:	Comparison	of Measurable	Compressive	Strength	and	Target
	Strength for	grade M-20 (ba	mboo Ash)			

Sample No	Concrete Grade	Measurable Compressive Strongth	Target Strength (MPa)	Curing Age	Remark
		(MPa)	(IVII <i>a)</i>	(Days)	
1(0%)	M-20	32.09	26.6	28	MCS>TS
2(5%)	M-20	34.77	26.6	28	MCS>TS
3(10%)	M-20	30.31	26.6	28	MCS>TS
4(15%)	M-20	25.06	26.6	28	MCS <ts< td=""></ts<>
5(20%)	M-20	21.44	26.6	28	MCS <ts< td=""></ts<>
6(25%)	M-20	22.92	26.6	28	MCS <ts< td=""></ts<>

Conclusion

Pozzolanic behavior of bamboo ash in partial cement replacement in concrete has been studied. By observing the EDXRF analysis of bamboo ash, it was found that bamboo ash contains high amount of silica and second dominant elements were potassium and calcium. The elements contain in bamboo ash and OPC were almost the same. For concrete grade M-15, according to MES's results, the measured value of maximum load and compressive strength of blended concretes did not exceed than OPC (0%) concrete. However, 5%, 10%, 15% and 20% blended concretes reached the target strength. For concrete grade M-20, from the results, the measured value of maximum load and compressive strength of 5% blended concrete was higher than that of OPC (0%) concrete. But, only 5% and 10% blended concretes reached the target strength. By observing the XRD patterns of 5% and 10% bamboo ash of concrete crushes, it was found that the hydration product, calcium silicate hydrate, C-S-H formed during the hydration of OPC and it was shown that the pozzolanic behavior of the bamboo ash. Fineness of bamboo ash is also the important factor affecting the compressive strength of concrete. So, grade M-20 for 5% and 10% of bamboo ash is quite suitable for partially cement replacements

Acknowledgements

I would like to express appreciation to Acting Rector Dr Theingi Shwe, Pro-rector Dr Khin May Aung and Dr Cho Cho Myint, Dawei University for their encouragement and kind permission to undertake the present research. I also would like to express my profound thanks to Professor Dr San San Aye, Head of Department of Physics, and Professor Dr Kyaw Myint Htoo, Department of Physics, Dawei University, for their kind permission to carry out this work, their encouragement and help during this work.

References

- Aigbodion V. S (2010), "Journal of Minerals & Materials Characterization & Engineering", Ahmadu Bello University, Samara, Zaria, Nigeria, Vol.9, 67-77.
- Anurag Nayak , Arehant S Bajaj , Abhishek Jain , Apoorv Khandelwal , (2013)
 "Replacement of Steel by Bamboo Reinforcement". IOSR Journal of Mechanical and Civil Engineering (IOSR-JMCE), Vol- 8, 50-61
- Dinesh Bhonde. P. B. Nagarnaik, D. K. Parbat, U. P. Waghe (2014) "Experimental Investigation of Bamboo Reinforced \ Concrete Slab", American Journal of Engineering Research (AJER) Vol.03, 128-131.
- Ernesto Villar-Cocina Ernesto ,Villar-Cocina a, ft, Eduardo Valencia Morales a, Sergio F. Santos b, Holmer Savastano Jr. b, Moises Friasc (2011) ,"Pozzolanic behavior of bamboo leaf ash Characterization and determination of the kineti parameters", Cement & Concrete Composites Journal ,Voi.33 ,68-73.
- Jigar K. Sevalia , Nirav B. Siddhpura , Chetan S. Agrawal , Deep B. Shah , Jai V. Kapadia, (2013) "Study on Bamboo as Reinforcement in Cement Concrete", International Journal of Engineering Research and Applications (IJERA) Vol. 3.1181-1190.
- Kawade U.R (2013),"International Journal of Innovative Research in Science", Engineering and Technology, Pravara Rural Engineering College, India, Vol.2.
- Toshi Bhavsar (2015) "Preparation and Characterization of BRC with Different Types of Concrete", International Journal of Latest Trends in Engineering and Technology (IJLTET), Vol.5, 390-401.

Zongjin Li (2011) "Advanced concrete technology".

ESTIMATE OF UNCERTAINTY OF MEASUREMENT IN THE DETERMINATION OF Cu, Zn, Fe IN PROFICIENCY TEST (PT) DRINKING WATER SAMPLE

Kyauk Khe Sein¹, Ye Chan²

Abstract

Nowadays, the testing and calibration laboratories have to provide high confidence and globally acceptable of measurement results in order to support the important action or decision based on it, especially for international trade and customer satisfaction. Therefore, according to guide ISO/IEC 17025, the measurements should be carried out by using validated method of analysis, defining the internal quality control procedures, participating in proficiency testing schemes and establishing the traceability and uncertainty of the measurement results. For this reason the determination of metals in drinking water requires the use of validated methods which demonstrating their robustness and reliability. In this context the estimate of uncertainty is an important tool allowing the identification the influence of each step of the analytical protocol in the overall quality of the results. In this paper, it was discussed the estimate of uncertainty during the measurement of metals (Cu, Zn and Fe) in proficiency test (PT) drinking water sample by atomic absorption spectrometry in flame mode. The concentration of Cu, Zn, Fe found in PT drinking water is 1.601 \pm 0.043 mg/L, 1.061 \pm 0.202 mg/L and 0.179 \pm 0.095 mg/L respectively. The total uncertainty for Cu, Zn and Fe were 3%, 19%, 53% respectively.

Keywords: uncertainty, AAS, proficiency test, ISO/IEC 17025

Introduction

Nowadays, the testing and calibration laboratories have to provide high confidence and globally acceptable of measurement results in order to support the important action or decision based on it, especially for international trade and customer satisfaction. Therefore, according to guide ISO/IEC 17025, the measurements should be carried out by using validated method of analysis, defining the internal quality control procedures, participating in proficiency testing schemes and establishing the traceability and uncertainty of the measurement results. The importance for uniform

¹ Assistant Lecturer, Universities' Research Centre, University of Yangon

² Professor, Head of Universities' Research Centre, University of Yangon

approach of measurement in estimation of uncertainty and its reporting has attracted metrologist globally. An evaluation, or at least full consideration, of all identifiable components that contribute to the uncertainty of a test result will allow valid results to be obtained and indicate the aspects of the test that require attention to improve procedures. In addition, systematic assessment of the factors influencing the results and its uncertainty forms a key of validation method.

According to EURACHEM/CITAC, the uncertainty can be defined as 'a parameter associated with the result of measurement, which characterizes the dispersion of the values that could reasonably be attributed to the measurand'. In the other word, the estimation of uncertainty is a result of the various components which affects to the measurement. The evaluation of uncertainty requires the analyst to look closely at all the possible sources of uncertainty. Many possible sources of uncertainty may be arisen in practice such as sampling, sample effects (matrix effects and interferences), instrument reagent purity, effects, storage conditions, assumed stochiometry, measurement condition, uncertainties of masses and volumetric equipment, reference values, computational effect, blank correction, operator effect, and random effect. In estimating the overall uncertainty, it may be necessary to take each source of uncertainty and treat it separately to obtain the contribution from that source. Each of the separate contributions of uncertainty is referred to as an uncertainty component, and known as standard uncertainty if it is expressed as a standard deviation. For a measurement result, the total uncertainty, termed combined standard uncertainty is calculated and obtained by combining all the uncertainty components. Furthermore, an expanded uncertainty should be used for most purposes in analytical chemistry. The expanded uncertainty provides an interval within which the value of measurand is believed to lie with a higher level confidence.

A good estimation of uncertainty can be made by concentrating effort to the largest contribution of source of uncertainty because the value obtained for the combined uncertainty is almost entirely controlled by the major contribution. Further, once uncertainty value evaluated for a given method applied in particular laboratory (i.e. particular measurement procedure), the uncertainty estimation obtained may be reliably apply to subsequent results obtained by the method in the same laboratory, provided that this is justified by the relevant quality control data. No further effort should be necessary unless the procedure itself or the equipment used is changed, in which case the uncertainty estimation would be reviewed as part of the normal revalidation. In the other hand, the observed differences in result may be accounted for by the uncertainty associated with the result rather than real difference in properties or performance. Thus if two competent laboratory examine different sub samples from the same sample source by the same method and obtain numerically different results, these results may not be different when uncertainty of measurement is taken into account (Harry Budiman, et.al., 2009).

This paper describes the evaluation of uncertainty of measurement in determination of Cu, Zn, Fe content in drinking water PT sample using flame atomic absorption spectrometry. The specification of measurand, source of uncertainty, standard uncertainty, combined uncertainty and expanded uncertainty from this measurement were evaluated and accounted. The purpose of the evaluation of uncertainty in this measurement is to provide the bias taken place which depended on the various components or measurands that effect to the measurement. This is required for the laboratory participating in the Proficiency Testing Scheme: Analysis of drinking water and waste water by Universities' Research Centre, University of Yangon. The estimation of uncertainty measurement of each laboratory is needed by proficiency testing provider for comparison with the standard deviation for proficiency assessment (σ P) that represents fitness-for-purposes over a whole application sector in proficiency testing scheme.

The objective of a measurement is to assign a magnitude to the measurand, the quantity intended to be measured. The assigned magnitude is considered to be the best estimate of the values of the measured. For a given result there is not one value, but an infinite number of values dispersed about the result within an interval. Hence measurement of a parameter is meaningless unless the width of interval within which the reported value of the measured is expected to disperse is specified. Material used for army purpose is to be tested in proper way because the chemical composition of material is most affecting factor in performance of final product. While testing

chemical composition the final result get affect by various factors so the composition result may not be so correct.

Experimental Section

2.1 Atomic Absorption Spectrophotometer

Atomic Absorption (AA) occurs when a ground state atom absorbs energy in the form of light of a specific wavelength and is elevated to an excited state. The amount of light energy absorbed at this wavelength will increase as the number of atoms of the selected element in the light path increases. The relationship between the amount of light absorbed and the concentration of analytes present in known standards can be used to determine unknown sample concentrations by measuring the amount of light they absorb. Simplified diagram of principle of AAS is shown in Fig. 1.



Figure 1: Simplified diagram of principle of AAS

The liquid sample is reduced to a vapor mist of atomic population by a nebulizer with support gas. Mixed with proper fuel, it is sprayed over the flame. The reference beam going around the flame is not affected because the energy of sample beam going through the flame is absorbed by the sample element present in the liquid sample and amount of absorption being proportional to the element concentration. Both these beam are combined together before entering the monochromatic region which selects the appropriate resonance line and direct it to the wide range photo multiplier tube. The electronics there after separates reference and sample signal in time reference single is used to compensate for drift in lamp intensities and sample signal is processed for photometric computation of the result. The atomic absorption Spectrophotometer (Perkin Elmer 900H) is as shown in Fig. 2.



Figure 2: Atomic Absorption Spectrophotometer AAS (Perkin Elmer 900H)

2.2 Material

All chemicals were purchased from SIGMA-ALDRICH as shown in Fig. 3 and for analysis grade. Pure deionized water was used for all solution preparation. Calibration of standard Cu, Zn, Fe solution was prepared by the dilution of titrisol of Cu, Zn, Fe solution 1000 \pm 4 mg/L as stock solution. The test sample is clean water for drink which prepared and distributed by LIPI Indonesia as shown in Fig. 4.



Figure 3: Cu and Zn Standard for calibration



Figure 4: Proficiency test (PT) sample

2.3 Principle of working

When a liquid sample containing a chemical constituent element of interest is reduced to a spray mist of atomic vapour, mixed with proper fuel and burn over a burner head and if light radiation of the same element from a emitting source is passed through the flame, as atoms of the element in the sample vapour are present in ground state of unexcited condition they absorb amount of corresponding radiation passing through the flame. Amount of absorption by the analyst depend on its concentration in the sample and are directly proportional to each other. Hence measurement of absorption value forms the base for calculation of its concentration in sample (EURACHEM/ CITA Guide CG4, 2012).

2.4 Method of Analysis

Every time when an element is estimated, the system is calibrated by aspirating a set of different strength standard solution of known concentration of the element and graphical representation of absorbance verses concentration is made to get a liner graph for the standard solution. When an unknown sample is aspirated in the same condition, with reference to its measured absorbance and the standard graph concentration of the element in test sample is displayed in part per million (ppm) or mg/L.
Result and Discussion

3.1 Identification of sources of uncertainty

The sources of uncertainty for the method were identified by constructing a cause-and-effect (fish bone) diagram Fig.5 widely cited by some authors EURACHEM/CITAC Guide CG 4.



Figure 5: Sources of uncertainty fish bone diagram

3.1.1 Concentration of aliquot sample, C_x

As shown in Fig. 5 the uncertainty associated with the concentration of the Cu, Zn, Fe in the sample aliquot is estimated from calibration curve. The uncertainty of aliquot sample analyzed, represented by $\mu(Cx)$, is given by EURACHEM/ CITA Guide CG4. And equation (1) and (2) is used to calculate the uncertainty of aliquot sample.

$$S_{y/x} = \sqrt{\frac{\Sigma(Yi - Yc)^2}{(n-2)}} \tag{1}$$

$$\mu(C_x) = \frac{S_{y/x}}{b} \sqrt{\frac{1}{m} + \frac{1}{n} + \frac{(Y_{Spl} - Y_{mean})^2}{b^2 \cdot \Sigma(X_i - X_{mean})^2}}$$
(2)

Where, b = slope of the calibration curve,

m = number of measurements to determine Co,

n = number of measurements for the calibration,

Sy/x = residual standard deviation.





(iii)

Figure 6: Standard calibration curve graph for (i) Copper (Cu) (ii) Zinc (Zn) (iii) Iron (Fe)

3.1.2 Recovery (Rec.)

The uncertainty from recovery is calculated by using equation (3) as percentage recovery from comparable reference material. The recovery, R, has an uncertainty associated with the certified reference material value used and with the variability of the particular measurement of the solution analyzed.

$$\mu(\operatorname{Re} c) = \operatorname{Re} c \cdot \sqrt{\left(\frac{\mu(X_{Obs})}{X_{Obs}}\right)^2 + \left(\frac{\mu(X_{CRM})}{X_{CRM}}\right)^2} \tag{3}$$

3.1.3 Repeatability (Rep)

Fig.5 shows two major contributions to the uncertainty associated with the repeatability, instrument drift and precision associated with the dilution of calibration solutions.

3.1.4 Stock Standard (C0.5)

The uncertainty from stock standard is calculated by using equation (4).

$$C_{0.5} = C_{1000} \times \frac{v_1}{v_{100}} \tag{4}$$

Table 1: Calculated standard uncertainty arising from uncertainty sources

	Standard	Uncertainty	Uncertainty	Uncertaint	Combined		
	uncertainty	arising from	arising from	from Stock	from Stock Standard		
	arising from	Repeatability	Recovery	Туре А Туре В		C _s (mg/L)	
	$C_x \left(mg/L\right)$	(Rep)	(Rec.) (%)	(mg/L)	(mg/L)		
Cu	0.0032	0.0049	1.1682	0.0005	4	0.022	
Zn	0.0989	0.0113	1.3330	0.0005	4	0.101	
Fe	0.0472	0.0278	1.1680	0.0005	4	0.048	

3.2 Combined Standard Uncertainty

The value of parameters for calculation of Cu, Zn, Fe concentration in sample, equation (1), their standard uncertainties and their relative standard uncertainties were summarized in Table 1. According to the data of combined

uncertainty, it is fount that Fe is more error percent than Cu and Zn elements and Cu is least error.



Figure 7: Comparison of error in PT sample

Fig. 7 shows the comparison of error percentage of estimate assigned error and estimate the test error in PT sample. It is found that the error of Fe element is greater than other elements but Cu is smaller for our calculation because relative standard deviation of Fe is greater than Cu in the calibration curved. This is due to chemical interference on atomization process.



Figure 8: Comparison of concentration in PT sample with assigned value and test value without using uncertainty

Fig. 8 shows the comparison of concentration in PT sample with assigned value and test value without using uncertainty. It is found that the concentrations of elements of our test value are nearly equal to the assigned value of PT coordinator.

Moosuvands	Assigned value with uncertainty	Test value with uncertainty			
Measuranus	(mg/L)	(mg/L)			
Copper (Cu)	1.58 ± 0.14	1.601 ± 0.043			
Zinc (Zn)	1.12 ± 0.11	1.065 ± 0.202			
Iron (Fe)	0.21 ± 0.06	0.178 ± 0.095			

 Table 2: Comparison of assigned value of PT coordinator and our test

 value with uncertainty

It is found that the concentration results of the determination of Cu, Zn, Fe in PT sample are reliable with assigned value when measurement uncertainty is added as shown in Table 2.

Conclusion

The Cu, Zn, Fe content in drinking water PT sample analyzed by Flame AAS was 1.601 ± 0.043 mg/L, 1.065 ± 0.202 mg/L, 0.178 ± 0.095 mg/L at 95% confidence level. The total uncertainty for Cu, Zn and Fe were 3%, 19%, 53% respectively. The sources of uncertainty in the determination of Cu, Zn, Fe in sample by AAS were the uncertainties of concentration of Cu, Zn, Fe obtained by AAS, the uncertainties of mass of sample, the uncertainties of dilution factor, the uncertainties of the volume of sample, the uncertainties of repeatability and the uncertainties of recovery. The uncertainty estimation of different sources in analysis Cu, Zn and Fe demonstrated that the calibration curve was the major contribution to the uncertainty of the final results. Even if the result of the measurement is not perfect, it is possible to obtain reliable information, since the result of the measurement is associated with its respective uncertainty. The success in estimating uncertainty of measurement depends on correct analysis of the whole measuring process. Estimation of measurement uncertainty is very important for reliability of measurement data. This paper shows the effects of individual factors and its importance on final result. Evaluation of uncertainty gives idea about various factors affecting the test results. Accordingly proper actions can take to reduce the effect of factor which is affecting more. This helps to improve the quality of testing and calibration method. In case of AAS repeatability is affecting more, so while performing the test standard procedure should be followed which help to minimize the uncertainty of measurement.

References

- Ellison, S.L.R., Rosslein, M., and Williams, A., *EURACHEM/CITAC Guide CG 4*, (2012), "Quantifying Uncertainty in Analytical Measurement", Third Edition.
- Harry Budiman*, Fransiska Sri H. Krismastuti, and Nuryatini, (2009), "Estimation of Measurement Uncertainty in the Determination of Fe Content in Powdered Tonic Food Drink Using Graphite Furnace Atomic", Research Centre for Chemistry, Indonesian Institute of Sciences, Kawasan PUSPIPTEK Serpong, Banten 15314, Indonesia.
- Kirkup, L., (2007), "Calculating and Expressing Uncertainty in Measurement", University of Technology, Sydney.
- Neha S. Mahajan et al., (2012), "Analysis of Uncertainty Measurement In Atomic Absorption Spectrophotometer", International Journal of Engineering Science and Technology (IJEST), ISSN : 0975-5462 Vol. 4.
- V. J. Barwick, S. L. R. Ellison, B. Fairman, (1999), "Estimation of uncertainties in ICP-MS analysis: a pratical methodology", Analytica Chimica Acta 394, pp. 281-291.

SYNERGIC SYNTHESIS ROUTE FOR THE FABRICATION OF ORGANIC-INORGANIC COMPOSITE FILM

Nyunt Win¹, Cho Cho Thet² and Ye Chan³

Abstract

Synergic synthesis for organic-inorganic hybrid matrices has been significantly interested for a wide range of optoelectronic applications. Regarding this, efficient synthesis route for the fabrication of $P(Py-2FPy)/TiO_2$ composite film has been studied. While inorganic TiO₂ nanoparticle solution was synthesized by low temperature solution method, the fabrication of composite film was prepared by *ex-situ* chemical copolymerization through spin coating technique. The synergic assembly of composite film was identified and characterized by FT-IR, UV-Vis and XRD. The resulted films show that the inorganic TiO₂ nanoparticles can be successfully incorporated into the organic copolymer matrix. In addition, the new fabricated organic-inorganic composite films are scalable. Thus, it can be applied in industry and will be major interest in the area of nanocomposite materials.

Keywords: polypyrrole, 2- formyl pyrrole, TiO₂, *ex-situ* chemical copolymerization and composite film

Introduction

The mixing of organic polymers and inorganic nanoparticles is opening pathways for engineering flexible composites materials that show a better magnetic, electrical, optical, or mechanical property. New strategies to engineer materials that combine the desirable properties of polymers and nanoparticles for the formation of polymer-inorganic nanocomposites have been attempted for last decades. However, there were many challenges for the synthesis techniques since nanoparticles are typically aggregated which can hinder the fabrication of nanocomposites. The nanoparticles must be integrated in a way leading to isolated, well-dispersed primary nanoparticles inside the matrix. There is no debt to establish the processing techniques that are effective on the formation of composites. Thus, synthetic strategies for composite with a high homogeneity are really a challenge. Synthesis of

¹ Lecturer, Department of Physics, Pathein University

² Lecturer, Universities' Research Centre, University of Yangon

³ Professor, Head of Universities' Research Centre, University of Yangon

composites can be classified into two major groups, chemical and physical methods respectively.

Chemical methods are direct mixing and melt processing of particles with polymers often lead gradients of the incorporated fillers in the matrix. However, this method leads to turbidity/translucency of composite materials because of the agglomeration of the nanoparticles. As a result, *in-situ* polymerization and *in-situ* nanoparticle formation methods have been developed to overcome these problems. Inorganic nanoparticles were directly dispersed in the monomer solution prior to a polymerization processing in *in-situ* polymerization. In this process, inorganic particles tend to phase separate and sediment quickly from the organic polymer. For the good link/interaction at the interface, specific groups have to be linked onto their surface to stabilize nanoparticle dispersions (Althues *et al.*, 2007).

Physical or *ex-situ* polymerization methods are based on liquid particle dispersions. It implies that particles are dispersed into a polymer melt and then composites are obtained by extrusion. Casting methods use a polymer solution as a dispersant and solvent evaporation yields the composite material (Althues *et al.*, 2007). The *ex-situ* synthesis method is more suitable for large-scale industrial applications than the *in situ* method (Guo *et al.*, 2014). The advantages of this method include resulting of higher dispersibility of nanoparticles in the polymer and have long-term stability against aggregation.

The polymer inorganic composites comprise inorganic nanoparticles which are uniformly dispersed in and fixed to a polymer matrix. The interfacial surface area of composite was increased due to higher surface area of nanoparticles. In addition, smaller particle size allows a much more homogeneous distribution of a composite material. However, this may tend to aggregation of the nanoparticles to energetically stabilize composites, thus lowering the homogeneity of particle distribution. In order to minimize interface energies between particles and polymer matrix, several nanocomposites of polymer and nanoparticles surface modification/f unctionalization and stabilization techniques have been developed that are mainly used in chemical methods. Recently, *in-situ* polymerization and sol-gel methods were used to fabricate a new class of composite polymer with

transparent nano-fillers. This type of material is also sometimes called polymer-inorganic hybrid/nanohybrid. (Zhang *et al.*, 1997; Yuwono *et al.*, 2004; Li *et al.*, 2007).

Depending on the applications, inorganic components including metals (Hopf *et al.*, 1997; Macanas *et al.*, 2007), metal alloys (Fang et al., 2002), metal oxides (Ahmad *et al.*, 2008), ferric oxide (Gangopadhyay *et al.*, 1999; Gass *et al.*, 2006) and ferrite (Prabhakaran *et al.*, 2008) and carbon based materials (Grossiord *et al.*, 2008; Agarwal *et al.*, 2008) and organic matrix including industrial plastics conducting polymers and transparent polymers usually chosen. However, there is no work for fabrication of copolymer composites film according to our concerns.

In this work, $P(Py-2FPy)/TiO_2$ composites films were prepared *ex-situ* chemical polymerization through spin coating for the electrical application aspects of composite. The synergic synthesis route for the fabrication of composite film is presented by investigating with UV-Vis, FT-IR and XRD measurement. The incorporation of TiO₂ improved the structural, morphological, and conductivity properties of the composite.

Experimental Details

Preparation of the Organic Monomer Solution

(200 mg, 3 mmol) of Py and (286 mg, 3 mmol) of FPy were mixed and dissolved in 2 mL of chloroform (CHCl₃) in a conical flask. They were stirred at the room temperature for 30 min to obtain the monomer solution.

Preparation of the Inorganic TiO₂ Precursor Solution

In the synthesis of TiO₂, titanium isopropoxide (TTIP), 2-propanol and hydrochloric acid (HCl) are used as the precursor, catalyst and solvent. Typically, the first solution of 0.0138 M, 2.53 mL 2-propanol (IPA) was mixed with 2 M, 35 μ L HCl were prepared. Then another solution was prepared by adding 0.23 M, 369 μ L TTIP in 0.0138 M, 2.53 mL, 2-propanol. Then, the first solution is slowly added drop wise to the second solution and was stirred at 800 rpm. After being stirred for six hours at the room temperature, a clear and transparent TiO_2 nanoparticle dispersion solution was successfully obtained.

Preparation of the Composite Films

486 mg of as-synthesized TiO_2 solution was added to 486 mg of monomer solution. Thus, the weight ratio of inorganic to organic is 1:1. The mixture was continuously stirred for 24 h. Then, the solution containing (13 mmol) trifluoroacetic acid (TFA) and (2 mL) CHCl₃ was additionally put to composite solution at room temperature. After that, the mixed solution was spin-coated onto the Petri dish at 20 rpm using a home-made spin coater until the complete formation of copolymerization. After that, the film was successively washed by excess deionized water and acetone and dried in a vacuum oven for 12 h. Figure 1(a) illustrates the synthesis route scheme of the composite films. The photo of composite film casted in the Petri dish was exhibited in Figure 1(b). The film was a metallic greenish black and insoluble in several solvents.

Characterization Tools

The UV-Vis was performed in order to examine the absorbance values of all synthesized samples. The UV-Vis spectra were obtained by using Shimadzu UV-1800 UV-Vis spectrophotometer. The crystal structure and crystallite size of the samples were confirmed by XRD (model RIGAKU-RINT 2000) using CuK_a radiation (40 kV, 40 mA) over a 2 θ range from 10° to 70° on a powder type X-ray diffractometer equipped with a diffracted-beam graphite monochromator. The identification of functional group was investigated by FT-IR. The spectra formations of TiO₂, pure copolymer and composite films were obtained by FT-IR 8400 Shimadzu spectrophotometer using a KBr pallet in the mid IR radiation (4000 cm⁻¹ - 400 cm⁻¹) range with a resolution of 4.0 cm⁻¹.



Figure 1:(a) *Ex-situ* synthesis schemes for the preparation of nanocomposites films



Figure 1: (b) Photo showing copolymer/TiO₂ composite film

Results and Discussion

The formation of TiO₂ nanoparticles and copolymer film was monitored by ultraviolet-visible (UV-Vis) spectroscopy. The maximum absorption wavelength occurred at 271 nm in Figure 2(a) was confirmed that the product is TiO₂ nanoparticles (Vebber *et al.*, 2016).UV-Vis spectrum of pure copolymer film is shown in Figure 2(b). It was noted that characteristic absorption band of the π - π * transition of polypyrrole is appeared at around 492 nm. This fact indicated that the FPy group was incorporated into the chemical structure of the conjugated polymer chains. Since Py and FPy had no absorption band at about 500 nm, this could be assigned with π - π * transition of the C=C double bond, which was formed by the copolymerization. In addition, weaker and broader band was appeared at about 700 nm. This strongly implied that the bipolaron state of polypyrrole was present in the films. This indicated that such strong acid (TFA) strongly interacted with pyrrole segments to form bipolaron state (Hoshina *et al.*, 2012).



Figure 2: (a) UV-Vis absorption Figure 2: (b) UV-Vis absorption spectrum of as- synthesized TiO_2 spectrum of pure copolymer film nanoparticles

The functional groups for all investigated samples were identified by FT-IR. The spectra were shown in Figure 3.The spectrum (a) is for TiO₂ nanoparticles. In this spectrum, the peaks at 3400-3500 cm⁻¹ and 1622-1633 cm⁻¹ in the spectra are due to the stretching and bending vibration of the -OH group. The peak at 1458 cm⁻¹ corresponds to the Ti-O-Ti vibration (Saravanan *et al.*, 2010). The peak at 1354 cm⁻¹ corresponds to the C-H deformation (Colthup *et al.*, 1964., Bellamy *et al.*, 1975). The peak at 1203 cm⁻¹ corresponded to the V₁ and V₃ (degenerate splitting) modes that correspond to symmetric and asymmetric stretching modes respectively (Lane 2007). The peaks at 522.73 cm⁻¹ show stretching vibration of Ti-O (Vetrivel *et al.*, (2014-2015)). Absorption peaks found at 480 cm⁻¹ correspond to Ti-O-Ti peak frequency since the regions from 400 to 800 cm⁻¹ are dominated with weak and broad peaks identified to have the frequencies corresponding to bulk titania skeletal (Kuma *et al.*, 2000).



Figure 3: FT-IR spectra of (a)TiO₂ nanoparticles (b) pure copolymer P (Py-2FPy) films without nanoparticles and (c) P(Py-2FPy)/TiO₂ composite films

The FT-IR spectrum (b) shows the pure copolymer film. The peak observed at 3383 cm⁻¹ was due to the N-H stretching vibration. The peak at 3128 cm⁻¹ was aromatic C-H stretching. The peaks of C=N stretching at 1483-1402 cm⁻¹ were attributed to the formation of the conjugated structure in the film. The peak observed at 1258 cm⁻¹ was assigned to -C=CH- stretching from methine group of the copolymer. The peak at 1203 cm⁻¹ can be related to C-N stretching of amine group. The peak of C=N appeared at 1138 cm⁻¹. The peak at 1051 cm⁻¹ can be attributed to C-H in plane deformation. The peak of the aromatic C-H out-of-plane deformation vibration appeared at 1006-800 cm⁻¹, respectively (Yusuke *et al.*, 2012).

In the spectrum (c), composite film, characteristic peaks of copolymer are observed in the composite films, indicating the formation of copolymer. The two peaks at 2875 and 2825cm⁻¹ correspond to C-H stretching vibration (asymmetric) and C-H stretching vibration (symmetric) from the remaining organic-moiety (Sabzi *et al.*, 2009). In addition to this, the presence of the new peaks at 522.73 and 445.57 cm⁻¹ confirmed that inorganic component was well resident in the polymer matrix. The obvious spectral differences between pure polymer and the composite indicate that polymer exhibits a different polymer chain structure and there are physicochemical interactions between the TiO_2 nanoparticles and PPy-FPy copolymer.

XRD measurement was carried out in order to confirm the crystal structure of TiO₂ nanoparticles. TiO₂ has amorphous structure at the room temperature (Guo et al., 2012). In order to obtain the TiO₂ crystals, assynthesized TiO₂ was annealed at different temperatures (500°C, 600°C and 700 $^{\circ}$ C). The crystal phases of TiO₂ nanoparticles were observed by XRD measurement. Figure 4 represents the XRD patterns of TiO₂ nanoparticles annealed at 500°C, 600°C and 700 °C. The generated TiO₂ nanoparticles contained the phase type anatase, rutile, and brookite. The important roles in the formation of the resulting TiO₂ crystal phases were depended on the starting material, its composition, deposition method and annealing temperature (Mechiakh et al., 2010). Crystallization is often performed by calcination at temperatures above 400 °C since as-synthesized TiO₂ is amorphous (Liao et al., 2010). Only the crystal form of pure anatase was obtained at the annealing temperature 500 °C and a partial phase anatase and rutile was resulted at 600 °C since the weak diffraction peak (110) started to generate in this sample. However, the diffraction peak (110) is more prominent and the (101) peak was weaker when the annealing temperature was increased to 700 $^{\circ}$ C. This can result the more rutile phase of TiO₂ nanoparticles. Rutile phase can totally transform above 800 °C (Mechiakh et al., 2010). Thus, annealing temperature has one of the major impacts on the crystal phase because the kinetics of reactions taking place was changed and the amount of OH- was varied by temperature and acid (Yin et al., 2004; Cheng et al., 1995; Liet al., 2002).



Figure 4: XRD patterns of TiO₂ nanoparticles annealed at 500 $^{\circ}$ C, 600 $^{\circ}$ C and 700 $^{\circ}$ C



Figure 5: XRD spectrum of pure P(Py-FPy) copolymer film

XRD spectrum in Figure 5 shows the standalone P(Py-Fpy) copolymer film. No diffraction peaks could be detected except only for the broad peak around at the diffraction angle around 23° C which is corresponding to amorphous polymer.

Conclusions

The new synthesis route of composite films comprising of TiO₂ nanoparticles in the P(Py-2FPy) copolymer matrix has been presented. While the TiO₂ nanoparticles were synthesized by low temperature solution method, the fabrication of composite film was prepared by chemical copolymerization through spin coating technique. The integration of inorganic components in polymer matrix was confirmed by FT-IR analysis. It can be remarkable that a suitable synthetic method of inorganic nanoparticles is firstly required in order to well dissolve in monomer solutions. Secondly, the enough stirring time is necessary for the homogeneous composite solution. The most important issue is the preparation technique of composite film formation. In this case, it is very important to consider the polymerization methods which are uncomplicated and possibility of film formation. In conclusion, by exploiting the physics of the inorganic nanoparticles, organic polymer and polymeric nanocomposites, the novel and functional composites can be designed and fabricated for new interesting applications such as optoelectronic and magneto-optic applications. It is expected that the use of a new functional composites as P(Py-2FPy)/TiO₂ materials will lead to nanocomposites with the unique combination of inorganic an organic properties.

Acknowledgements

The authors sincerely thank to Prof Dr Khin Khin Win, Head of Department of Physics, for her permission of this work. I do specially thank you to my Supervisor, Dr Ye Chan, Professor and Head of URC, for his guidance of my work. I am also greatly indebted to my Co-advisor, Dr Cho Cho Thet, Lecturer, Universities' Research Centre, who gives me valuable comments and suggestions and a large number of excellent discussions. Our special thanks go to URC staff for their interest and excellent discussion.

References

- Agarwal S., M. M. K Khan and R. K. Gupta, (2008) "Thermal conductivity of polymer nanocomposites made with carbon nanofibers." *Polymer Eng Sci*, **48**, 2474-2481.
- Ahmad S., S.A. Agnihotry and S. Ahmad, (2008) "Nanocomposite polymer electrolytes by in situ polymerization of methyl methacrylate: for electrochemical applications." J Appl Polymer Sci, **107**, 3042-3048.
- Althues H., J. Henle and S. Kaskel, (2007) "Functional inorganic nanofillers for transparent polymers." Chem Soc Rev, 36, 1454-1465.
- Cheng H., J. Ma, Z. Zhao and L. Qi, (1995) "Hydrothermal preparation of uniform nanosize rutile and anatase particles." Chem. Mater., **7**, 663-671.
- Colthup, N. B., S. E. Wiberley, (1964) "Introduction to Infrared and Raman Spectroscopy." *Academic Press: New York*, 191-298.
- Fang J., L. D. Tung, K. L. Stokes, J. He, D. Caruntu, W.L. Zhou and C. J. O'Connor. (2002) "Synthesis and magnetic properties of CoPt-poly(methylmethacrylate) nanostructured composite material." J Appl Phys, 91, 8816-8818.
- Gangopadhyay R. and A. De (1999) "Polypyrrole-ferric oxide conducting nanocomposites I: synthesis and characterization." *Eur Polymer J*, **35**, 1985-1992.
- Gass J., P. Poddar, J. Almand, S. Srinath and H. Srikanth, (2006) "Superparamagnetic polymer nanocomposites with uniform Fe_3O_4 nanoparticle dispersions." Adv *Funct Mater*, **16**, 71-75.
- Grossiord N., J. Loos, L. van Laake, M. Maugey, C. Zakri, C.E Koning, A.J. Hart, (2008) "High-conductivity polymer nanocomposites obtained by tailoring the characteristics of carbon nanotube fillers." *Adv Func Mater*, 18,3226-3234.
- Guo Q., R. Ghadiri, T. Weigel, A. Aumann, E. L. Gurevich, C. Esen, O. Medenbach, W. Cheng, B. Chichkov and A. Ostendorf, (2014)"Comparison of *in situ* and *ex Situ* methods for synthesis of two-photon polymerization polymer nanocomposites." Polymers 6, 2037-2050.
- Guo, Q., R. Ghadiri, S.Xiao, C. Esen, O. Medenbach and A. Ostendorf, (2012) "Laser direct writing of high refractive index polymer/TiO₂ nanocomposites." *In Proceedings* of SPIE Photonics West, San Francisco, CA, USA.
- Hopf H., G.N. Gerasimov, S.N. Chavalun, V.I. Rozenberg, E.L. Popova and E.V. Nikolaeva, E. I. Grogoriev, S.A. Zavjalov and L. I. Trakhtenberg, (1997) "Metal-containing poly (p-xylylene) films by CVD: poly (p-xylylene) with germanium crystals." *Chem Vap Deposition*; 3, 197-200.
- Kumar P. M., S. Badrinarayanan and M. Sastry, (2000) Thin Solid Films, 58, 122-130.
- Li S, M.S. Toprak, Y.S. Jo, J. Dobson, D.K. Kim, and M. Muhammed (2007) "Bulk synthesis of transparent and homogeneous polymeric hybrid materials with ZnO quantum dots and PMMA." *Adv Mater*, **19**, 4347-4352.

- Li, Y., Y. Fan and Y. Chen, (2002) "A novel method for preparation of nanocrystalline rutile TiO₂ powders by liquid hydrolysis of TiCl₄." *J. Mater. Chem.*, **12**, 1387-1390.
- Liao. Y and W. Que, (2010) "Preparation and photocatalytic activity of TiO₂ nanotube powders derived by a rapid anodization process." J. Alloys Compd.,**505** (1) 243-248.
- Macanas J., J. Parrondo, M. Munoz, S. Alegret, F. Mijangos and D.N. Muraviev. (2007) "Preparation and characterisation of metalpolymer nanocomposite membranes for electrochemical applications." *Phys Stat Sol (a)*; **204**, 1699-1705.
- Mechiakh R., N. Ben Sedrine, R. Chtourou, and R. Bensaha, (2010). "Correlation between microstructure and optical properties of nano-crystalline TiO₂ thin films prepared by sol-gel dip coating." *Appl. Surf. Sci.* 257 (3), 670-676.
- Prabhakaran T., J. Hemalatha, (2008) "Synthesis and characterization of magnetoelectric polymer nanocomposites." J Polymer Sci B Polymer Phys, 46, 2418-2422.
- Saravanan L., R. Mohan Kumar, A. Pandurangan and R. Jayavel, (2010) "Synthesis and photophysical studies of PVP capped Titania Nanostrips for photocatalytic applications." *Optoelectronics and Advanced Materials-Rapid Communications*, 4 (11) 1676-1680.
- Sabzi M., S. M. Mirabedini, J. Zohuriaan-Mehr and M. Atai, (2009). "Surface modification of TiO₂ nano-particles with silane coupling agent and investigation of its effect on the properties of polyurethane composite coating." Progr. Org. Coating. 65 (2), 222-228.
- Vebber M.C., A. C. R. Faria, N. Dal' Acqua, L. L. Beal,G. Fetter, G. Machado, M. Giovanelaand J. S. Crespo,(2016) "Hydrogen production by photocatalytic water splitting using poly (allylamine hydrochloride)/poly(acrylic acid)/TiO₂/ copper chlorophyllin self-assembled thin films" *International Journal of Hydrogen Energy*, **41**(40)17995-18004.
- Vetrivel V., K. Rajendran and V. Kalaiselvi (2014-2015) "Synthesis and characterization of Pure Titanium dioxide nanoparticles by Sol-gel method." *Int.J. ChemTech Res.*, 7 (3), 1090-1097.
- Yin, S., H. Hasegawa, D. Maeda, M. Ishitsuka and T. Sato, (2004) "Synthesis of visible-lightactive nanosize rutile titania photocatalyst by low temperature dissolutionreprecipitation process." J. Photochem. Photobiol. A Chem., 163, 1-8.
- Yusuke H. and T. Kobayashi, (2012) "Effect of Acidic Catalyst on Properties of Novel Conductive Copolymer Films Made of Pyrrole and Formyl Pyrrole." *Engineering*, 4, 139-145
- Yuwono A.H., B. Liu, J. Xue, J. Wang, H.I. Elim, W. Ji, Y. Li and T.J. White, (2004) "Controlling the crystallinity and nonlinear optical properties of transparent TiO₂-PMMA nanohybrids." *J Mater Chem*, **14**, 2978-2987.
- Zhang J., S. Luo and L. Gui L, (1997) "Poly(methyl methacrylate)-titania hybrid materials by sol-gel processing." J Mater Sci, **32**, 1469-1472.

ACOUSTIC PROPERTY OF POLYURETHANE-TiO₂ COMPOSITE FOAMS

Ei Shwe Sin Oo¹, MyoAung² and Ye Chan³

Abstract

The acoustic property of polyurethane foam and polyurethane composite foams reinforced with different concentration (0wt%, 2wt%, 4wt% and 6wt %) of TiO₂ particles were investigated. The particle size of TiO₂ particle was analyzed by X-ray diffraction (XRD). The morphology of polyurethane composite foams was characterized by using optical microscopy. The acoustic property of polyurethane composite foams was measured using one microphone impedance tube method. The result show that polyurethane foam reinforced by TiO₂ particles have better the sound absorption properties than pure polyurethane foam and 6 wt% of TiO₂ particles reinforced in polyurethane composite foam obtain the maximum value of the sound absorption coefficient.

Keywords: polyurethane foam, TiO₂ particles, impedance tube, acoustic absorption coefficient

Introduction

Nowadays, rapid developments of modern industries and transportations lead to serious noise pollutions, which have significant adverse effects on the environment and personal health. Therefore, research and development of efficient and environmentally friendly sound absorbing materials is important (Yonghua W. et.al, 2013). The sound absorbing material is one of the major requirements for human comfort today, especially in automobiles and manufacturing environment and it is the relationship between the acoustic energy that is absorbed by the material and the total incident impinging upon it.

Polymer-based foams are widely used in industry to benefit from their mechanical, electrical, thermal and acoustic properties. Polyurethane (PU) is one of the polymers with the largest and most versatile applications having the ability to easily change its properties by changing the chemical composition or adding filler reinforcement agents. It is commonly used in automotive

^{1.} Assistant Lecturer, Department of Physics, Technological University of Mawlamyine

^{2,3} Universities' Research Centre, University of Yangon

industry as sound absorbing material (Yuvaraj L., Vijay G., and Jeyanthi S., 2016). Shuming et al. (Shuming C, 2014) improved the sound absorption ability of PU foams with addition of nano-silica, results showed that with increase of nano-silica content, the sound absorption ratio of PU/nano-silica foams increased over the entire frequency range. Ancuţ a-Elena Tiuca (Anctua-Elena T. et.al, 2015) studied on acoustic properties improvement of rigid polyurethane closed-cell foam, by incorporating various quantities of textile waste into the matrix. It was observed that the composite materials obtained have better sound absorption properties compared to rigid polyurethane foam.

The sound absorption coefficient is measured by using the phenomenon of reflection of sound waves. Sound waves are generated within a medium and transmitted towards the test sample. By measuring the incident and reflected waves, reflection coefficient and the acoustic absorption coefficient can be calculated. There are three standard methods for determining the absorption coefficient which are Reverberation method, Standing Wave Ratio (SWR) method and Transfer function method. Standing wave ratio method and transfer function method are also called impedance tube method. (NireshJ et.al, 2016)

This study focuses on the studying of acoustic property of polyurethane foam with the different concentration of weight percentage (0wt%, 2wt%, 4wt% and 6wt%) of TiO₂ particles. First of all, the polyurethane foam was synthesized by free-rising method. And then, TiO₂ particles were added to the PU foam to make PU composite foam. The particles size of TiO₂ particle was analyzed by X-ray diffraction (XRD). After that, the morphology of polyurethane-TiO₂ composite foams has been characterized by optical microscopy. Finally, the acoustic property of Polyurethane-TiO₂ Composite foams was analyzed by using one microphone impedance tube method.

Design and Construction of Impedance Tube

The experimental setup includes computer, data acquisition board, power amplifier, a speaker and a 1/4inch electret condenser microphone is shown in Figure 1 and Figure 2.The one microphone impedance tube was designed for the frequency range 100 Hz to 2000 Hz. The tube was constructed using commercial circular PVC pipe with the thickness of the pipe close to 5% of the tube diameter (Kin Ming et al. 2005). The tube also had to be long enough to ensure the development of sound waves between the sound source and the sample. The interior section of the tube can be circular or rectangular but should be constant dimension from one end to another. The tube should be straight and its inside surface should be smooth, nonporous, and free from dust to maintain low sound attenuation. Length of the tube should be greater than the thrice the diameter of the tube (L>3d). The distance between the sample and microphone is should be greater than the half of the tube diameter for the flat sample surface. The sound source, speaker was fixed at one end of the pipe and the sample was attached at the left of the impedance tube. For measuring the incident and reflected waves, microphone is required to be positioned and be able to measure the sound pressure levels inside the tube. The sample with diameter equal to that of impedance tube was placed above the surface of the rigid plate which was in the sample holder. Temperature of the surrounding had to be maintained constant throughout the experiment (Rick et al. 2004 & Suhanek et al. 2005).

The speaker was connected to the AUDIO OUT channel of NI my DAQ. The sound wave from the speaker was guided through a straight pipe of PVC tube. The microphone was connected to the AUDIO IN channel of the NI my DAQ board which was programmed to be synchronized and had the sampling rate of 5.4 kHz. The speaker was driven by NI my DAQ as the signal generator and the microphone captured the standing wave which was the superposition of incident and reflected wave from the sample. The sample was placed vertically at the end of the straight pipe, backed by a rigid plate. The NI myDAQ was used for both signal generation to the speaker and data acquisition of the microphone output. Once the microphone response was recorded, the desired acoustic property is calculated in Matlab. In this research, material was analyzed at the frequency ranging from 100 Hz to 2600 Hz.

The sound pressure at any position in the tube can be written as

$$p = \frac{sink(l-x) - izcosk(l-x)}{coskl + izsinkl}i\rho cv_0$$
(1)

The acoustic impedance can be calculated by the following equation

$$z = \frac{p(x,\omega)coskl - i\rho cvsink(l-x)}{\rho cvcosk(l-x) - ip(x,\omega)sinkl}$$
(2)

The specific acoustic impedance ratio can be expressed as

$$\frac{Z}{\rho c} = \frac{p(x,\omega) \cosh l - i\rho \cosh (l-x)}{\rho \cosh (l-x) - ip(x,\omega) \sinh l}$$
(3)

$$Z = \rho c \frac{1+R}{1+R} \tag{4}$$

The reflection factor (R) can be solved as

$$R = \frac{\frac{Z}{\rho c} - 1}{\frac{Z}{\rho c} + 1} = \frac{\frac{p(x, \omega) \cosh l - i\rho cv sink(l - x)}{\rho cv cosk(l - x) - ip(x, \omega) sinkl} - 1}{\frac{p(x, \omega) coskl - i\rho cv sink(l - x)}{\rho cv cosk(l - x) - ip(x, \omega) sinkl} + 1}$$
(5)

where 1 is the length of the tube, x is the distance between sample and microphone, ρ is the air density and c is the velocity of sound.

The sound absorption coefficient (α) can be calculated by the following

$$\alpha = 1 - \left| \frac{p(x, \omega) \cos kl - i\rho \cos k(l - x)}{\rho \cos k(l - x) - ip(x, \omega) \sin kl} - 1 \right|^{2}$$

$$(6)$$

$$\alpha = 1 - \left| \frac{p(x, \omega) \cos k(l - x) - ip(x, \omega) \sin kl}{\rho \cos k(l - x) - ip(x, \omega) \sin kl} + 1 \right|^{2}$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

$$(6)$$

Figure1: (a) Block diagram of data acquisition



Figure 2:(a) Experimental setup of impedance tube



Figure 2: (b) Schematic diagram of data acquisition with LabVIEW

Synthesis of Polyurethane-TiO₂ Composite Foams

The polyol (polyether polyol, viscous yellow liquid, containing additives such as catalyst, blowing agent and surfactant) and isocyanate (Methylene diphenyl diisocyanate (MDI), dark blown liquid) were used for polyurethane (PU) foam formulation. Commercial TiO₂particles were used as filler in polyurethane foam. The PU composite foam with and without varied content of TiO₂particles were prepared by free-rising method. The PU foam was prepared by mixing the polyol and isocyanate at a ratio of 1:1. The proportion ratio of polyol, isocyanate and TiO₂ particles is shown in Table 1.

Table 1: Proportion of polyol, isocyanate and TiO₂

wt% of TiO ₂	Polyol (g)	Isocyanate (g)	TiO ₂ particles(g)		
0% TiO ₂	15	15	0		
2% TiO ₂	15	15	0.6		
4% TiO ₂	15	15	1.2		
6% TiO ₂	15	15	1.8		

To fabricate the polyurethane foam, the combination of isocyanate (part A) and polyol(part B) were measured. For the PU foam, different weight

percentage of TiO₂ (0wt%,2wt%,4wt% and 6wt%) was first mixed with part B about 30 minutes to get homogeneous mixture by using magnetic stirrer hot plate 85-2 equipment. Figure 3 shows basic schematic of polyurethane-TiO₂ composite foams production. Then, part A was mixed with part B that also contains the filler and stirred together using a stir stick. During that mixing, exothermic reaction occurs. When the mixture started to get really warm to touch, the mixture was ready to place in the plastic mold (Anika et.al, 2017). A series of polyurethane foams with and without TiO₂ particles with loading fraction of 2wt%, 4wt% and 6wt% were also prepared by the above procedure. The formation of foam processing conditions is given below.

4	Ratio (polyol to isocyanate)	: 1:1
4	Cream time	:9 s
4	Rise time	:14 s
4	Gel time	:7 s

The mixed liquids were poured for foaming to a plastic mold with dimensions 5 cm \times 5 cm \times 5cm. After the foaming and curing process (at least 72 h at room temperature), samples were cut from the center of the block to characterize them. The flow chart of the process of polyurethane foam with different concentration of TiO₂particle is illustrated in Figure 4.



Figure 3: Schematic of polyurethane-TiO₂ composites foam production



Figure 4: Process of production of polyurethane-TiO₂ composites foam

Results and Discussion

XRD Analysis of TiO₂ particles

The particle size of commercial TiO_2 particles was analyzed by Multiflex 2kW, Rigaku (Japan) X-ray diffraction(XRD). The X-ray diffraction pattern of the TiO₂ particles is shown in Figure 5. The intensity of XRD peaks of the sample reflects that the formed particles are crystalline. From this study, considering the peak at degrees, average particle size has been estimated by using Debye-Scherer formula. The average particle size of TiO₂ particle was about 372 nm.



Figure 5: XRD analysis of TiO₂ particles

Morphological Structure of Polyurethane Foam Reinforced with TiO₂ Particles

The optical microscopy is used to analyze the surface morphology of polyurethane foams with different concentration (0wt%, 2wt%, 4wt% and 6wt%) of TiO₂particles which is shown in Figure 6. The samples were prepared as 1 mm ×1 mm ×1 mm sizes to see their surface with an optical microscopy. The cells (bubbles) appeared spherical and closed. The purpose of the optical microscopy analysis was to determine the size of the cells affected by the reinforced of TiO₂ in PU foams. The morphology of polyurethane- TiO₂ composite foams was evaluated by optical microscopy. The average cell size of the PU-TiO₂ composite foam was measured by using imageJ software. The average cell size of polyurethane foam with different concentration of TiO₂particles is shown in Table 2. According to the figure, it is observed that the cell size reduces when TiO₂ particles are added. The reason for the cell size reduction is due to TiO₂ particles act as nucleation agents and promote cell nucleation because of an effective decrease in the required energy for creating bubbles.



(c)

- (d)
- **Figure 6:** Morphology image of polyurethane –TiO₂ composite foams (a) pure PU foam (b) 2wt% PU-TiO₂ composite foam(c) 4wt% PU-TiO₂ composite foam(d) 6 wt.% PU-TiO₂ composite foam

Ta	ble	e 2	:/	Average	cell s	size o	f pol	lyuret	hane-	TiO	2 comp	osite	foams
----	-----	-----	----	---------	--------	--------	-------	--------	-------	-----	--------	-------	-------

wt% of TiO ₂	Average cell size (µm)
0%	325
2%	238
4%	174
6%	98





Acoustic Absorption Coefficient Measurement

The acoustic absorption test was carried out using impedance tube with one fixed microphone apparatus. The signal generator and data acquisition were performed using National Instruments Labview. The NI my DAQ was used both for signal generation to the speaker and for data acquisition of the microphone output. Once the microphone response was recorded, Matlab was used to calculate the desired acoustic property. To validate the impedance tube setup constructed, the 6 mm thick polyurethane foam was measured and compared with the result of standard material such as glass which was 6 mm thick. This comparison result is shown in Figure 8.

The acoustic absorption coefficient of polyurethane foam with different concentration of TiO_2 particles is presented in Figure9.The comparison of estimated acoustic absorption coefficient of different concentration of TiO_2 particles reinforced in polyurethane composite foams is presented in Figure 10. According to figure, it can observed that composite foams have better sound absorption properties compared to the pure polyurethane foam but the 6wt% polyurethane-TiO₂ composite foam has the best sound absorption property reaching a value of maximum 0.9 of sound absorption coefficient on the whole analyzed frequency ranges. This is due to the absorption coefficient of composite foams depending on the concentration

of TiO_2 particles and frequency of the acoustic which strikes the surface of the composite foams.



Figure 8: Comparison of estimated acoustic absorption coefficient of glass and Polyurethane foam



Figure 10: Comparison of acoustic absorption coefficient of different concentration of TiO₂ in polyurethane-TiO₂ composite foams

Noise Reduction Coefficient (NRC)

The noise reduction coefficient, NRC, is the arithmetic average of a material's sound absorption coefficients at 250 Hz, 500 Hz, 1000 Hz and 2000 Hz. The NRC was used to compare the acoustical property of different concentration of TiO_2 particles reinforced and non-reinforced in rigid polyurethane foam is illustrated in Figure 11. It can also observe that with the increase of concentration of TiO_2 particles percentage, the value of noise reduction coefficient (NRC) also increases. The 6wt% TiO_2 particles reinforced in polyurethane composite foam has the maximum NRC value of about 0.65 (it absorbs 65 percent of the sound hitting it and 35 percent bounces back), while rigid polyurethane foam has only about 0.59 (it absorbs 59 percent of the sound hitting it and 41 percent straight back).



Figure 11: Comparison of noise reduction coefficient of different concentration of TiO₂ in polyurethane-TiO₂ composite foams

Conclusion

This study investigated an impedance tube with one fixed microphone which was used to determine the acoustic absorption coefficient of the polyurethane composites foam reinforced with different concentration (0wt%, 2wt%, 4wt% and 6wt%) of TiO₂ particles as sound absorbent materials. It was observed that the average cell size of polyurethane composite foams decreases when the concentration of TiO₂ particles increases. According to experimental result, the polyurethane foam and polyurethane-TiO₂ composite foams have

approximately the same acoustic absorption coefficient at different frequency. The polyurethane-TiO₂ composite foams have more enhancement sound absorption property them pure polyurethane foam. Among them, 6wt% polyurethane composite foam has the best capacity to absorb noise, reaching a value of maximum 0.9 of sound absorption coefficient on the whole analyzed frequency ranges. With decreasing their cell size, the sound absorption coefficient of polyurethane composite foams increases. It can be concluded that foams with small cell size absorb sound better than the foams with large cell size. Therefore, the polyurethane-TiO₂ composite foams can be used not only in the indoor but also outdoor environment as sound absorbing material.

Acknowledgements

The authors are grateful to Dr Khin Khin Win, Professor and Head of the Department of Physics, University of Yangon for her kind permission to carry out this work. The authors are grateful to Headmaster Dr Min Zaw Aung, Principle, Technological University of Mawlamyine for his kind permission to carry out this work.

References

- Ancuţ a-Elena T., Horaţ iu V., Timea G., Ovidiu V., (2015), "Improved sound absorption properties of polyurethane foam mixed with textile waste", Sustainable Solutions for Energy and Environment, EENVIRO - YRC 2015, Romania
- ASTM standard 10534–2, (1998), "Acoustics determination of sound absorption coefficient and impedance in impedance tube" Part 2: Transfer function method
- Ayesha .K, (2017), "Polyurethane Composite Foams in High-Performance Applications: A Review", Polymer-Plastics Technology and Engineering, Quaid-i-Azam University, Islamabad, Pakistan
- Chumwon .K, Junji .M and Kazuyuki .A, (2005), "A Comparison of the Standing Wave and Two Microphone Methods in Measuring the Sound Absorption Coefficient of Wood", Fukuoka 812-8581, Japan
- Guan .Q, (2015), "Analysis of Acoustic Damping in Duct Terminated by Porous Absorption Materials Based on Analytical Models and Finite Element Simulations", New Jersey
- Kamal .J, Vahid .B, (2012), "Investigating the design considerations of a standing wave type impedance tube", Tehran, Iran
- Niresh.J, Neelakrishnan .S and Subha Rani .S, (2016), "Investigation and correction of error in impedance tube using intelligent techniques", Coimbatore 641004, India
- Shuming C., Yang J., (2014), "The Acoustic Property Study of Polyurethane Foam With Addition of Bamboo Leaves Particles", State Key Laboratory of Automotive Simulation and Control, Jilin University, Changchun, China
- Yonghua .W, Chengchun .Z and Luquan .R,(2013), "Influences of Rice Hull in Polyurethane Foam on Its Sound Absorption Characteristics", POLYMER COMPOSITES
- Yuvaraj L., Vijay G., and Jeyanthi S., (2016), "Study of Sound Absorption Properties on Rigid Polyurethane Foams using FEA", Indian Journal of Science and Technology, Vol 9(33), ISSN (Print) : 0974-6846 ISSN (Online) : 0974-5645

FAST AND FACILE SYNTHESIS OF COPPER NANOWIRES AND THEIR APPLICATION AS CONDUCTIVE INK

Khin Win Mu¹, Nan Thidar Chit Swe² and Khin Khin Win³

Abstract

Copper nanowires (Cu NWs) were synthesized by a chemical reduction method under atmospheric pressure stirring at 700 rpm using Sodium Hydroxide(NaOH), Copper (II) Nitrate (Cu NO₃)₂, Hydrazine (N₂ H₄) and Ethylenediamine (C₂ H₈ N₂) at temperature 70 °C and the synthesis time of 5 minutes. The surface morphologies of Cu NWs are analyzed by Scanning Electron Microscopy (SEM). SEM results revealed that the lengths of CuNWs were up to 40 μ m ranging in diameter from 1 μ m to 2 μ m. The size of synthesized nanoparticles accompanied with nanowire are in the range of 100 nm to 300 nm. Finally, the as-synthesized Cu NWs are dispersed well in a 0.5 wt % PVP-based ink and then coated onto glass by a Meyer rod. The electrodes fabricated by this technique exhibited good performance (sheet resistance) of 30 Ω /sq.

Keywords: Copper nanowire, hydrazine, low sheet resistance, copper nanowire ink

Introduction

Copper (Cu) and the compounds of gold (Au), silver (Ag), palladium (Pd) and platinum (Pt) are widely used during these days (Bell et al, 2001). Copper has an excellent electrical conductivity. Nanoparticles of these metals have been interested extensively in recent years because of their unexpected physical and chemical properties shown at nanoscale (Ozin, 1992). Owing to extremely small size, copper nanoparticles exhibit enhanced properties when compared with bulk material including large surface area relative to their volume, ability to easily interact with other particles and increased antibacterial efficiency (Song et al, 2006). Because of its excellent electrical conductivity, catalytic behaviour, good compatibility and surface enhanced Raman scattering activity, copper nanoparticles have drawn the attention of scientists to be used as essential component in the future nano-devices (Pergolese et al., 2006). The general problems like aggregation and oxidation

¹ Lecturer, Department of Physics, Mawlamyine University

² Lecturer, Universities' Research Center, University of Yangon

³ Professor and Head of Department, Department of Physics, University of Yangon

of copper nanoparticles limit their usage. However, the usage of suitable separate stabilizing agent in the preparation rectifies this problem easily. Copper nanoparticles have been synthesized by different methods.

To date, thermal reduction, thermal decomposition, direct electrochemical reduction from CuO nanoparticles, mechano-chemical process, polyol process, chemical reduction, in-situ synthesis in polymers, electro-exploding wire (EEW) and ion beam radiation have all been developed to prepare nanostructured copper.

Moreover copper is only 6% less conductive than the most conductive element, silver, but it is 1000 times more abundant. Based on these facts, there has been recently a growing interest in the development of one-dimensional copper nanowires (Cu NWs). Several methods for preparing Cu NWs have been reported such as chemical vapour deposition, template assisted electrochemical synthesis or membrane processes. Surprisingly, fabrication of flexible transparent electrodes based on random networks of Cu NWs has been scarcely studied up to now. Wiley and co-workers have pioneered CuNWs based electrodes by preparing flexible films exhibiting sheet resistance of 30 Ω /sq at 85% transmittance. Transparent electrodes with remarkable optoelectronic performances were also obtained with the deposition of electrospun copper nanofibers or nanotrough networks.

In this paper, one pot synthesis of ethylenediamine-mediated processes have been used for the synthesis of ultralong copper nanowires. The stability against aggregation or precipitation of copper nanowires will be improved. Their influence on the different amount of hydrazine affects the nanowire solutions will be discussed. Moreover, optical and electrical properties of air dried ultralong CuNWs thin films are reported. Further, the structural, chemical properties of these two different structures of ultralong CuNWs were examined.

Experimental

2.1 Materials

Analytical grade (BDH, England) Copper (II) Nitrate $(CuNO_3)_2$, Sodium Hydroxide (NaOH), Ethylenediamine $(C_2H_8N_2)$, Hydrazine (N_2H_4) were used as starting precursor. All chemicals were used as purchased without further purification.

2.2 Synthesis of copper nanowire

In a typical copper nanowires synthesis Sodium Hydroxide (NaOH) (15 M, 20 mL), Copper (II) Nitrate(Cu $(NO_3)_2$) (0.15 M, 1 mL)and Ethylenediamine (EDA) (99 %, 8.5 mmol) were mixed for 3 minutes under stirring at 700 rpm. Hydrazine (N₂H₄) (50wt %,0.13 -0.22 mmol) was then added to the solution and the stirring was stopped after 5 minutes. The solution color changed from deep blue to clear and colorless to reddish cake floating on to top of the solution surface, indicating the formation of Cu NWs. Next, the Cu NWs were washed with the above solution many times with water until pH 7 was obtained. Finally the precipitation was washed with ethanol and 2 propanol by centrifuge at 2000 rpm, 5 min and stored in the same solution. The concentration of reducing agent Hydrazine (N₂H₄) is a critical parameter for anisotropic growth of NWs. Moreover, EDA is also a critical chemical. In this method, without EDA, only copper nanoparticles are achieved.

The initial mixing of Cu(NO₃)₂, NaOH, and EDA results in a blue complex, Cu(OH)₄ ²⁻. After the addition of N₂H₄, the blue solution turns white and then colorless, and is comprised mainly of Cu(OH)²⁻ with a small amount of Cu₂O nanoparticles. These Cu₂O nanoparticles are further reduced to metallic Cu aggregates which serve as seeds that sprout CuNWs via continuous reduction of Cu(OH)²⁻. The resultant solute was centrifuged many times to obtain pure Cu Nws precipitations. The results of an EDA-mediated CuNWs synthesis before and after centrifugation are shown in Figure 1(a) and (b). Three samples were synthesized by varying the concentration volume of Hydrazine from 0.13 mmol to 0.22 mmol. The result also reveals that the amount of hydrazine used in the synthesis take part a important role to the formation of CuNWs.




Figure1: Photograph of CuNWs growth solutions. (a) before and (b) after centrifugation

2.3 Characterization

Centrifuge machine (Kokusan H-200 series) was used to separate the colloid from the solutions. The influence of solvent on formation of Cu nanoparticles was confirmed UV _Vis spectrophotometer (Lamda35), X-ray powder diffractometer (Type: RIGAKU–RINT 2000), and Scanning Electron Microscope (Type: JEOL 15 kV).

Results and Discussions



3.1.UV-Vis Measurements



Figure2: UV- Vis spectra of Cu Nanowires solution by using ethylenediamine and hydrazine (a) 0.22 mmol (b) 0.17 mmol and (c) 0.13 mmol.

Figure 2 shows the UV-Vis spectra of the copper nanostructures in the range 250 nm - 700 nm. The results from the different amount of hydrazine (0.22 mmol, 0.17 mmol and 0.13 mmol) show a different response. At the hydrazine amount of 0.22 mmol, the absorption band in visible light region (250 nm - 700 nm, plasmon peak at 580 nm) is typical for copper nanoparticles (Hutter et al, 2001). Different peak at 666 nm and 470 nm shows that the sample has different size of nanostructure. The plasmon peak and the full-width of half-maximum (FWHM) depends on the extent of colloid aggregation (Yamamoto et al, 2004). Figure 2 (b) shows the two different absorption peak at 593 nm and 356 nm indicates that amount of copper nanoparticles decrease and the formation of nanowires are formed. The decrement of the hydrazine amount to 0.13 mmol (Figure 2c) produce a more relevant change in the response. At 0.13 mmol, the intensity of the peak is higher than the detection limit. So the dilution of the sample is needed to obtain the good UV-Vis spectrum. The good spectrum was obtained after diluting the sample to one tenth of original solution. As hydrazine at 0.13 mmol was added to synthesis procedure, the SPR peaks are around 356 nm 279 nm. The peak positioned at 356 nm could be considered as the optical signature of relatively long CuNWs. This implies that the final product synthesized under this particular condition that is using 0.13 mmol mediated gives a high of yield of Cu NWs. As it can be noted, the spectrum is broad and asymmetric and it has been suggested that this optical feature is due to the non-uniform size of the copper nanoparticles and nanowires, Figure 2.

3.2 SEM Measurements

After the preparation of the nanowires, the suspension of nanowires in ethanol was used for microscope analysis by fabricating a drop of suspension onto a clean glass substrate and allowing ethanol to completely evaporate. The surface morphology of Cu NWs were observed by using SEM. The SEM characterizations of the as-synthesized Cu NWs are shown in Fig.3 (a) (b) and (C). In Fig 3 (a), it was obviously shown that the wire and particles were distributed throughout the sample surface. 90 % of the sample is particles and other is wire. The SEM images suggested that the length of CuNWs were up to more than 40 μ m ranging in diameter from 1 μ m to 2 μ m. The sizes of synthesized nanoparticles accompanied with copper wires are in the range of 100 nm to 300 nm.



Figure 3: SEM micrograph of Cu Nanowires solution by using ethylenediamine with different amount of hydrazine (a) 0.22 mmol (b) 0.17 mmol and (c) 0.13mmol.

In Fig 3 (b), it was obviously shown that the amount of wire is increasing when the hydrazine amount decreased to 0.17 mmol Fig. 3 (C) show the lengths that could be increased by reducing amount of hydrazine 0.13 mmol. Cu NWs with particle-like structures along their lengths are also observed in this sample. Attaching Cu nanoparticles along the Cu NWs may cause the larger diameter of the wire and consequently increase the larger size distribution in the sample. According to these three experiments, a greater volume hydrazine produced CuNWs accompanied with more CuNPs. This means that there is an optimized condition in which the amount of hydrazine helping to transform the CuNPs into CuNWs.

3.3 XRD Measurements

To confirm the crystalline structure of the copper (Cu) nanostructures, the samples were analyzed on X-ray diffractometer (Model RIGAKU-RINT 2000). All samples give similar XRD spectrum. The polycrystalline properties for drop coated glass thin film of Cu nanostructure were analyzed by using Cu K- α 1 radiation (40 kV, 40 mA) in 2 θ range from 10°C to 70° C on a Rigaku powder X-ray diffractometer equipped with a diffracted-beam graphite monochromator. The crystallite domain diameters D were obtained from XRD peaks according to the Scherrer equation: where λ is the wavelength of the incident X-ray beam (1.54056 Å for Cu K- α 1), θ is the Bragg's reflection angle, ΔW is the width of X- ray pattern line at peak half peak height in radians. The Miller indices in XRD pattern reference of Cu (upper) and standard CuO and Cu₂O (lower) were shown in Fig 4. This pattern showed that two XRD peaks appeared at 43.092, 50.209° due to strong Bragg reflections from (111) and (200) planes of fcc (face centred cubic) copper respectively. All reflections are agreed with standard library file (ICDD-PDF#99-0034) of pure copper metal with fcc symmetry. Based on Scherrer equation, the average crystallite size of Cu NWs was found to be 28 nm. No peaks attributed to copper oxides such as CuO and Cu₂ O could be detected.



Figure 4: XRD plots obtained from CuNWs sample by using hydrazine 0.13 mmol to investigate the structures and crystallinity. Reference bulk reflections of pure Cu phases are shown at the bottom (ICDD-PDF#99-0034).

3.4 Preparation of copper nanowire ink

First, 0.5 wt % Polyvinylpyrrolidone (PVP)-based ink was prepared by dissolving 0.5 g of PVP-K30 in 100 ml of IPA. The stored Cu NWs were transferred to a 1.5 mL tube and washed once more with the 0.5 wt % PVPbased ink solution by centrifuging at 2000 rpm for 5 min. Lastly, depending on the desired concentration, there quired amount of PVP-based ink was pipetted into the tube containing the copper nanowires to make the final coating solution. Purified copper nanowire ink was deposited onto glass. The very first step before ink deposition is the washing of glass substrate in order to remove dirt and impurities that may have unknowingly settled on the glass substrate. This is done by washing in several substances, namely: acetone, distilled water, ethanol, distilled water again, hydrochloric acid (HCl) and lastly distilled water. These glass substrates are then dried in air blow at room temperature. The CuNWs ink was applied on glass substrates and then annealed at temperature 150 HC to evaporate the solvents. Finally, the coated film is dipped into acetic acid for 1 min at room temperature and left for 3 min to self-dry. Without any post-treatment, the conductivity between the copper nanowires is greatly confined by the incomplete contact between Cu nanowires and their small contact area because of their round cross section. Interestingly, the dried copper pastes exhibited low electrical resistance of 30Ω .



Figure 5: Copper nanowires ink deposited on glass substrate. Thin film of copper nanowires shows low sheet resistance 30 Ω .

Conclusion

In conclusion, highly dispersed Cu NWs possessing a long (entire length up to 40 μ m) and fine (average diameter of 1 μ m, 2 μ m) geometric nature have been successfully synthesized through chemical reduction by using hydrazine as the reducing agent. A series of experiments were carried out to clarify role of reducing agent (hydrazine) on the formation of NWs, which demonstrates that right amount of hydrazine play a key role in forming NW elongation and meanwhile restricting the lateral diameter and production of copper nanoparticles which are bi products of synthesis procedure. Finally, the as-synthesized Cu NWs are dispersed well in a 0.5 wt % PVP-based ink and then coated onto glass by a Meyer rod and the coated film is dipped into acetic acid for 1 min at room temperature and left for 3 min to self-dry. The electrodes fabricated by this technique exhibited excellent performance (sheet resistance) of 30 Ω /sq. In virtue of the superior properties, low cost and capability of mass synthesis, further improvement of the performance is believed to lead to a replacement of traditional ITO in the near future.

Acknowledgements

The authors greatly indebted to Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her kind permission to carry out this work. The authors wish to show our sincere thanks to Professor Dr Aye Aye Thant, Department of Physics, University of Yangon, for her fruitful discussions to this work.

References

- Choi, H.; Park, S.-H. Seedless Growth of Free-Standing Copper Nanowires by Chemical Vapor Deposition. J. Am. Chem. Soc. 2004, 126, 6248–9.
- Gao, T.; Meng, G.; Wang, Y.; Sun, S.; Zhang, L. Electrochemical Synthesis of Copper Nanowires. J. Phys. Condens. Matter 2002, 14, 355–363.
- Molares, M. E. T.; Busch mann, V.; Dobrev, D.; Neumann, R.; Scholz, R.; Schuchert, I. U.; Vetter, J. Single- Crystalline Copper Nanowires Produced Track Membranes. Adv. Mater.
- Rathmell, A. R.; Bergin, S. M.; Hua, Y.-L.; Li, Z.-Y.; Wiley, B. J. The Growth Mechanism of Nanowires and Their Properties in Flexible, Transparent Conducting Films. Adv. Mater. 2010, 22, 3558–63.
- Rathmell, A. R.; Wiley, B. J. The Synthesis and Coating of Long, Thin Copper Nanowires to Make Flexible, Transparent Conducting Films on Plastic Substrates. Adv. Mater. 2011, 23, 4798–4803.
- Shengrong Ye, et al (2016), How Copper Nanowires Grow and How To Control Their Pr Wu, H.; Hu, L.; Rowell, M, W.; Kong, D.; Cha, J, J.; McDonough, J.R.; Zhu, J.; Yang, Y.; Mcghee, M. D.; Cui, Y. Electrospun Metal Nanofiber Webs as High-Performance Transparent Electrode. Nano Lett. 2010, 10, 4242-8.
- Wu, H.; Kong, D.; Ruan, Z.; Hsu, P.-C.; Wang, S.; Yu, Z.; Carney, T. J.; Hu, L.; Fan, S.; Cui, Y. A Transparent Electrode Based on a Matel Nanotrough Network. Nat Nanotechnol. 2013, 8, 421-5.
- Zhao, Y.; Zhang, Y.; Li, Y.; Yan, Z. Soft Synthesis of Single-Crystal Copper Nanowires of Various Scales. New J. Chem. 2012, 36, 130.

SYNTHESIS OF COPPER NANOPARTICLES FOR APPLICATION OF CONDUCTIVE INK

Mi Mu Mu Khaing ¹, Nan Thidar Chit Swe ², Lwin Ko Oo³, Myo Aung⁴, Ye Chan⁵

Abstract

This paper focused on the preparation of copper (Cu) nanoparticles from copper (II) Nitrate as metal precursor. Sodium borohydride was used as a reducing agent and polyethylene glycol and ascorbic acid were used as stabilizer. The copper particles formed were identified by UV-Vis, XRD and SEM. Small spherical copper nanoparticles and the good dispersion of nanoparticles are observed from the samples. From XRD pattern, the average crystallize size of Cu nanoparticles is 38 nm as each particle observed from SEM is not a single crystallite of Cu but the agglomerates of many single crystallites. The aggregation of nanoparticles caused the inhomogeneous size distribution. Well-dispersed stable copper based conductive ink was prepared in which the copper nanoparticles possess a excellent dispersive, monodispersed size distribution and strong antioxidation. From UV analysis, the absorption band in visible light region (350 nm-700 nm, plasmon peak at 588 nm).

Keywords: Copper nanoparticles, spherical shaped nanoparticles, inhomogeneous size distribution

Introduction

During these years, conductive inks have attracted considerable attention due to their growing application in electrodes of silicon-crystal solar cells and the printed electronics industry such as smart labels, flexible displays, and radio frequency identification (RFID). Currently, silver inks have been commonly developed to enable outstanding conductivity and excellent printability. However, the high price and scarcity of such material limit wide industrial applications. In view of these, copper is a good alternative material for silver because of its high electrical conductivity and low price.

^{1.} Lecturer, Department of Physics, Hpa-an University

² Lecturer, Universities' Research Center (Physics), University of Yangon

³ Assistant Lecturer, Universities' Research Center (Physics), University of Yangon

⁴ Professor and Head of Department, Universities' Research Center, University of Yangon

Therefore, the synthesis of Cu nanoparticles has become of great interest from a scientific as well as an industrial point of view, due to its huge potential for replacing the expensive nano silver ink (Bell *et al*, 2001) (Hutter et al, 2001). Owing to extremely small size, copper nanoparticles exhibit enhanced properties when compared with the bulk material including large surface area relative to their volume, ability to easily interact with other particles and increased antibacterial efficiency (Carrol et al, 2011). Many research groups have been made to synthesize nano copper by wet chemistry, as well as by gas or solid phase methods. Such as the sonochemical method, microemulsion techniques, polyol processes, radiation methods, thermal reduction, reducing flame synthesis, metal vapor synthesis, vacuum vapor deposition and chemical reduction in solution (Ozin, 1992).

The synthesis method represented in this paper is a chemical reduction method which are based on the reduction of metal ions by reducing agents in liquid media. It is well suited for the preparation of nano-sized metal or oxide particles of various shapes. This method is simple, but the great attention must be needed to make stable and reproducible colloid. Many parameters such as solution temperature, concentrations of the metal salt and reducing agent, reaction time influence the particle size.

Experimental

2.1 Materials

Analytical grade (BDH, England) Copper (II) Nitrate $(Cu(NO_3)_2)$, Sodium Hydroxide (NaOH), Polyethylene glycol (PEG), Ascorbic Acid and Sodium borohydride (NaBH₄) were used as starting precursors. All chemicals were used as purchased without further purification.

2.2 Synthesis of copper nanoparticles

The copper nanoparticles were prepared by reduction of copper nitrate $[Cu(NO_3)_2]$ with polyethylene glycol (PEG) and ascorbic acid. Copper nitrate was used as a starting material, polyethylene glycol is used as a capping agent and ascorbic acid were used as a reducing agent. Sodium Hydroxide is used for faster the chemical reaction. Cu (NO₃)₂ (0.01 M) was dissolved in 10 ml distilled water. 10 ml of polyethylene glycol and 10 ml of ascorbic acid were added to Cu (NO₃)₂ solution. NaOH (0.1 M) with 10 ml distilled water was

added in that mixture. The solution colour was changed to yellow colour. And then sodium borohydride (NaBH₄) (0.1 M) with 10 ml of distilled water were mixed that mixture, the colour was changed to dark red. Then mixture of that solution was heated on a hot plate stirrer at temperature of 70 °C for 1 hr. The red coloured solution was removed from the heating magnetic stirrer and cooled down. Then, the colloidal solution was separately centrifuged for 15 min at 6000 rpm, the wet precipitates were dried at 70 °C overnight to obtain the Cu nanoparticles.

2.3 Characterization

Centrifuge machine (Kokusan H-200 series) was used to separate the colloid from the solutions. The influence of solvent on formation of Cu nanoparticles was confirmed

UV-Vis spectrophotometer (Lamda 35), X-ray powder diffractometer (Type: RIGAKU–RINT 2000), and SEM (Type: JEOL 15 kV).

Results and Discussions

Figure1 (b) shows the UV-Vis spectra of the copper colloid in the range 300 nm - 700 nm. The absorption band in visible light region (350 nm - 700 nm, plasmon peak at 588nm) is typical for copper nanoparticles (Hutter *et al*, 2001). The plasmon peak and the full-width of half-maximum (FWHM) depends on the extent of colloid aggregation (Yamamoto *et al*, 2004). As it can be noted, the spectrum is broad, asymmetric and it has been suggested that this optical feature is due to the non-uniform size of the copper nanoparticles.



Figure 1: (a) The photograph of copper nanoparticle solution (b)The UV-Vis spectra of Copper colloid, synthesis temperature at 70 °C

After UV analysis, SEM measurements were performed on dried Cu nanoparticles to investigate the size and surface morphology of figure 3(a)–(b) show the top-view SEM images of the prepared Cu samples after centrifugation and drying. According to SEM images, the size of copper nanoparticles are ranging in diameter from 100 to 200 nm, as each particle observed from SEM is not a single crystallite of Cu but the agglomerates of many single crystallites. The aggregation of nanoparticles caused the inhomogeneous size distribution.



Figure 2:(a) high and (b) low magnification of SEM images: The spherical nanoparticles are observed in high magnification SEM image in which the diameters are around 100 nm.

To confirm the crystalline structure, the prepared copper, (Cu) nanoparticles were analyzed on X-ray diffractometer (Model RIGAKU–RINT 2000). The polycrystalline properties for drop coated glass thin film of Cu powder were analyzed by using Cu / K- α_1 radiation (40 kV, 40 mA) in 20 range from 10° to 70° on a Rigaku powder X-ray diffractometer equipped with a diffracted-beam graphite monochromator. The crystallite domain diameters D were obtained from XRD peaks according to the Scherrer equation: $D = \frac{0.89\lambda}{\Delta W \cos \theta}$, where λ is the wavelength of the incident X-ray beam (1.5405 Å for Cu / K- α 1), θ is the Bragg's reflection angle, ΔW is the width of X- ray pattern line at peak half peak height in radians. The Miller indices in XRD pattern of Cu nanoparticles (upper spectrum) and standard Cu

particles (lower) were shown in Figure 5. This pattern showed that two XRD peaks appeared at 43.5° and 50.16°, due to strong Bragg reflections from (111) and (200) planes of fcc (face centred cubic) copper respectively. All reflections are agreed with standard library file (ICDD-PDF#04-0836) of pure copper metal with fcc symmetry. Based on Scherrer equation, the average crystallite size of Cu nanoparticles was found to be 38nm.



Figure3: XRD plots obtained from copper nanoparticles sample to investigate the structures and crystallinity. Reference bulk reflections of pure Cu phases are shown at the bottom (ICDD-PDF#04-0836).

Copper Nanoparticles Ink Deposition on Glass Substrates

Before copper nanoparticles ink deposition, the glass substrate was washed with deionized water, followed by acetone, methanol and isopropanol and dried with air blow. First, 0.5 wt % poly vinyl pyrrolidone (PVP)-based ink was prepared by dissolving 0.5 g of PVP-30 K in 100 ml of isopropyl alcohol (IPA ,99%). The stored Cu nanoparticles were transferred to a 1.5 ml tube and washed once more with the 0.5 wt % PVP-based ink solution by centrifuging at 2000 rpm for 5 min. Lastly, depending on the desired concentration, the required amount of PVP-based ink was pipetted into the

tube containing the copper nanoparticles to make the copper nanoparticle ink. The synthesized ink was ultrasonicated to break up the large agglomerates formed in the well dispersed copper nanoparticle ink. After sonication, the ink was deposited on glass substrates, which were preheated to 160°C. The copper films deposited on the glass substrate were dipped in an actic acid for 3 minutes to remove the oxide layer. Interestingly, the dried silver pastes exhibited low sheet resistance of 56 Ω (Figure 4).



Figure 4: copper paste on glass substrate show the sheet resistance 56 Ω

Conclusion

A simple, fast and economical chemical reduction method to synthesize copper nanoparticles is presented. There is no need to use high pressure, energy, temperature, toxic chemicals, downstream processing etc. Handling of the nanoparticles is also much easier than other methods. The synthesized copper nanoparticles are in spherical shape with particle size of around 100 nm. Their characterizations have been successfully done using XRD, SEM and UV-Vis spectroscopic techniques. Investigation on the conductive behavior of nanosized copper ink reveals high efficiency of copper nanoparticles as conductive ink. This synthesized copper nanoparticles can be useful as conductive ink in electronics.

Acknowledgement

The authors are grateful to Dr Khin Khin Win, Professor and Head of the Department of Physics, University of Yangon for her kind permission to carry out this work.

References

- Bell, W. C., and Myrick, M. L. (2001), 'Preparation and characterization of nanoscale silver colloids by two novel synthetic routes', *Journal of Colloid and Interface Science*, 242, 300 – 305
- Choi, S. H., Zhang, Y. P.,Gopalan, A., Lee, K. P., and Kang, H. D. (2005), 'Preparation of catalytically efficient precious metallic colloids by γ-irradiation and characterization colloids and surfaces A', *Physicochemical and Engineering Aspects*, 256, 165 – 170
- D. V. Goia and E. Matijevic, (1998), "Preparation of monodispersed metalparticles," New J.Chem., vol. 22, no.11, pp. 1203-1215.
- Hutter, E., Fendler, J. H., and Roy, D. (2001), 'Surface plasmon resonance studies of gold and silver nano particles linked to gold and silver substrates by 2-aminoethanethiol and 1,6 Hexanedithiol' J. Phys. Chem. B, 105, 11159-11168
- K. J. Carroll, J. U. Reveles, M. D. Shultz, S. N. Khanna, and E. E. Carpenter, (2011), "Preparation of ele-mental Cu and Ni nanoparticles by the polyol method: An experimental and theoretical approach," J. Phys. Chem. C, vol. 115, no. 6, pp. 2656–2664.
- Kuo, C.H., Chen, C.H., Huang, M.H. (2007): Seed-mediated synthesis of monodispersed Cu2O nanocubes with five different size ranges from 40 to 420 nm. Adv. Funct. Mater. 17, 3773–3780
- S. P. Wu and S. Y. Meng, (2006), "Preparation of micron size copper powder with chemical reduction method," Materials Letters, vol. 60, no. 20, pp. 2438–2443
- T. M. D. Dang, T. T. T. Le, E. Fribourg-Blanc, and M. C. Dang, (2011), "Synthesis and optical properties of copper nanoparticles prepared by a chemical reduction method," Adv. Nat. Sci: Nano-sci. Nanotechnol., vol.2, no.1, pp. 1-6.
- Ozin, G.A. (1992),' Nanochemistry Synthesis in diminishing dimensions' Advanced. Materials, 4, 612

SYNTHESIS OF SILVER NANOWIRES USING NACL ASSISTED ETHYLENE GLYCOL MEDIATED POLYOL METHOD

Saw Thiri¹, Nan Thidar Chit Swe² and Ye Chan³

Abstract

The synthesis of silver nanowires (AgNWs) from AgNO₃ through ethylene glycol mediated polyol process with the assisted of polyvinylpyrrolidone (PVP) and a NaCl. The surface morphologies and crystallinity of silver nanoparticles are analyzed by Scanning Electron Microscopy (SEM), XRD and UV-Vis. The UV-Vis spectra showed the typical surface plasmon absorption maxima around 465 nm, 436 nm, 414 nm, 399 nm and 350nm. SEM results revealed that the diameter of silver nanowires (AgNWs) were 100 nm and length up to 150 µm accompanied with silver nanoparticles (AgNps). XRD studies reveal a high degree of crystallinity and monophase silver nanowires (AgNWs). The polyol synthesis of silver nanowires (AgNWs) produce ultralong and thin nanowires.

Keywords: Polyol synthesis method, mediated salt, silver nanoparticles, silver nanowires

Introduction

Materials with high transparency, flexibility, and conductivity are important for progressing optoelectronic applications such as solar cells, infrared reflectors, flat panel displays, touch screens, and organic light emitting diodes. Ideally transparent electrodes would be highly transparent, easily fabricated, and serve as efficient electron acceptors with low resistivity. To date, the dominant material of the transparent conductive electrode (TCE) is indium tin oxide (ITO). However, limitation of ITO such as its scarcity, expensive price, brittleness and complicated process in the vacuum environment resulted in not only extremely intensive energy but also economically expensive of using ITO during thin film fabrication process. Moreover, flexing of ITO electrodes alters the homogenous coverage over the flexible substrate resulting in cracking and reduced performance over time. Therefore, there are some emerging alternatives, such as carbon nanotubes, graphene, conducting polymers, and metal nanowires with high conductivity

¹ Demonstrator, Department of Physics, Kalay University

². Lecturer, Universities' Research Center, University of Yangon

³ Professor and Head of Department, Universities' Research Center, University of Yangon

and transmissivity to replace with ITO. One-dimensional (1-D) metallic nanostructure, namely silver nanowires (AgNWs), has exhibited for their unique materials in building macroscale flexible conductors because of their high conductivity, good flexibility, and mature preparation technology, and various flexible conductive materials and devices have been fabricated on the basis of silver nanowires. However, in order to implement the optical and electrical features required for flexible and transparent electrodes, there is still a need to develop more effective processes for synthesizing AgNWs with controllable shapes and sizes, which can be grown continuously up to get long and thin AgNWs. For wider industrial applications of AgNWs, a simple and scalable preparation process is required.

Various synthetic methods for AgNWs have been investigated over the past decade. Until now, the most widely used methods is polyol method. The polyol method is becoming the most promising synthesis for preparing AgNWs by virtue of their various advantages such as their homogeneous reaction. This method is simple, but the great attention must be needed to make stable and reproducible colloid. Solution temperature, concentrations of the metal salt and reducing agent, reaction time influences particle size. Controlling size and shape of metal nanoparticles remains a challenge.

Silver nanowires preparing by this methods strongly depends on the parameters of the synthesis procedure such as the reaction temperature, the molar ratio between PVP and AgNO₃, PVPs with different chain lengths, the seeding condition and shielding gas, the additive of the control agents and the stirring speed.

In this paper, one pot synthesis of modified polyol-mediated processes have been used for the synthesis of ultralong silver nanowires within reaction time one hour after completing the all reagents. Moreover, optical and electrical properties of air dried ultralong AgNWs thin films are reported. Further, the structural, chemical properties of these two different structures of ultralong AgNWs were examined.

Experimental

Silver Nitrate (AgNO3, 99.9 %), Ethylene Glycol (EG, 95.5 %), Polyvinyl pyrrolidone (PVP) (MW: 1300,000), and sodium chloride (NaCl anhydrous, 99.0%), anhydrous ethanol (EtOH), Acetone were used as received without any purification.

Silver nanowires were synthesized by reducing AgNO₃ as metal precursor salt in Ethylene Glycol (EG) which was used as not only reducing agent but also solvent and PVP as a capping agent. The first sample (Sample 1) was synthesized without any mediated salt, NaCl. AgNO₃ solution (94 mM, in EG) and PVP solution (1300K) (147 mM, in EG) were completely dissolved by using magnetic stirring at room temperature. First, 30 mL of EG in a flask was heated at 170°C in a heating mantle with stirring rate 150 rpm for 30 minutes. After 30 minutes, NaCl solution was dropped into heated EG and then the reaction temperature was reduced to 110°C. After 10 minutes, mixed PVP/ethylene glycol was added to prepared solution, followed by AgNO₃ /ethylene glycol drop wise to the solution over dropping at a rate of 1 ml min^{-1} . The magnetic stirring was completely stopped when the AgNO₃ solution was added. After adding all reagents, the mixture turned yellow indicating the appearance of AgNps. The reaction mixture was maintained at 110°C for 10 minutes until all AgNO₃ had been completely reduced. And then, the temperature was increased to 170°C within 10 minutes for nanowire growth and the solution became gray gradually. The reaction continue to down at 150°C for 40 minutes until the reaction finished completely with formed slightly gray-white suspensions. The sample marked as Sample S1 (S1). For Sample 2 (S2), Sample 3 (S3) and Sample 4 (S4) was synthesized by using Sodium Chloride (NaCl 10 mM, 20 mM and 30 mM, in EG) as a mediated salt before adding starting precursor. The synthesis procedure was exactly the same as Sample 1 (S1). The product was diluted with acetone (1:5 by volume) and centrifuged at 3000 rpm for 20 minutes. The supernatant containing silver particles could be removed using a pipette. This centrifugation procedure could be repeated three times with ethanol until the supernatant became colorless. The collected precipitates redispersed in ethanol for further used and some were dried oven at 60°C for further characterization.

Centrifuge machine (Kokusan H-200 series) was used to separate the nanowires from the solutions. The surface morphology of AgNWs were observed by using Scanning Electron Microscope (JEOL- JSM 5610 LV) with the accelerating voltage of 15 kV, the beam current of 50 mA and 10000 time of photo multiplication. The crystalline properties for drop coated glass thin film of silver nanostructures were analyzed by using Cu K- α 1 radiation (40 kV, 40 mA) in 2 θ range from 10°C to 70° C on a Rigaku powder X-ray diffractometer (RINT 2000) equipped with a diffracted-beam graphite monochromator.

Results and Discussions

The merit of this research provide the easiest way to synthesize thin and long AgNWs with high yield within one hour after adding all reagents. Different aspect ratios of AgNWs were obtained by using different amount of NaCl with exactly the same experimental procedure.

After the preparation of samples, the suspension of nanowires in ethanol was used for SEM analysis by fabricating a drop of suspension onto a clean glass substrate and allowing ethanol to completely evaporate. The crystallite domain diameters D were obtained from XRD peaks according to the Scherrer equation: $D = \frac{0.9\lambda}{Wcos\theta}$ where λ is the wavelength of the incident X-ray beam (1.54056 Å for Cu K- α 1), θ is the Bragg's reflection angle, ΔW is the full width at half maximum. Crystallinity is evaluated through comparison of crystallite size as ascertained by SEM particle size determination. Crystallinity index Equation is presented as following $I_{crystal} = \frac{D_{p(SEM,TEM)}}{D_{XRD}}$ where $I_{crystal}$ is the crystallinity index; D_p is the particle size (obtained from either TEM or SEM morphological analysis); D_{XRD} is the crystallite size (calculated from the Scherrer equation).



Sample 1

Figure1:(a) The UV-Vis absorption spectrum of AgNps without any mediated salt (b) XRD pattern of purified AgNps (c) low (d) high magnification SEM micrograph of AgNps solution without any mediated salt

Figure 1(a) shows the absorption spectra of silver nanostructures by using the precursor of PVP to AgNO₃ without mediated salt. The appearance of surface plasmon resonance (SPR) which can be attributed to the collective oscillation of conduction electrons that is induced by an electromagnetic field at 465 nm indicated the formation of AgNps. The symmetric shape of the SPR band indicates the formation of spherically shaped Nps, and the long tail in the red region indicates the formation of polydisperse size of Nps. The X-ray diffraction pattern of the silver nanoparticles synthesized by polyol method is shown in Figure 1 (b). A number of strong Bragg reflections can be seen which correspond to the (111), (200), and (311) reflections of FCC silver. No spurious diffractions due to crystallographic impurities are found, only monophase silver agrees with the XRD data (ICDD-PDF#04-0783). The high intense peak for FCC materials is generally (111) reflection, which is observed in the sample. The lattice constant calculated from the diffraction pattern was 0.4086 nm, which is in agreement with the reported value of silver (JCPDS 04-0783). From XRD data, the ratio of intensity between (111) and (200) peaks reveals a relatively same value of 2.25 compared to the theoretical ratio value of 2.5. The crystallite size of the silver nanoparticles estimated from the Debye–Scherrer formula is 24 nm. SEM images show that the spherical shaped silver nanoparticles have relatively uniform average diameter equal to 100 nm.

Sample 2

Figure 2(a) shows the UV-Vis absorption spectra of AgNWs with NaCl 10 mM as mediated agent. As NaCl salt 10 mM was added to synthesis procedure, the SPR peak around 465 nm (sample 1) is blue-shifted to 414 nm. This implies that the final product synthesized under this particular condition that is using mediated salt was a mixture of AgNps and AgNWs. The UV spectrum had a main absorption at 414 nm with a shoulder at 350 nm. These two absorption bands were ascribed to the surface plasmon resonance bands of the transverse and longitudinal modes of the silver nanowires and nanoparticles. Figure 2(b) XRD pattern reveals that the ratio of intensity between (111) and (200) peaks reveals a relatively high value of 4.5. It is obvious that using of NaCl 10 mM as mediated agent affected ratio of intensity between panels and it shows the crystallinity in this method increased. Figures 2(c) and 2(d) show high and low magnification SEM images of silver nanostructures synthesized with NaCl 10 mM as mediated agent. SEM images show that the high yield of spherical shaped silver nanoparticles accompanied with some nanowires. AgNWs with very low yield and relatively uniform average diameter equal to 100 nm length around 10 µm.



Figure 2: (a) The UV-Vis absorption spectrum of AgNWs : at 414 nm and 350 nm were attributed to the plasmon resonance peaks of silver with various origins: surface plasmon of nanoparticles, long nanowires similar to the bulk silver (b) XRD pattern of purified silver nanostructure (c) low and (d) high magnification SEM micrograph of Ag nanostructure solution with 10 mM of NaCl mediated salt

Sample 3

Figure 3(a) shows the UV-Vis absorption spectra of AgNWs with NaCl 20 mM as mediated agent. As NaCl salt 20 mM was added to synthesis procedure, the SPR peak around 414 nm (sample 2) is blue-shifted to 399 nm.

The peak positioned at 399 nm could be considered as the optical signature of relatively long AgNWs. This implies that the final product synthesized under this particular condition that is using 20 mM mediated gives a high of yield of AgNWs. Figure 3(b), XRD pattern reveals that the ratio of intensity between (111) and (200) peaks reveals a relatively high value of 6.5. It is obvious that using of NaCl 20 mM as mediated agent affected ratio of intensity between panels and it shows the crystallinity in this method increased. Figures 3(c) and 3(d) show high and low magnification SEM images of silver nanostructures synthesized with NaCl 20 mM as mediated agent. SEM images show AgNWs with very high yield and relatively uniform average diameter equal to 100 nm and length up to 150 μ m.



Figure 3: (a)The UV-Vis absorption spectrum of AgNWs: at 399, and 350 nm were attributed to the plasmon resonance peaks of silver with various origins: transverse mode of nanowire, long nanowires similar to the bulk silver (b) XRD pattern of purified silver nanostructure (c) low and (d) high magnification SEM micrograph of AgNWs solution with 20 mM NaCl mediated salt

Sample 4

Figure 4(a) shows the UV-Vis absorption spectra of AgNWs with NaCl 30 mM as mediated agent. As the NaCl salt amount increases from 20 mM to 30 mM, the SPR peak around 399 nm is red-shifted to 411 nm. The UV spectrum had a main absorption at 418 nm with a shoulder at 380 nm and 350 nm. The main absorption 418 nm indicated the formation of AgNps and shoulder peak at 380 nm and 350 nm ascribe to the surface plasmon resonance bands of the transverse and longitudinal modes of the AgNWs. The final product synthesized under this particular condition that is using 30 mM of mediated salt gives mixture of nanowires and nanoparticles. Figure 4(b) the ratio of intensity between (111) and (200) peaks reveals a relatively high value of 6.8. It is obvious that using of NaCl 30 mM as mediated agent affected ratio of intensity between panels and it shows the crystallinity in this method increased. Figures 4(c) and 4(d) show high and low magnification SEM images of silver nanostructures synthesized with NaCl 30 mM as mediated agent. SEM images show AgNWs with very low yield and relatively uniform average diameter equal to 88 nm.





Figure 4 (a) The UV-Vis absorption spectrum of AgNWs: at 399, and 350 nm were attributed to the plasmon resonance peaks of silver with various origins: transverse mode of nanowire, long nanowires similar to the bulk silver (b) XRD pattern of purified silver nanostructure and the intensity of two distinct peaks show high aspect ratio (c) low and (d) high magnification SEM micrograph of AgNWs solution with 30 mM NaCl mediated salt

Different amounts (0 mM, 10 mM, 20 mM and 30 mM) of NaCl mediated salts in the synthesis procedure give the maximum SPR peak around 465 nm, 414 nm, 399 nm and 418m. The maximum of the plasmon peaks ~ 418 nm, ~ 399 nm, and 414 nm which were always described as the transverse mode of AgNWs or nanorods. The shoulder peaks at 350 nm could be considered as the optical signature of ultralong AgNWs. This implies that the final product synthesized under this particular condition that is using mediated salt was a mixture of AgNps and AgNWs. Moreover, with fragmentation of rod-like branches, the trunks of silver dendrites can convert into long NWs, which would support a blue-shift optical style of the plasmon peak. These results are consistent with the XRD results: with increasing the aspect ratio, the transverse SPR band shifts slightly to the blue side. By using 20 mM salt in the synthesis procedure, the plasmon peak shifts to ~ 399 nm and the plasmon band becomes relatively narrow.

SEM showed that the structure and yield silver products varied with the molarity of mediated salts used in the AgNO₃/PVP/mediated salts/Ethylene glycol system. The SEM images show that there are no mediated salt in synthesis procedure, the AgNWs are not achieved, and the majority of the structures are AgNps. By using 10 mM NaCl mediated salt, the main products are the spherical AgNps (96%) besides there are different length of silver nanostructure. Figure 3(c) and (d) show the SEM image of AgNWs with NaCl (20 mM,in EG) as the mediated agent. The image reveals that the product is entirely composed of AgNWs. The diameter of the nanowire is around 100 nm and length up to 150 μ m. As the NaCl salt amount increases from 20 mM to 30 mM, the main products are the spherical silver nanoparticles (50%) besides there are different shaped of metal nanostructure. The average diameter of the nanowire is equal to 88 nm and length up to 100 μ m.

According to XRD results, all the reflections correspond to pure silver metal with face centered cubic symmetry. The high intense peak for FCC materials is generally (111) reflection, which is observed in the sample. The intensity of peaks reflected the high degree of crystallinity of the silver nanoparticles. The calculation results shows that the crystallinity index of the sample that scored higher than 4.0 by using mediated salt; NaCl. If $I_{crystal}$ value is close to 1, then it is assumed that the crystallite size represents monocrystalline whereas a polycrystalline have a much larger crystallinity index greater than 1. The silver nanostructures show poly crystalline nature. The intensity ratio of (111) to (200) of around 6.5 is much larger than the theoretical value of 2.2, indicating that the intensity of the (200) peak was much smaller than expected. The XRD data suggest that the silver nanowires grew preferentially along the [110] direction.

Conclusion

In conclusion, a simple, fast, and economical polyol method to synthesize silver nanoparticles is presented. There is no need to use high pressure, energy, temperature, toxic chemicals, downstream processing etc. Handling of the nanowires is also much easier than other methods. AgNWs were successfully synthesized by using polyol technique with mediated agents. It was found that the addition of NaCl to the polyol reduction of $AgNO_3$ in the presence of PVP greatly facilitated the formation of AgNWs. Without the mediated agents, the final product synthesized was AgNps. A certain amount mediated salts produce high yield of ultralong AgNWs, otherwise, a mixture of AgNps and AgNWs were obtained. The right amount of NaCl mediated salt is crucial for the successful production of AgNWs. The synthesized AgNWs are in diameter of around 100 nm and length up to 150 μ m. Their characterizations have been successfully done using XRD, SEM and UV-Vis spectroscopic techniques. XRD studies reveal a high degree of crystallinity and monophase silver nanoparticles.

Acknowledgements

The authors greatly indebted to Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her kind permission to carry out this work. The authors wish to show our sincere thanks to Professor Dr Aye Aye Thant, Department of Physics, University of Yangon, for her fruitful discussions to this work.

References

- Bao, L-R, Wei. B and Xiao, Y.A. (2007)." Conductive Coating Formulations with Low Silver Content," *Electronic Components and Technology Conference*.
- Chun, K-Y., Oh, Y., Rho, J., An, H-H., Kim, Y-J., Choi, H. Y. and Baik, S. "Highly conductive, printable and stretchable composite films of carbon nanotubes and silver", *Nature Nanotechnology*, vol 5, pp 853
- Chou1, K-S., Huang, K-C. and Lee, H-H. (2005) "Fabrication and sintering effect on the morphologies and conductivity of nano-Ag particle films by the spin coating method," *Nanotechnolo*, 16, pp 779–784
- Dang, T. M. D., Le, T., Fribourg-Blanc, E. and Dang, C. M., (2012). "Influence of surfactant on the preparation of silver nanoparticles by polyol method" Advances in Natural sciences: *Nanoscience and Nanotechnology*, 3, 035004 (4pp)
- Gudikandula. K and Maringan,C.S. (2016). "Synthesis of silver nanoparticles by chemical and biological methods and their antimicrobial properties", *Journal of Experimental Nanoscience*, Vol. 11, No. 9, 714-72.
- Hao, E and Schatza, C. G. (2004). "Electromagnetic fields around silver nanoparticles and dimers", *Journal of Chemical Physics*, vol 120, No. 1, pp 357-366

- Hutter, E., Fendler, J. H., and Roy, D. (2001)." Surface plasmon resonance studies of gold and silver nano particles linked to gold and silver substrates by 2aminoethanethiol and 1,6-Hexanedithiol", Journal of Physical Chemistry. B, 105, 11159-11168
- Jakubowska, M. J., Kieł basinski, K. and Mł oniak, A. (2011). "New conductive thick-film paste based on silver nanopowder for high power and high temperature applications," *Microelectronics Reliability*, vol. 51, no. 7, pp. 1235–1240
- Kooa, H. Y., Yia, H. J., Kima, H. J., Koa, Y. N, Junga, S. D., Kanga, C.Y., Leeb, J-H, (2010). "Conductive silver films formed from nano-sized silver powders prepared by flame spray pyrolysis", *Materials Chemistry and Physics*, 124, 959– 963
- Landage S.M., Wasif A. I. and Dhuppe P, (2014) Synthesis of nanosilver using chemical reduction method,vol3, No. 5, pp 14-22

CHEMICAL BATH DEPOSITION OF ZINC OXIDE NANOFLOWER FILM ON SILVER NANOPARTICLE SEED LAYER

Su Myat Aung¹, Myo Aung² and Nan Thidar Chit Swe³

Abstract

Zinc oxide nanoflower with hexagonal structure was achieved by using chemical bath deposition method under atmospheric pressure by using zinc nitrate hexahydrate $[Zn(NO_3)_2.6H_2O]$ and hexamethylene-tetramine $(C_6H_{12}N_4)$ at constant temperature 93°C and the deposition time of 2 h. The prepared the film was grown on the suface of silver nanoparticles. The surface morphologies and the structural characterization of zinc oxide (ZnO) nanoflowers and silver nanoparticles were characterized by Scanning Electron Microscope (SEM) and X-ray Diffraction (XRD) technique. The SEM results revealed that the petal lengths of the zinc oxide (ZnO) nanoflowers were up to more than 2 nm in diameter from 200 nm to 300 nm. The XRD pattern of the sample revealed that ZnO nanoflowers have hexagonal crystallite structure.

Key words: Zinc Oxide nanoflowers, silver nanoparicles, seed layer

Introduction

Zinc oxide (ZnO) is a wide direct band gap (3.37eV) semiconductor which possesses high dielectric constant and excitation with high binding energy (60 MeV) at room temperature. The melting point of zinc oxide (ZnO) is 1954 °C, this determines high thermal and chemical stability. It also shows piezoelectricity. It is nontoxic material which is cheaply available. ZnO is also biocompatible, biodegradable, and biosafe for medical and environmental applications (Xia *et al*, 2003). Due to these properties, ZnO is a material of huge technological importance. Due to their remarkable performance in electronics, optics, and photonics, ZnO nanostructures are attractive candidates for many applications such as UV lasers, light-emitting diodes, solar cells, nanogenerators, gas sensors, photodetectors (Cao *el al*, 2006).

Variety of nanostructures of ZnO can be grown by using different methods. In general, there are two distinct approaches to create

^{1.} Demonstrator, Department of Physics, Loikaw University

^{2.} Lecturer, Universities' Research Center, University of Yangon

^{3.} Lecturer, Universities' Research Center, University of Yangon

nanostructures: top-down and bottom-up strategies. The top-down approach, etching and lithography in bulk materials is created to form functional devices. In the bottom-up approach, functional nanostructures are assembled from well-defined chemically and/or physically synthesized building blocks (Feng L *et al*, 2010).

There are various techniques to synthesize zinc oxide (ZnO) nanostructures such as metal organic chemical vapor deposition (MOCVD) (Park et al, 2002), molecular beam epitaxy (MBE), pulse laser deposition (PLD) and chemical vapor deposition (CVD). But these techniques are very expensive, highly toxic, high cost in environmental disposal and they need high vacuum equipment (Samanta P et al, 2009). Nonetheless, it is essential to find another technique to grow zinc oxide (ZnO) nanostructures that offers low cost and does not need high vacuum equipment. One of the most interesting method of ZnO synthesis is chemical bath deposition (CBD) (Yi S-H et al, 2007). (.It does not need complicated and expensive instruments and it allows for deposition of ZnO on different substrates. Nowadays, it is believed that chemical bath deposition (CBD) technique might be the cheapest method to deposit ZnO nanostructures. It does not require sophisticated instruments while the starting chemicals are commonly available and cheap, and the preparation parameters are easily controlled. And this technique does not need high vacuum equipment (Gowthaman P et al, 2011). In this paper, zinc oxide (ZnO) nanostructures such as nanoflowers and nanorods are synthesized by a bottom-up approach.

Experimental

2.1 Materials

Analytical grade (BDH, England) Zinc Nitrate Hexahydrate $[Zn(NO_3)_2.6H_2O]$, Hexamethylenetetramine $(C_6H_{12}N_4)$, Silver Nitrate (AgNO₃, 99.9%), Ethanol (EtOH) Polyvinylpyrroli done (PVP), Ethylene Glycol (EG) were used as starting precursor. All chemicals were used as purchased without further purification.

2.2 Cleaning Procedure of Glass Substrate

The very first step before the CBD proper is the washing of glass substrate in order to remove dirt and impurities that may have unknowingly settled on the glass substrate. This is done by washing in several substances, namely: acetone, distilled water, ethanol, distilled water again, hydrochloric acid (HCl) and lastly distilled water. These glass substrates are then dried in air blow at room temperature.

2.3 Synthesis of Silver nanoparticles (Ag NPs) and fabrication of Ag seeding layer

Silver nanoparticles were synthesized by reducing AgNO₃ as metal precursor salt in Ethylene Glycol (EG) which was used as not only reducing agent but also solvent and PVP as a capping agent. AgNO₃ solution (94 mM, in EG) and PVP solution (30K) (147 mM, in EG) were completely dissolved by using magnetic stirring at room temperature. First, 30 mL of EG in a flask was heated at 170 °C in a heating mantle with stirring rate 150 rpm for 30 minutes. Mixed PVP/ethylene glycol was added to prepared solution, followed by AgNO3 /ethylene glycol drop wise to the solution over dropping at a rate of 1ml min⁻¹. After adding all reagents, the mixture turned yellow indicating the appearance of Ag nanoparticle. (Nan *et al*, 2018). The reaction continue for 40 minutes until the reaction finished completely with formed slightly gray-white suspensions.

The product was diluted with acetone (1:5 by volume) and centrifuged at 10000 rpm for 20 min. The supernatant containing organic residues could be removed using a pipette. This centrifugation procedure could be repeated three times with ethanol. Purified Silver nanoparticles solution was mixed with 2-propanol (1:1v/v) and sonicated for 15 minutes to get homogenous ink solution for making seed layer. This solution was coated on glass substrates by rod coating method. After being placed in the air for few minutes at room temperature, the Ag nanoparticle layer was achieved as a solid and thin layer on the glass substrate.



Figure 1: (a) Silver nanoparticle (b) Silver nanoparticles seed layer coated on glass slide

2.3 Chemical Bath Deposition (CBD) Method

For chemical bath deposition (CBD) growth process, the aqueous solution of zinc nitrate hexahydrate $[Zn(NO_3)_2.6H_2O],$ and hexamethylenetetramine ($C_6H_{12}N_4$) were first prepared. The concentrations of both were fixed at 0.1M. The aqueous solutions of zinc nitrate hexahydrate $[Zn(NO_3)_2.6H_2O]$ (100 mL) and hexamethylenetetramine (C₆H₁₂N₄) (100 mL) were mixed together in 250 mL beaker. The bath is stirred at a constant rate of 360 RPM by magnetic stirrer for 30 minutes at room temperature. The beakers containing the bath solutions and the substrates were put on the hot plate for 2 h at a constant temperature of 93°C. After the growth, the substrates were removed from the solutions, rinsed with acetone, distilled water, ethanol then acetone and dried at room temperature. A post growth annealing was performed for the substrates (samples) at 150°C for 1 h and then quenched to room temperature (Li Z et al, 2008).



Figure 2: The schematic diagram of chemical bath depesotion of ZnO nanostructure

2.4 Characterization

Centrifuge machine (Kokusan H-200 series) was used to separate the colloid from the solutions. Silver nanoparticles and ZnO nanostructures such as nanoflowers and nanorods were confirmed X-ray powder diffractometer (XRD) (Type: RIGAKU–RINT 2000), and Scanning Electron Microscope (SEM) (Type: JEOL 15 kV).

Results and Discussions

3.1. UV and XRD Analysis of silver seed for CBD

Before fabricating the seeding layer, UV and XRD analysis are performed to determine the nature of Ag nanoparticles.





In Figure 3 (a) shows the uV-vis spectra of silver nanoparticles. The appearance of surface plasmon resonance (SPR) which can be attributed to the collective oscillation of conduction electrons that is induced by an electromagnetic field at 465 nm indicated the formation of AgNps. The symmetric shape of the SPR band indicates the formation of spherically shaped NPs, and the long tail in the red region indicates the formation of The X-ray diffraction pattern of the silver polydisperse size of NPs. nanowires synthesized by polyol method is shown in Figure 3 (b). A number of strong Bragg reflections can be seen which correspond to the (111), (200), and (311) reflections of FCC silver. No spurious diffractions due to crystallographic impurities are found, only monophase silver agrees with the XRD data (ICDD-PDF#04-0783). The high intense peak for FCC materials is generally (1 1 1) reflection, which is observed in the sample. The lattice constant calculated from the diffraction pattern was 0.4086 nm, which is in agreement with the reported value of silver (JCPDS 04-0783). From SEM data, SEM images show that spherical shaped silver nanoparticles have relatively uniform average diameter equal to 100 nm.

To compare ZnO nanostructures grown on different seed layers, SEM images of ZnO nanostructures on three types of Ag film were performed, as shown in Fig. 4, 5 and 6. The SEM characterizations of the seed layers and assynthesized zinc oxide (ZnO) nanostructures are shown in Figure: 4, 5 and 6.



Figure 4:(a) Top-view SEM images of sample S1 (a) silver seed layer which is coated onetime on the glass substrate (b) ZnO nanorod which is grown on thin seed layer



Figure 5: (a) Top-view SEM images of sample S1 (a) silver thickseed layer which is coated two times (b) ZnO nanorod which is grown on thicker seed layer



Figure 6: (a) Top-view SEM images of sample S3 (a) silver thick seed layer which is coated three times on the glass substrate(b) ZnO nanoflowers which is grown on thicker seed layer.

The SEM results revealed that the formation of nanorods and nanoflowers are formed in these samples. It is observed that the size of the nanorod and nanoflowers is depend on the seed layer. In Figure 3(b) SEM image shows that the length of the zinc oxide (ZnO) nanorods is 2μ m in diameter from 200 nm to 300 nm. Figure 4(b) and 5(b) show that the lengths of zinc oxide (ZnO) nanoflowers were up to more than 2 μ m and the diameter around 500 nm. It could be seen that the shape of ZnO nanoflowers resembled star-like morphology and the edges of ZnO petal were not smooth and were composed of assemblies of smaller nanocrystallites.

Ag seed films show symmetric and spherical NPs where the particles are uniformly distributed on the glass substrate. With increasing film thickness, more numbers of particles are deposited on top of each particle forming arrays of Ag NPs. The bottom Ag layer greatly influences the growth of ZnO nanostructure concerned to their aspect ratio, orientation, and density. With an increase in Ag seed layer film thickness, ZnO nanorods starts to grow in multiple directions leading to form flower like morphology could be called as nanoflower (i.e. growing more than 10 ZnO rods in a different direction ori- ginated from a single point) at thicker seed layer (Park WI *et al*, 2002).

The structural properties of the zinc oxide (ZnO) nanorods were characterized by X- ray diffraction (XRD). X-ray diffractomer, operated at 40kV and 40mA, with a Cu-K α radiation ($\lambda = 1.54056$ Å) in the range of 2 θ between 10° and 70° as shown in Figure: 6. The upper site of (XRD) profile represented the observed XRD pattern while the lower site indicated the standard (reference) #PDF-76-0704 (Powder Diffraction File) Library file. The X-Ray Diffraction analysis shows that ZnO nanorod has a hexagonal crystallite structure with lattice parameters; a=b=3.2699 and c=5.2219 (a=b≠c), which agrees with the condition for a lattice structure to be hexagonal. The Debye-Scherrer's equation (equation 1) used to estimate the average crystallite size. The crystallite domain diameters *D* were obtained from XRD peaks according to the Debye-Scherrer's equation:

$$D = k\lambda/\beta \cos\theta \tag{1}$$

where, k is known as Scherrer's constant which is dependent on the crystallite shape and can be considered as 0.9, λ is the X-ray wavelength of the incident Cu K α radiation, which is 0.154056 nm, β is the full width at half maximum of the respective peak and θ represents the diffraction peak angle. The calculated average crystallite size for zinc oxide (ZnO) nanoflower is 50 nm. The result showed that the (ZnO) nanorods that was prepared through the chemical bath deposition method presented a remarkably strong diffraction peak at the (002) plane, which is located between 34.23°. This finding indicated that of the (ZnO) nanoflower possessed hexagonal structure with high c-axis orientation. There is a significant increase in the intensity of the diffraction peak corresponding to the (002) plane perpendicular to the substrate. Meanwhile, the weak diffraction peaks of (100) and (101) also appear, as shown in the figure 4. The relative intensity ratio of I(002), defined as I(002) = I(002)/[I(100)+I(002)+I(101)], of the (ZnO) nanoflowers is 0.37. The XRD pattern exhibited that of the (ZnO) nanoflowers had remarkably excellent crystal quality and high c-axis orientation.



Figure 6:XRD plots obtained from ZnO nanostructures sample to investigate the structures and crystallinity. Reference bulk reflections of pure Ag and Ag2O3 phases are shown at the bottom (ICDD-PDF#07-0719), (ICDD-PDF#72-0607).
According to XRD result, ZnO nanostructures were heterogeneously grown on oxidized Ag layers. The ZnO nanostructure (lattice constant 1.5) are grown on a lattice-mismatched Ag/Ag_2O_3 (lattice constant 4.9) seed layer. These results explicit that ZnO nanorods can grow vertically on an oxidized Ag layer. Basically, the ZnO nucleation occurs at stable sites with lowest surface energy. The sites with large lattice mismatch between ZnO and metal substrate are forced to separate ZnO nucleus due to their high surface energy. To reduce surface energy and lattice mismatch, water molecules can oxidize the ionized metal layer using environmental thermal energy given by M++ OH-, \square M(OH), \square MO⁻ + H⁺, where M is metal. Usually, ionized metal atoms result from oxidized metal atoms, which have been exposed and oxidized in ambient air. These oxidation processes on metal surfaces are used to happen non-uniformly. In addition, the lattice constant of a metal oxide layer seriously affects the growth of ZnO nanostructures on itself. Therefore, when the both requirements are met, ZnO nanorod can be successfully grown on the metal oxide (Kashif M et al, 2012).

For the growth of the ZnO nanoflower following the growth of the nanorods, nucleation sites are formed on the surface of the ZnO nanorods with greater height because of the radial growth preference of the nanorods which is less spatially hindered. After the formation of the nucleation sites, many ZnO nanorods grow radially which finally results in the ZnO nanoflower structure (Karami H *et al*, 2011). Whereas non-uniformly localized metal oxide sites collect ZnO nucleus and grow ZnO nanowires along with the morphology of ZnO nucleus, Ag+ ions can oxidize metal surface very uniformly and metal atoms are negatively ionized easily to meet Zn2+ ions when Ag+ ions are detached (Lee GJ *et al*, 2010). Once ZnO islands are formed, ZnO nanoflowers are grown further on those islands following c-plane of ZnO.

Conclusion

Silver nanoparticles were synthesized by reducing $AgNO_3$ as metal precursor salt in Ethylene Glycol (EG) which was used as not only reducing agent but also solvent and PVP as a capping agent. In conclusion, zinc oxide (ZnO) nanoflowers were synthesized by a chemical bath deposition (CBD) method with wide range of size and various shapes. The petal lengths of the zinc oxide (ZnO) nanoflowers were up to more than 2 μ m and the diameter around 500 nm. It was observed that the length and alignment of (ZnO) nanoflowers were strongly related to the thickness of the seed layers.

Acknowledgements

The authors greatly indebted to Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her kind permission to carry out this work. The authors wish to show our sincere thanks to Professor Dr Aye Aye Thant, Department of Physics, University of Yangon, for her fruitful discussions to this work. The authors acknowledge Professor Dr Ye Chan, Universities' Research Center, University of Yangon, for his advice and suggestions to this research and kind permissions to carry out laboratory facilities in URC.

References

- Cao HL, Qian XF, Gong Q, Du WM, Ma XD, Zhu ZK: Shape- and size controlled synthesis of nanometre ZnO from a simple solution route at room temperature. Nanotechnology 2006, 17:3632.
- D.H. Kim, H-J. Koo, J.S. Jur, M. Woodroof, B. Kalanyan, K. Lee, C.K. Devine, and G.N. Parsons, *Nanoscale*, 4 (2012) 4731-4738.
- Feng L, Liu A, Ma Y, Liu M, Man B: Fabrication, structural characterization and optical properties of the flower-like ZnO nanowires. Acta Physiol Pol 2010, 117:512– 517.
- Gowthaman P, Saroja M, Venkatachalam M, Deenathayalan J, Senthil TS: Structural and optical properties of ZnO nanorods prepared by chemical bath deposition method. Aust J Basic Appl Sci 2011, 5:1379–1382.
- Hossain M, Ghosh S, Boontongkong Y, Thanachayanont C, Dutta J: Growth of zinc oxide nanowires and nanobelts for gas sensing application. J Metastable Nanocrystalline Mater 2005, 23:27–30.
- J. Liu, S. Xie, Y. Chen, X. Wang, H. Cheng, F. Liu, and J. Yang, *Nanoscale Res. Lett.*, 6 (2011) 619.
- Karami H, Fakoori E: Synthesis and characterization of ZnO nanorods based on a new gel pyrolysis method. J Nanomater 2011, 2011:11.
- Kashif M, Hashim U, Ali ME, Ali SMU, Rusop M, Ibupoto ZH, Willander M: Effect of different seed solutions on the morphology and electro optical properties of ZnO nanorods. J Nanomater 2012. 2012:6.
- Li Z, Huang X, Liu J, Li Y, Li G: Morphology control and transition of ZnO nanorod arrays by a simple hydrothermal method. Mater Lett 2008, 62:1503–1506

- L-W. Ji, S-M. Peng, J-S. Wu, W-S. Shih, C-Z. Wu, and I-T. Tang, J. Phys. Chem. Solids, 70 (2009) 1359.
- Lee GJ, Lee Y, Lim HH, Cha M, Kim SS, Cheong H, Min SK, Han S,H: Photoluminescence and lasing properties of ZnO nanorods. J Korean Phys Soc 2010, 57:1624–1629.
- Nan TD, Lwin KO, Thida M, Ye C: Polyol Synthesis of Silver Nanoparticles for Flexible Electronic Circuit. Universities Research Journal, 2018, Vol.11.
- Park WI, Kim DH, Jung S-W, Yi G-C: Metalorganic vapor-phase epitaxial growth of vertically well-aligned ZnO nanorods. Appl Phys Lett 2002,80:4232–4234.
- Samanta P, Patra S, Chaudhuri P: Visible emission from ZnO nanorods synthesized by a simple wet chemical method. Int J Nanosci Nanotech 2009, 1:81–90.
- Xia Y, Yang P, Sun Y, Wu Y, Mayers B, Gates B, Yin Y, Kim F, Yan H: One dimensional nanostructures: synthesis, characterization, and applications. Adv Mater 2003, 15:353–389.
- Yi S-H, Choi S-K, Jang J-M, Kim J-A, Jung W-G: Low-temperature growth of ZnO nanorods by chemical bath deposition. J Colloid Interface Sci 2007, 313:705–710.

GPS-GSM BASED LOCATION AND POSITION TRACKING SYSTEM

Aung Zaw Oo^{*}

Abstract

This research work reveals the location and position tracking system based on GPS (Global Positioning System) and GSM (Global System for Mobile Communication) modules. Location and position tracking system is constructed with NEO-7M GPS Module, SIM900A GSM module, MPU-6050 gyroscope sensor and Arduino Mega microcontroller. The constructed system is used for vehicle tracking system. Arduino microcontroller is used as main control device. GPS module connects the GPS satellites and receives geographic coordinate data at regular time interval. MPU-6050 senses the position of object. GSM module transmits the GPS location and position of the system to mobile phone through SMS (Short Message Service). GPS location and position of system can be viewed on Google map with the help of software via the internet.

Keyword: GPS module, GSM module, MPU-6050 gyroscope sensor, Google map

Introduction

Tracking system uses the GPS (Global Positioning System) to determine the precise location of a vehicle or person to which the device is attached. The tracking system offers its location information and records the data. The recorded data are transmitted to data base server or sends SMS to predetermined phone number.

Constructed system includes hardware and software components to track the location and position of vehicle or person. NEO-7M GPS Module, SIM900A GSM module, MPU-6050 gyroscope sensor and Arduino Mega microcontroller are used as hardware component. MySQl server and Google map are used as software components.

Arduino Mega is interfaced serially to a GSM module and GPS sensor. MPU-6050 gyroscope sensor measures the position of the vehicle and NEO-7M GPS Moduleprovides the location. The SIM900A GSM module is used to

^{*} Lecturer, Department of Physics, Pyay University

send the data in terms of latitude and longitude via SMS and these data are sent to database server on domain. The location and position of vehicle can be viewed on Google map.



Figure1: Block diagram of GPS-GSM based location and position tracking system

Material and Method

Constructed system is based on hardware and software components to track the location and position of vehicle or person.

Arduino Mega 2560 Microcontroller

Arduino Mega 2560 microcontroller board is used as main controller device. Arduino Mega is based on Atmel ATmega2560 microcontroller. Mega 2560 board has 54 digital input/output pins, 16 analog inputs, 4 UARTs (hardware serial ports), a 16 MHz crystal oscillator, a USB connection, a power jack, an ICSP header (In-Circuit Serial Programming), and a reset button. Photograph of Arduino Mega board is shown in Figure 2.



Figure 2: Photo of Arduino Mega 2560 microcontroller board

NEO-7M GPS Module

The Waveshare NEO-7M GPS Module provides location, heading, and speed and comes in a compact package. It comes with a high-gain active antenna, but also includes an IPX interface for connecting a different active antenna. A rechargeable backup battery will hold data when powered down, but perhaps more importantly it supports hot starts for a fast satellite lock time. A 5-wire cable with a SIP socket on one end and individual sockets on the other makes it easy to connect the Waveshare NEO-7M GPS module. Figure 3 shows the NEO-7M GPS Module.



Figure 3: NEO-7M GPS Module

SIM900A GSM Module

Global system for mobile communications (GSM) is digital cellular system used for mobile devices. It is an international standard for mobile which is widely used for long distance communication. SIM900A module allows users to send/receive data over GPRS, send/receive SMS and make/receive voice calls. The GSM/GPRS module uses USART communication to communicate with microcontroller or PC terminal. AT commands are used to configure the module in different modes and to perform various functions like calling, positing data to a site.Figure 4 shows the SIM900A GSM module.



Figure 4: SIM900A GSM Module

MPU 6050 Sensor

MPU 6050 is the combination between a MEMS 3-axis gyroscope and a 3-axis accelerometer on the same silicon die together with an onboard Digital Motion Processor[™] (DMP[™]) capable of processing complex 9-axis MotionFusion algorithms, the MPU-6050 does away with the cross-axis alignment problems that can creep up on discrete parts. Figure 5 shows MPU 6050 sensor.



Figure 5: MPU 6050 sensor

Domain Name

A domain name is an identification string that defines a realm of administrative autonomy, authority or control within the Internet. Domain names are formed by the rules and procedures of the Domain Name System (DNS). Any name registered in the DNS is a domain name. Domain names are used in various networking contexts and for application-specific naming and addressing purposes. In general, a domain name represents an Internet Protocol (IP) resource, such as a personal computer used to access the Internet, a server computer hosting a web site, or the web site itself or any other service communicated via the Internet.

cPanel

cPanel is an online Linux-based web hosting control panel that provides a graphical interface and automation tools designed to simplify the process of hosting a web site. cPanel utilizes a three-tier structure that provides capabilities for administrators, resellers, and end-user website owners to control the various aspects of website and server administration through a standard web browser. It is designed to function either as a dedicated server or virtual private server. Application-based support includes Apache, PHP, MySQL, Postgre SQL, Perl, and BIND (DNS). Email-based support includes POP3, IMAP, and SMTP services. cPanel is accessed via https on port 2083.



Figure 6: cPanel from domain

Hardware Interface

Tx pin (Yellow wire) of GPS module is directly connected to digital pin No.10 of Arduino. Rx pin (Green wire) of GPS module is directly connected to digital pin No.11 of Arduino. Ground pin (Black wire) is directly connected to digital pin GND of Arduino. Vcc pin (Red wire) is directly connected to digital pin 3.3V of Arduino as shown in Figure 5.

Circuit connections of GSM module is Tx pin (Green wire) of GSM module is directly connected to digital pin Rx of Arduino. Rx pin (Yellow wire) of GSM module is directly connected to digital pin Tx of Arduino. SDA and SCL pins of MPU6050 are connected to pin 20 and 21 of Arduino respectively.

Ground pin (Black wire) is directly connected to digital pin GND of Arduino. GSM module is also powered by 12V supply.



Figure 7: Circuit diagram of tracking system

Software Interface

Creating Database in MySql

phpMyAdmin is a free software tool written in PHP, intended to handle the administration of MySQL over the Web. phpMy Admin supports a wide range of operations on MySQL and Maria DB. Frequently used operations (managing databases, tables, columns, relations, indexes, users, permissions, etc) can be performed via the user interface, while you still have the ability to directly execute any SQL statement. Figure 7 shows the database in MySql server.

Creating PHP Script

PHP is a general purpose scripting language that is well suited to web development and can be embedded into HTML. To send measured data to database server, PHP script is created as shown in Figure 8.

🍯 cPanel - Main 🛛 🗙 🗙	🙀 sg2.fcomet.	:om / localhost	/ azow 🗙	+						
← → ♂ @	🛈 🔒 ht	tps://sg2. fco r	met.com:208	3/cpsess	9439419079	9/3rdparty/php!	/lyAdmin/sql	.php?server=	1&db=azowea	th_testdata&d
ohoMuAdmin	← 🗐 Ser	er: localhost	3306 » 📄 D	atabase	azoweath_	_testdata » 📷 T	able: gps_tr	aek		
<u>≙</u> © ⇒ ¢	Brow	se 🥻 St	ructure [SQL	🔍 Se	arch 📑 ir	isert 🖷	Export	Import	Operations
Recent Pavontes	+ Options									
■ azoweath_DB	←T→		∇	id tin	ie		latitude	latitudeD	longitude	longitudeD
azoweath_test	🗆 🥜 E	dit 📑 Copy	Oelete	602 20	18-06-30 02	2:27:52.601529	18.76825	N	95.22460	E
Zoweath_testdata	🗆 🥜 E	lit 📑 Copy	Oelete	589 20	18-06-27 05	5:54:25.698500	18.81626	N	95.21778	E
🕀 🌈 data	🗆 🥜 E	dit 📑 Copy	Oelete	590 20	18-06-27 05	5:55:21.424708	18.81750	N	95.21558	E
flood_data	🗆 🥜 E	lit 📑 Copy	Oelete !	591 20	18-06-27 05	5:56:17.531821	18.82052	Ν	95.21571	E
+ gps_track	🗆 🥜 E	lit 🚮 Copy	Oelete 4	592 20	18-06-27 05	5:57:17.684916	18.82224	N	95.21701	E
azoweath_wp935	□ <i>⊘</i> E	dit 👫 Copy	Oelete !	593 20	18-06-27 05	5:58:08.448533	18.82487	N	95.21784	E
❶→→→ ● information_schema	□ <i>⊘</i> E	lit 🚮 Copy	Oelete 4	594 20	18-06-27 05	5:59:04.631660	18.82703	N	95.21896	E
	🗆 🥜 E	lit 📑 Copy	Oelete 4	595 20	18-06-27 06	6:00:00.318468	18.82660	N	95.22144	E
	🗆 🥜 E	lit 📑 Copy	Oelete 4	596 20	18-06-29 00):59:28.591263	18.77491	N	95.22179	E
	🗆 🥜 E	lit 📑 Copy	Oelete	597 20	18-06-29 01	1:00:32.974196	18.77476	N	95.22186	E
	🗆 🥜 E	lit 📑 Copy	Oelete 4	598 20	18-06-30 02	2:24:09.612423	18.77008	N	95.21907	E
		lit 🚮 Copy	Oelete 4	599 20	18-06-30 02	2:25:06.427525	18.76829	N	95.21940	E
	0 /E	dit 👫 Copy	Oelete (600 20	18-06-30 02	2:26:01.350693	18.76712	N	95.21931	E
	E	lit 👫 Copy	O Delete	588 20	18-06-27 05	5:53:29.758784	18.81622	N	95.22104	E
	E	dit 👫 Copy	Delete 4	587 20	18-06-27 05	5:52:35.227072	18.81715	N	95.22323	E
		lit 👫 Copy	Delete 4	586 20	18-06-27 05	5:51:40.379097	18.81907	N	95.22275	E
		dit 3∔i Copv	Delete 4	585 20	18-06-27 05	5:50:42.729455	18.82009	N	95,22303	E
		lit 📑 Copy	O Delete	584 20	18-06-27 05	5:49:46.832870	18.82109	N	95.22600	E

Figure 8: Creating Database in MySql database server



Figure 9: PHP code for accessing data (GET method)

Results and Discussion

This research work is designed using ATmega1280 microcontroller which is used as main control device for tracking the location and position of any vehicle by using GPS and GSM modules.

Figure 10 shows the serial output of the Arduino when program runs the tracking system. GPS module sends the location information including latitude, longitude, altitude, date, satellites as shown in Figure 10.Table 1 shows the coordinates of location collected from SMS message. Table 2 shows the location data in Excel format. MPU-6050 gyroscope sensor measures the position of the vehicle and sensor's data are shown in Table 3.

GPS Visualizer as shown in Figure 11 is an online utility that creates maps and profiles from geographic data. Input can be in the form of GPS data (tracks and waypoints), driving routes, street addresses, or simple coordinates. These data are sent to GPS Visualizer web page and export it to Google Earth. Figure 12shows the location tracking of exported data on Google maps output. Figure 13 shows SMS message from GPS tracking system. Figure 14 shows the photos of constructed system.

💿 COM23 (Arduino/Genuino Uno) —		×
		Send
\$GPGGA,030111.50,1849.56150,N,09513.44491,E,1,04,14.32,25.7,M,-47.4,M,,*70		î
\$GPGGA,030111.75,1849.56148,N,09513.44518,E,1,04,14.33,25.7,M,-47.4,M,,*7F		
\$GPGGA,030112.00,1849.56157,N,09513.44538,E,1,04,14.34,25.6,M,-47.4,M,,*74		
\$GPGGA,030112.25,1849.56160,N,09513.44565,E,1,04,14.35,25.6,M,-47.4,M,,*7E		
\$GPGGA,030112.50,1849.56157,N,09513.44588,E,1,04,14.35,25.6,M,-47.4,M,,*7B		
\$GPGGA,030112.75,1849.56153,N,09513.44602,E,1,04,14.36,25.6,M,-47.4,M,,*7A		
\$GPGGA,030113.00,1849.56169,N,09513.44538,E,1,04,14.37,25.5,M,-47.4,M,,*78		
\$GPGGA,030113.25,1849.56184,N,09513.44523,E,1,04,14.38,25.5,M,-47.4,M,,*79		
\$GPGGA,030113.50,1849.56186,N,09513.44522,E,1,04,14.39,25.5,M,-47.4,M,,*79		
\$GPGGA,030113.75,1849.56175,N,09513.44524,E,1,04,14.39,25.5,M,-47.4,M,,*74		
\$GPGGA,030114.00,1849.56159,N,09513.44522,E,1,04,14.40,25.4,M,-47.4,M,,*76		
\$GPGGA,030114.25,1849.56161,N,09513.44528,E,1,04,14.41,25.4,M,-47.4,M,,*71		
\$GPGGA,030114.50,1849.56174,N,09513.44538,E,1,04,14.42,25.4,M,-47.4,M,,*75		
\$GPGGA,030114.75,1849.56183,N,09513.44525,E,1,04,14.43,25.4,M,-47.4,M,,*77		
\$GPGGA,030115.00,1849.56189,N,09513.44514,E,1,04,14.43,25.3,M,-47.4,M,,*7B		
\$GPGGA,030115.25,1849.56182,N,09513.44507,E,1,04,14.44,25.3,M,-47.4,M,,*72		
\$GPGGA,030115.50,1849.56185,N,09513.44500,E,1,04,14.45,25.3,M,-47.4,M,,*71		×
No line ending v 115200 baud v	Clear	output

Figure 10: GPS data shown on serial output of Arduino

No	SMS link
1	http://google.com/maps/place/18.77481,95.22179\r\n
2	http://google.com/maps/place/18.78514,95.22205\r\n
3	http://google.com/maps/place/18.78374,95.22226\r\n
4	http://google.com/maps/place/18.78200,95.22282\r\n
5	http://google.com/maps/place/18.78029,95.22299\r\n
6	http://google.com/maps/place/18.77856,95.22320\r\n
7	http://google.com/maps/place/18.77666,95.22318\r\n
8	http://google.com/maps/place/18.77537,95.22321\r\n
9	http://google.com/maps/place/18.77515,95.22218\r\n
10	http://google.com/maps/place/18.77517,95.22217\r\n
11	http://google.com/maps/place/18.77518,95.22215\r\n
12	http://google.com/maps/place/18.77479,95.22181\r\n
13	http://google.com/maps/place/18.77480,95.22187\r\n
14	http://google.com/maps/place/18.77475,95.22184\r\n

Table 1: Location data collected from SMS messages

Table 2: Location data in Excel Format

No	Latitude	Longitude
1	18.77475	95.22184
2	18.7748	95.22187
3	18.77479	95.22181
4	18.77518	95.22215
5	18.77517	95.22217
6	18.77515	95.22218
7	18.77537	95.22321
8	18.77666	95.22318
9	18.77856	95.2232
10	18.78029	95.22299
11	18.782	95.22282
12	18.78374	95.22226
13	18.78514	95.22205
14	18.77481	95.22179

No	Position
1	Normal
2	Normal
3	Normal
4	Normal
5	Normal
6	Normal
7	Normal
8	Normal
9	Normal
10	Normal
11	Normal
12	Normal
13	Normal
14	Normal

Table 3: Position of Vehicle



Figure 11: GPS Visualizer web page



Figure 12: Location Tracking on Google Maps output



Figure 13: Received SMS message and viewed on Google map



Figure 14: Photo of GPS-GSM Based Location and Position Tracking System

Conclusion

The GSM modem was configured and tested in the tracking system to monitor the vehicle's location via SMS and online on Google map. To display the position on Google map it needs the Google map API. The Arduino is the brain of the system and the GSM modem is controlled by AT commands that enable data transmission over GSM network while the GPS provide the location data. Whenever the GPS receives a new data it is updated in the database and hence tracking of object can be seen on Google map.

Acknowledgements

I would like to thank Professor Dr Soe Soe Nwe, Head of Department of Physics, Pyay University, Professor Dr Naw Htoo Lar Phaw, Pyay University, Dr Aung Aung Min, Rector from Pyay University, for their kind permission to do this work.

We would like to express our deepest gratitude to Rector (YU) Dr Pho Kaung, Professor Dr Khin Khin Win (Head of Department of Physics, YU) and Professor Dr Aye Aye Thant (YU) for their permission to present this research report.

I am also indebted to Dr Ye Chan, Professor of Physics, Universities' Research Center, University of Yangon, for his guidance and thought to complete this research work.

References

Delisle M., (2008) Mastering php My Admin 2.11 for Effective MySQL Management (Packt Publishing)

DuBois, (2013) P., *MySQL* (Addison-Wesley)

- Fleischer P, Nelson A, Sowah R and Bremang A, (2012) Design and Development of GPS/GSM Based Vehicle Tracking and Alert System for Commercial Inter-City Busses, IEEE 4th International Conference on Adaptive Science & Technology (ICAST)
- Gertz E., Di Justo P., (2012)*Environmental Monitoring with Arduino* (Sebastopol, California: O'Reilly Media)

Sklar D., Trachtenberg A., (2003) PHP Cookbook (Sebastopol, California: O'Reilly Media)

https://dev.mysql.com/doc/refman/5.1/en/what-is-mysql.html

http://www.microchip.com/downloads/en/devicedoc/39662a.pdf

http://php.net/manual/en/index.php

CHARACTERIZATION OF PEROVSKITE-TYPE XSnO₃ (WHERE X= Ca, Sr AND Ba) CERAMICS

Zin Bo Htut¹, Phyu Phyu Khaing², Wai Khaing Moe³, Win Kyaw⁴ & Soe Soe Nwe⁵

Abstract

Perovskite-type CalciumTin Oxide (CaSnO₃), Strontium Tin Oxide (SrSnO₃) and Barium Tin Oxide(BaSnO₃) were prepared by solid state reaction method. Analytical reagent (AR) grade CaCO₃, SrCO₃,BaCO₃ and SnO₂ were used as the starting materials with equal molar ratios. The samples were characterized by XRD and SEM.XRD patterns indicated that the samples belong to orthorhombic structure for CaSnO₃ and SrSnO₃ ceramics and cubic for BaSnO₃. The lattice parameters were obtained as a = 5.4982 Å, b = 5.6356 Å and c = 7.8651 Å for CaSnO₃, a = 5.7079 Å, b = 5.7072 Å and c = 8.0708 Å for SrSnO₃ and a = b = c = 4.1114 Å for BaSnO₃ respectively. The crystallite sizes were also obtained as 42.17 nm for CaSnO₃,47.34 nm for SrSnO₃ and 51.75 nm for BaSnO₃ and the obtained crystallite sizes showed that the samples were nanosized ceramic materials. From the SEM micrographs, the grain sizes were obtained as in the range of 0.55 μ m – 0.58 μ m. Electrical conductivities of the samples were investigated in the temperature range of 303 K - 773 K. Electrical conductivity and activation energy of the samples were studied.

Keywords: CaSnO₃, SrSnO₃, BaSnO₃, Perovskite-type, XRD and SEM

Introduction

The double oxides of the general formula ABO_3 (where A =Ca, Sr and Ba) formed between the oxides of alkaline – earth metals and those of some of the group IV elements are great industrial and technological importance. These "A" carbonates are the precursors for this research[Abdul-Majeed Azad, (1997)]. This paper is the synthesis and characterization of Alkaline earth stannates from these carbonates and tin oxides (SnO₂). Most of the alkaline-earth stannates have the perovskite structures and they perform the dielectric characteristics because they have one set of electrical conductivity (having both donor and acceptor ions). This work intends to support the

^{1.} Demonstrator, Department of Physics, Pyay University

² Dr, Assistant Lecturer, Department of Physics, Pyay University

³ Dr, Demonstrator, Department of Physics, Pyay University

⁴ Dr, Associate Professor, Department of Physics, Pyay University

⁵ Dr, Professor& HOD, Department of Physics, Pyay University

finding applications in pure form (intrinsic) such as thermally stable capacitors in electronics because of their attractive dielectric characteristics. Moreover, in doped form, these stannates have also been investigated as potential sensor materials for a host of gases, including CO, HC, H₂, Cl₂, NO₂ and humidity etc. In addition they can be used as the transparent solar cells on the window glasses and buildings because of their transparent properties (e.g. having the smaller optical band gap) [Abdul-Majeed Azad, (1999)]. These stannates were also used to investigate the p-type (advance used in electronics devices including flat panel displays, solar cells) and n-type semiconductor (in pure state) [Cerda, (2001); Khuong, P.Ong, (2015)]. In this work, as the alkaline-earth (AE) carbonates BaCO₃, CaCO₃ and SrCO₃ were selected and mixing each with tin oxide (SnO₂) by dry mix. The whole experimental routine are processed and synthesized by the conventionally much-used solid state reaction technique. Characterization method, XRD was used to analyze the phase identification of the samples. Another characterization technique SEM (Scanning electron microscopy) is used to ascertain the reaction pathways leading to the formation of the target compound, particles size and their distribution and, to systematically follow the development of microstructure in the sintered bodies. Thus, in this paper, details of synthesis, processing and micro structural and electrical evolution of the investigated CaSnO₃, SrSnO₃ and BaSnO₃ samples are presented.

Experimental Details

Preparation of CaSnO₃, SrSnO₃ and BaSnO₃ Ceramics

Firstly, the starting materials of $CaCO_3$, $SrCO_3$, $BaCO_3$ and SnO_2 powders were weighed with molar ratios and mixed in crucible. The mixed powder was grounded by an agate mortar and pastel for 2 h to be homogeneous and fine powder. The fine powder was heated at 1200°C for 3 h to obtain the desired materials. The residual samples(SrSnO_3, BaSnO_3) are prepared by this procedure. Figure 1 shows the flow diagram of the preparation of CaSnO_3sample.

XRD, SEM and Electrical Conductivity Measurements

X-ray diffraction (XRD) is used to investigate structural properties of crystalline materials. Powder XRD patterns of the $CaSnO_3$, $SrSnO_3$ and $BaSnO_3$ samples were observed by RIGAKUMULTIFLEX X-ray Diffractometer.

The microstructural properties of the material have an important role in determining the electrical transport properties. SEM micrographs of CaSnO₃, SrSnO₃andBaSnO₃ were observed by JEOL JSM-5610LV Scanning Electron Microscope (SEM).



Figure 1: Flow diagram of the preparation of CaSnO₃ sample

For the temperature dependent electrical conductivity measurement, the samples were made into pellets by SPECAC hydraulic pellet-maker using 5 ton (~70 MPa). The silver paste was made over the sample to ensure good electrical contacts. The electrical resistances of the samples were observed by FLUKE 45 DUAL DISPLAY MULTIMETER in the temperature range of 303 K – 773 K. CAHO SR-T903 Temperature Controller and K-type thermocouple were used as Temperature Controller and Temperature Sensor. 300 W heater rod was used as the heating element. The electrical conductivity

 σ was evaluated by using $\sigma = \frac{l}{RA}$ where *l* is the distance between two electrodes, *A* is the cross-sectional area of the electrodes and *R* is the resistance. The dimensions of the sample are 1.14×10^{-4} m² in diameter and 3.83×10^{-3} m in thickness. Photograph of the experimental setup of electrical conductivity measurement and schematic diagram are shown in Figure 2 and Figure 3.



Figure 2: Photograph of the experimental setup for the temperature dependent electrical resistance measurement



Figure 3: Schematic diagram of the experimental setup for the temperature dependent electrical resistance measurement

Results and Discussion

XRD Study

Figure 4 shows the powder XRD pattern of the CaSnO₃. It is found that the many sharp peaks appeared in which the most sharp peaks (dominant) is (112) plane at the diffraction angle 32.15°. The observed peaks could be indexed since they are in complete agreement with standard XRD pattern of CaSnO₃ (JCPDS card no.01-074-7233) indicating the formation of crystalline phase pure CaSnO₃. Therefore it can be assumed that the crystallinity of CaSnO₃ crystallizes be obtained. XRD pattern shows that the CaSnO₃ analogous to orthorhombic structure. The calculated lattice parameters are shown in Table 1 and Table 2. Because the lattice parameters 'a' and 'b' have the nearly equal values and 'c' has the higher value but the lattice angle has the 90°. The crystallite size of CaSnO₃ is 42.17 nm.



Figure 4: XRD pattern of CaSnO₃

XRD pattern of the SrSnO₃ is shown in Figure 5. This figure shows that the intended target sample SrSnO₃ is obtained because the sharp peaks are found as the (002), (020), (004), (114), (312) and (224) planes. All the observed peaks could be indexed since they are in complete agreement with reported XRD pattern of SrSnO₃ (JCPDS card no. 01-0704389) indicating the formation of crystalline phase pure SrSnO₃. XRD pattern indicates that the single phase orthorhombic structure. The most dominant peak is the (020) plane at the 2θ value of 31.32°. The lattice parameters are presented in Table 1 and Table 2. The crystallite size is obtained as 47.34 nm and hence it is the nanosized polycrystalline mate.

XRD pattern of $BaSnO_3$ is shown in Figure 6. The observed XRD lines were identified by the standard $BaSnO_3$ (JCPDS card no. 00-015-0780). The appearance of very sharp diffraction peaks further indicates the quite small crystallite size in the powder. It can be seen that the most intense peak is (110) plane at the 30.76°.





The absence of diffraction peaks due either to the starting materials or second phase in the Ba-Sn-O system showed the powder obtained, to be of high quality. According to the XRD pattern, the dominant peaks (especially planes orientation) and the interplaner spacing (d_{hkl}) or lattice spacing, the lattice parameter "a", "b" and "c" can be calculated as shown in Table 1 and it is seen that the all of lattice parameters are in nearly equal to 4.1111 Å. The BaSnO₃sample belongs to cubic structure. The lattice parameters are presented in Table 1.



Figure 6: XRD pattern of BaSnO₃

Name	Maximum peak (hkl)	Lattice constant 'a' (Å)	Unit cell volume 'V' (nm) ³	Crystallite size 'D' (nm)
CaSnO ₃	(112)	5.4982	0.0244	41.7684
SrSnO ₃	(020)	5.7079	0.0263	46.9505
BaSnO ₃	(110)	4.1111	0.0695	49.0361

 Table 1: The lattice parameters and crystallite sizes of perovskite type

 CaSnO₃, SrSnO₃ and BaSnO₃

 Table 2: The lattice parameters of CaSnO₃, SrSnO₃ and BaSnO₃

Name	a (nm)	b (nm)	c (nm)
CaSnO ₃	0.5498	0.5636	0.7865
SrSnO ₃	0.5708	0.5707	0.8071
BaSnO ₃	0.4111		

Microstructural Characteristics of the Samples

From the SEM micrograph of the CaSnO₃ powders heated at 1200° C for 3 h is shown in Figure 7, it is observed that the grain sizes are uniform and homogeneous. The grain size is 0.56μ m and its average crystallite size is 42.1709 nm. So it can be suggested that the crystallite size is about 10 times smaller than that of the grain size. So the grain size is very small.

SEM micrograph of SrSnO₃prepared at 1200°C was shown in Figure 8, where it can be seen clear that the surface morphology is so good because the grain sizes are uniform and homogeneously. The average grain size is 0.60 μ m, so it is very small and the interconnectivity between the grains is very closer and it has some porosity in the sample.

SEM micrograph of BaSnO₃ is shown in Figure 9. It can be seen that sintering at 1200°C for 3 h, the grain size is ranging from the submicron to as large as $\approx (0.6 \ \mu m$, i.e., 6×10^{-7} m). It is observed that all the grains are the uniform and homogeneous grain size and it is estimated by using the line intercept method. In addition, it is the narrowing of grain size distribution and good interconnectivity. Thus it has some porosity in the sample. According

the XRD investigation, the cubic perovskite type $BaSnO_3$ crystallizes has the lattice constant of about 4.1111 Å. Therefore it appears that the grains on average are grown to an extent of about 100 times of the unit cell dimension. The obtained average grain sizes are tabulated in Table 3. Presence of some porosity provides the charged ions to move freely so it may cause the ionic current in the sample. Because of some porosity, these samples can adsorb the humidity or other gases so that it can be used as Humidity of gas sensor by measuring its sensitivity.



Figure 7: SEM micrograph of the CaSnO₃



Figure 8: SEM micrograph of the SrSnO₃



Figure 9: SEM micrograph of the BaSnO₃

Sample	Grain size (µ m)
CaSnO ₃	0.5610
SrSnO ₃	0.5534
BaSnO ₃	0.5874

Table 3: The grain sizes of CaSnO₃, SrSnO₃ and BaSnO₃

Electrical Conductivity Study

Electrical conductivity of a ceramic with temperature obeys an Arrhenius expression $\sigma = \sigma_0 \exp(-E_a/kT)$, where σ is the conductivity, $\sigma \partial is$ the pre-exponential factor, E_a is the activation energy for ionic conduction, k is the Boltzmann constant and T is the absolute temperature. In the present work, Arrhenius plots of the variation of dc electrical conductivity of the CaSnO₃, SrSnO₃ and BaSnO₃ samples in the temperature range 303 K - 773 K are shown in Figures10(a – c). According to the theory of ionic conductivity, the slope of the electrical conductivity in each of the figure, e.g., in Figure10(a) for CaSnO₃ sample, corresponding to the sample. The electrical conductivity σ of the sample can be written in the form:

$$\sigma = \sigma_0 \exp(-E_a / kT)$$
$$\ln(\sigma) = -E_a / kT + \ln \sigma_0$$
$$= (-E_a / k)(1/T) + \ln \sigma_0$$

Comparing the above equation with the experimental linear equation, y=mx+c where the value of slope will give the value of $(-E_a/k)$. From Fig 3(a), the activation energy E_a can be obtained by using the slope of the $\ln(\sigma)$ versus $10^3/T$ graph.

$$E_{a}/k = 5.8981 \times 1000$$

$$E_{a} = 5.8981 \times 1000 \times k$$

$$E_{a} = 5.8981 \times 1000 \times 1.38\text{E-}23$$

$$E_{a} = 8.14 \times 10^{-20} \text{ J}$$

$$E_{a} = 0.5087 \text{ eV}$$

As shown in Figures10(a -c), temperature dependent electrical conductivities of the sample increased with increased in temperature. The activation energies of the samples were evaluated and listed in Table 4.

From the experimental results, the samples exhibited as super ionic conductors at high temperature because their electrical conductivities are found as $\sigma \ge 10^{-3}$ S m⁻¹. In the ln σ – 1000/T graphs, the starting point (temperature) of superionic phase of the samples indicates with the colored circle. It is obvious that the conductivity of the samples increase with increase in temperature so that the samples behave like as semiconductor behavior.



Figure 10: (a) Arrhenius plot of the dc electrical conductivity of the CaSnO₃



Figure 10: (b) Arrhenius plot of the dc electrical conductivity of the SrSnO₃



Figure 10: (c) Arrhenius plot of the dc electrical conductivity of the BaSnO₃

Sample	Slope	E_a (eV)
CaSnO ₃	5.8981	0.5087
SrSnO ₃	6.5342	0.5636
BaSnO ₃	5.9035	0.5092

Table 4: The activation energies of the CaSnO₃, SrSnO₃and BaSnO₃

Conclusion

Perovskite-type CaSnO₃, SrSnO₃ and BaSnO₃ceramics were successfully prepared by solid state reaction method. Structural phase identification of the samples were examined by XRD. The variation of lattice parameters, unit cell volume and crystallite size were investigated. The crystal structure of BaSnO₃ is cubic and that of CaSnO₃ and SrSnO₃ are orthorhombic structure. The smallest value of crystallite size has been found as CaSnO₃ and the smallest grain size has been observed SrSnO₃. The grain size of are found to be nearly equal. From the temperature dependent electrical conductivity investigation, the samples exhibited as the superionic conductors. The activation energies are obtained as less than 1 eV. According to literature, the superionic conductors with the activation energies less than 1 eVcan be applied as the solid oxide fuel cell (SOFC) materials.

Acknowledgement

The authors would like to acknowledge Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her valuable discussions and comments on this work.

References

- Abdul-Majeed Azad, et. al.(1997). Characterization of BaSnO₃ based ceramics Part.1. Synthesis, processing and micro structural development, Department of Physics, University of Putra Malaysia.
- Abdual-Majeed Azad, et. al.(1999). The AC electrical characterization of the solid- state reaction derived CaSnO₃, *Journal of Materials Science*, 34, pp. 3375-3396.
- Cerda, J.et. al.(2001). Synthesis of perovskite-type BaSnO₃ particles obtained by a new simple wet chemical route based on a sol-gel process, Department of Electronica, University of Barcelona.
- Khuong, P.Ong, et. al.(2015) Transparent Conducting properties of SrSnO₃ and ZnSnO₃, AIP Publishing.

SYNTHESIS AND CHARACTERIZATION OF MAGNESIUM-ZINC FERRITE PREPARED BY FLASH-COMBUSTION TECHNIQUE

Wai Khaing Moe¹, Phyu Phyu Khaing², Zin Bo Htut³,

Win Kyaw⁴ & Soe Soe Nwe⁵

Abstract

Magnesium-Zinc Ferrite, $Mg_{1-x}Zn_xFe_2O_4$ (where x=0.50) was prepared by flash-combustion technique. The sample was characterized by XRD, SEM and FTIR-spectroscopy to study the structural, microstructural and vibrational characteristics. XRD pattern revealed that the sample analogous to cubic structure with the lattice parameters a=b=c=8.3512 Å. The crystallite size was obtained as 47.96 nm and showed that the sample was the nanosized material. SEM micrograph showed that the grain shape of the sample was spherical with the grain sizes of 0.20 µm – 0.50µm. Vibrational characteristics of tetrahedral site and octahedral site atoms were studied from the collected FTIR spectrum. Temperature dependent electrical conductivity and humidity sensitive electrical properties of the sample were observed for the applications of humidity sensing materials.

Keywords: Magnesium-Zinc Ferrite, Flash-Combustion, XRD, SEM, FTIR, humidity sensing materials

Introduction

Ferrites are still of interest as promising materials for many applications. For these reasons engineers and scientists are keenly interested in determining their characterization [Bhattacharjee, (2011)]. Since ferrites behave as low gap semiconductors and as insulators at low temperature, they have been used in number of technological applications [Gadkari, (2013)]. These applications include sensors, transformer core, microwave devices, magnetic and magneto-optic recording, data storage etc. [Maria1, (2013)].

Ferrite particles in nano scales can be produced by a large number of methods. These include soft chemical methods such as flash combustion

^{1.} Dr, Demonstrator, Department of Physics, Pyay University

² Dr, Assistant Lecturer, Department of Physics, Pyay University

³ Demonstrator, Department of Physics, Pyay University

⁴ Dr, Associate Professor, Department of Physics, Pyay University

⁵ Dr, Professor& HOD, Department of Physics, Pyay University

technique, co-precipitation method, sol gel synthesis, hydrothermal synthesis and mechano-synthesis approach of ball milling [Brito, (2010)] etc. Ferrites belong to a special class of magnetic material consisting of metal oxide xand ferric oxide as their main compositions [Vagolu, (2013)]. The novel magnetic, electric and dielectric properties possessed by them have made ferrites more attractive to the current field of science and technology [Khot, (2011)]. These properties are largely dependent on chemical composition, method of synthesis, synthesis conditions, grain size and surface morphology.

This work preferred the Mg based ferrite from the two following reasons: (i) it is a slight porous ceramic and (ii) the stability of Mg^{2+} ions avoid the appearance of Fe²⁺ ions (essential require to obtain high resistivity). In the present work, Magnesium-Zinc ferrite, $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50) was prepared by flash-combustion technique and their structural, microstructural and vibrational characteristics were studied by using XRD, SEM and FTIR methods. Temperature dependent electrical properties were also investigated. Furthermore, humidity sensitive electrical resistances, dc voltages and capacitances were investigated in the relative humidity range of 36 RH% – 98 RH%.

Materials and Method

Preparation of Magnesium-Zinc Ferrite

In the present work, the cubic form of $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50) was prepared by flash-combustion technique. The raw materials used in this preparation were Magnesium Nitrate Hexahydrate [Mg(NO₃)₂.6H₂O], Zinc Nitrate Hexahydrate [Zn(NO₃)₂.6H₂O] and Ferric Nitrate Nonahydrate [Fe(NO₃)₂.9H₂O]. Urea [CO(NH₂)₂] was used as the fuel. De-ionized (DI) water was used as the solvent. According to the desired stoichiometric proportion, the pure nitrate solutions were weighed and mixed. Urea was added to the mixture (as fuel). The mixture was heated at 100°C. The mixture reacted leading to combustion and the reaction was complete in 30 min. A foamy and highly porous precursor mass was obtained. The ferrite precursor was dried at room temperature for 24 h and the dried powder was heated at 900°C for 4 h for ferrite crystalline formation. The heat treatment of the precursor solution was performed in vacuum chamber (160 mmHg) by using

DELTA A Series Temperature Controller DTA4896. The K-type thermocouple was used as the temperature sensor to read-out the real temperature of the sample in the chamber. The desired as-prepared Mg-Zn mixed ferrite, $Mg_{0.5}Zn_{0.5}Fe_2O_4$ was obtained. Flow diagram of the sample preparation procedure is shown in Figure 1. Photographs of the starting materials, solutions of starting materials, precursor solutions, DELTA A Series Temperature Controller DTA4896 and experimental setup of sample preparation system are shown in Figures 2(a – f).



Mg_{0.5}Zn_{0.5}Fe₂O₄ ferrite


Figure 2: Photographs of the (a) weighed starting materials and DI water,(b) mixed solution, (c) foamy and highly porous precursor, (d) dried ferrite precursor, (e) DELTA A Series DTA4896 temperature controller and (f) experimental setup of sample preparation system

XRD, SEM and FTIR Measurements

Powder XRD pattern of the sample was investigated by RIGAKU MULTIFLEX X-Ray Powder Diffractometer. The X-ray diffractometry is mainly used for the identification and qualification of compounds by their diffraction patterns. SEM micrograph of the sample were observed by using JEOL JSM-5610LV SEM with the accelerating voltage of 15 kV, the beam current of 50 mA and 5500 times of photo magnification. FTIR transmission spectrum of the sample was recorded on PC-controlled SHIMADZU FTIR-8400 Spectrophotometer with Potassium Bromide, KBr, pellet method.

Temperature Dependent Electrical Resistance and Humidity Sensitive Electrical Properties Measurements

The sample was made into pellet by SPECAC hydraulic pellet-maker using 5 ton (~70 MPa). The silver paste was made over the sample to ensure good electrical contacts. The electrical resistance and capacitance of the sample were observed by FLUKE 45 DUAL DISPLAY MULTIMETER and FUKE DM6013A CAPACITANCE METER in the temperature range of 299 K - 773 K. CAHO SR-T903 Temperature Controller and K-type thermocouple were used as Temperature Controller and Temperature Sensor. 300 W heater rod was used as the heating element. The electrical conductivity

 σ and dielectric constant ε_r of the sample were evaluated by using $\sigma = \frac{l}{RA}$

and $\varepsilon_r = \frac{Cl}{\varepsilon_0 A}$ where *l* is the distance between two electrodes, *A* is the cross-

sectional area of the electrodes, *R* is the resistance, *C* is the capacitance, and ε_0 is the permittivity of free space (8.8541 × 10⁻¹² F m⁻¹).Photograph of the experimental setup of electrical conductivity measurement is shown in Figure 3. The dimensions of the sample are 1.14×10^{-4} m² in diameter and 3.83×10^{-3} m in thickness.



Figure 3: Photograph of the experimental setup for the temperature dependent resistance and capacitance measurement

Humidity-sensitive electrical properties of the sample were investigated in the increasing and decreasing relative humidity ranges 36 RH% - 98 RH% and 98 - 36 RH% for the application of humidity sensor. Area and thickness of the pellet were $1.14 \times 10^{-4} \text{ m}^2$ and $2.37 \times 10^{-3} \text{ m}$. Electrical resistance, dc voltage and capacitance of the sample were observed. In this measurement, Oktimer TDK0302LA Humidity Meter was used as the humidity sensing element. UNI-T UT802 digital multimeter was used as the digital resistance meter, voltmeter and capacitance meter. The refrigerator (TOSHIBA) was used as the humidity sensitive electrical property measurement are shown in Figure 4.



Figure 4: Photograph of the experimental setup of humidity sensitive electrical properties measurement

Results and Discussion

XRD Study

XRD pattern of Magnesium-Zinc ferrite, $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50) is shown in Figure 5. The observed XRD lines were identified by using standard JCPDS data library files of (i) Cat. No. 88-1936> Magnesioferrite, syn – MgFe_2O_4 and (ii) Cat. No. 73-1963 > ZnFe_2O_4 – Zinc Iron Oxide. The observed XRD data of diffraction angle (°), atomic spacing (Å), miller indices (hkl), Full Width at Half Maximum (°)and peak height (%) of the sample are tabulated in Table 1. The appearance of the diffraction lines in the observed XRD patterns shows that the investigated sample is a single phase Magnesium-Zinc ferrite, $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50) with spinel structure.

The diffraction line at 35.68° or (311) plane indicated that the crystallites were preferentially



Figure 5: XRD pattern of $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50)

oriented along (311) plane. The lattice parameters are evaluated by using crystal utility of the equation of $\frac{\sin^2 \theta}{(h^2 + k^2 + l^2)} = \frac{\lambda^2}{4a^2}$ where θ is the diffraction

angle (°), (hkl) is the miller indices, λ is the wavelength of incident X-ray (Å) and *a* is the lattice parameter of the samples (Å). The obtained lattice parameters and the unit cell volume of the sample are obtained as a = b = c = 8.3512 Å and 582.43 (Å)³ respectively. Khot, S. S.et. al. (2011) has reported that the lattice parameters of the Mg_{0.5}Zn_{0.5}Fe₂O₄ferrite prepared by coprecipitation method are 8.3560Å. Thus, the obtained lattice parameters in the present study are found to be agreed with the results of Khot, S. S.et.al..

The broad peaks in the XRD patterns indicate a fine particle nature of the materials. In the present work, the particle size of Mg-Zn ferrite sample was calculated by using Scherrer's formula: $D = \frac{0.9\lambda}{B\cos\theta}$, where *D* is the crystallite size(nm), λ is the wavelength (Å), θ is the diffraction angle of the peak under consideration at FWHM (°) and B is the observed FWHM (radians). The crystallite size of the sample is obtained as 47.96 nm by using

the strongest diffraction line of (311) plane. The result shows that the sample is ananosized material.

Line No	2θ (°)	(hkl)	d(Å)	FWHM (°)	Height (%)
1#	30.19	(220)	2.96	0.187	8.50
2^*	30.36	(220)	2.94	0.156	36.60
3*	35.68	(311)	2.51	0.174	100.00
4*	37.27	(222)	2.41	0.213	6.50
5#	43.27	(400)	2.09	0.136	26.80
6*	53.58	(422)	1.71	0.176	11.80
7^*	57.06	(511)	1.61	0.164	43.10
8^*	62.62	(440)	1.48	0.191	42.50

Table 4.1: XRD data of Mg_{0.5}Zn_{0.5}Fe₂O₄ ferrite

#ZnFe₂O₄, *MgFe₂O₄

SEM Investigation

Figure 6 shows the SEM micrograph of as-prepared sample. As shown in figure, the grain shape sample is spherical and the sizes are obtained in the range of 0.20 μ m – 0.50 μ m. Also, the image shows that the Mg_{0.5}Zn_{0.5}Fe₂O₄ sample composed of agglomerated particles with poor grain boundary.



Figure 6: SEM micrograph of $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50)

FTIR Analysis

The vibrational wavenumbers of pure MgFe₂O₄ are mainly 565 cm⁻¹ and 581 cm⁻¹ for A atoms on tetrahedral sites (v_1 -mode) and 406 cm⁻¹ and 433 cm⁻¹ for B atoms on octahedral sites (v_2 -mode). Also, vibrational frequencies of pure Zinc Ferrite, ZnFe₂O₄, are mainly 550 cm⁻¹ and 555 cm⁻¹ for A atoms on tetrahedral sites (v_1 -mode) and 415 cm⁻¹ for B atoms on octahedral sites (v_2 -mode).

FTIR transmission spectrum of the sample is shown in Figure 7. As shown in observed FTIR spectrum, four absorption lines are mainly observed and these lines are represented by the vibrational characteristics of as-prepared $Mg_{0.5}Zn_{0.5}Fe_2O_4$. The lines at the wavenumber 417 cm⁻¹ and 448 cm⁻¹ indicate the B atoms on octahedral sites and assigned as v₂-mode. The lines at 556 cm⁻¹ and 586 cm⁻¹ represent the vibrational characteristic of A atoms on tetrahedral sites and assigned as v₁-mode. The appearances of the collected lines represent the vibrational characteristics of as-prepared Mg_{0.5}Zn_{0.5}Fe₂O₄ material in which others lines, e.g., starting materials and solvent, not appeared.



Figure 7: FTIR transmission spectrum of $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50)

Temperature Dependent Electrical Properties Study

Electrical properties of ferrites such as resistivity and conductivity generally depend upon the composition and preparation parameters of the synthesized materials. The electrical conductivity of a ferrite obeys an Arrhenius expression: $\sigma = \sigma_0 \exp(-E_a/kT)$, where σ is the conductivity, σ_0 is the pre-exponential factor, E_a is the activation energy for ionic conduction, k is the Boltzmann constant and T is the absolute temperature. The temperature dependence of d.c. electrical conductivity in the temperature range of 299 K – 773 K is shown in Figure 8. It is observed that the electrical conductivity of the sample increases with increase in temperature. The slope of the graph is fitted by linear regression method due to the analytical solving of Arrhenius expression and obtained as -4.4241. Then, the activation energy of the sample is evaluated as,

$$\frac{-E_a}{k} = -4.4241 \times 1000$$
$$E_a = 4.4241 \times 1000 \times 1.3806 \times 10^{-23}$$
$$E_a = 0.3818 \text{ eV}$$

The d.c. electrical conductivities are obtained as in the range of 3.8894×10^{-8} Sm⁻¹(at 299 K) – 6.5607×10^{-4} S m⁻¹(at 773 K). It shows that the sample is a normal ionic conductor.

Plot of the variation of dielectric constant as a function of temperature of the sample in the temperature range 299 K - 773 K is shown in Figure 9. From the plot, dielectric constant increased with increase in temperature.



Figure 8: Temperature dependence of d.c. electrical conductivity of $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50)





Humidity Sensitive Electrical Properties Investigation

The electrical resistance, dc voltage and capacitance of the Magnesium-Zinc ferrite, $Mg_{0.5}Zn_{0.5}Fe_2O_4$, sample under investigation were measured in the relative humidity ranges of 36 RH% – 98 RH% and 98 RH% – 36 RH% with the step of 1 RH%. Variations of the humidity sensitive resistance, R_H, with relative humidity RH%, dc voltage, V_H, with relative humidity RH%, and capacitance, C_H, with relative humidity RH% of the

sample are shown in Figures10(a – c) for the increasing humidity range of 36 RH% – 98 RH% and Figures 11(a - c) for the decreasing humidity range of 98 RH% – 36 RH%.

As shown in Figure 10(a) and Figure 11(a), the $R_Hvs RH\%$ curves were fitted by linear type. The slopes of the sample were obtained as 0.092 M Ω /RH% in36 RH%– 98 RH% and 0.0483 M Ω /RH% in 98 RH% – 36 RH% respectively. On inspection of figure, it was found that the resistance of the sample decreases with increase in humidity, as seen from slope of curve in Figure 10(a). Since, the sample can allow water molecules to pass through easily to reach the sensing surface, and can hold back condensation water from condensing directly on the surface of the sensing surface.

As presented in Figure 10(b) and Figure 11(b) of $V_H - RH\%$ graphs, under whole humidity ranges (36 RH% – 98 RH% and 98 RH% – 36 RH%), water adsorption on sample surface is likely the dominant factor for electrical conduction. Thus, the surface area would provide more sites for water adsorption and produce more charge carriers for electrical conduction.

As shown in Figure 10(c) and Figure 11(c), the capacitance of the sample increases with increase in RH, it changes a little in about 40 RH% – 85 RH%, and changes greatly at high RH (85 RH% – 98 RH%). In 40 RH% – 85 RH% conditions, the resistance of the sample slightly decreased, but in high RH conditions it is greatly increased. It can be said that, as an electrolyte, the water molecule is not only physically absorbed in the active group of the copolymer, but also can be polarized. The effect can generate space charge and dipoles, and then accumulate and degenerate between electrodes. The result is the increase of capacitance with increasing RH. The sensitivity factor S_f of the sample was evaluated by using the equation and obtained as S_f = R₃₆ RH% / R_{98 RH%} = 1.72.



Figure10: Plots of the variations of (a) resistance R_{H} ,(b) dc voltage V_{H} and (c) capacitance C_{H} with relative humidity RH% of $Mg_{1-x}Zn_{x}Fe_{2}O_{4}$ (where x = 0.50)in increasing humidity range of 36 RH% – 98 RH%





Figure11: Plots of the variations of (a) resistance R_H , (b) dc voltage V_H and (c) capacitance C_H with relative humidity RH% of $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50)in decreasing humidity range of 98RH% – 36 RH%

Conclusion

Nanosized Magnesium-Zinc ferrite, $Mg_{1-x}Zn_xFe_2O_4$ (where x = 0.50) was successfully prepared by flash-combustion technique. XRD pattern indicates that the sample is single phase cubic spinel structure with the lattice parameters a = b = c = 8.3512 Å. The crystallite size of the sample is obtained as 47.96 nm. From the SEM micrograph, the grain shape is spherical and the sizes are obtained as in the range of 0.20 μ m – 0.50 μ m. From the FTIR spectrum, the bands observed in the wavenumber ranges of $420 \text{ cm}^{-1} - 480 \text{ cm}^{-1}$ and 520 cm⁻¹ – 590 cm⁻¹ correspond to octahedral and tetrahedral sites molecules. The electrical conductivity and dielectric constant of the sample increase with increase in temperature. The sample exhibits the normal ionic conductor with the activation energy 0.3818 eV. Humidity sensitive electrical resistance decrease with increase in humidity and the dc voltage and capacitance increase with increase in humidity. The sensitivity factor S_f of the sample was obtained as 1.72. According to experimental results, the sample can be used as humidity sensing materials due to its sensitivity and sensitivity factor are comparable with the ferrite humidity sensor.

Acknowledgement

The authors would like to acknowledge Professor Dr Khin Khin Win, Head Department of Physics, University of Yangon, for her valuable discussions and comments on this work.

References

- Bhattacharjee, K., Ghosh, C.K., MITRA, M.K. & DAS, G.C. (2011). Novel synthesis of Ni_xZn_{1-x}Fe₂O₄(0 ≤ x `1) nanoparticles and their dielectric properties. *Journal of Nanoparticles Research*, 13, pp. 739–750.
- Brito, V.L.O. (2010). EVALUATION OF A Ni-Zn FERRITE FOR USE IN TEMPERATURE SENSORS. Progress in Electromagnetic Research Letters, 13, pp. 103–112.
- Gadkari, A.B., Shinde, T.J. & Vasambekar, P.N. (2013) Liquid petroleum gas sensor based on nanocrystallite Mg_{0.6}Cd_{0.4}Fe₂O₄. *Advanced Materials Letters*, 4(7), pp. 573–576.
- Maria1, K.H., Choudhury, S. & Hakim, M.A. (2013) Structural phase transformation and hysteresis behavior of Cu-Zn ferrites. Khot, S. S. &Watawe, S. C. (2011). EFFECT OF TEMPERATURE OF SYNTHESIS ON X-RAY, IRPROPERTIES OF MG-ZN FERRITES PREPARED BY OXALATECO-PRECIPITATION METHOD. International Journal of Advances in Engineering & Technology, 1(4), pp. 422 – 429.

International Nano Letters, 3, pp. 1–10.

Vagolu, V.K. &Samatha, K. (2013) Studies on Structural and Electrical Properties of Cobalt Substituted Nickel-Zinc Ferrites Prepared from Soft Chemical Method. International Journal of Innovative Research and Studies, 2(8), pp. 99–113.

PHANTOM SCALAR FIELDS AND ITS PHYSICAL IMPLICATIONS

Tin Tin Htay¹, Thant Zin Naing²

Abstract

Equations of state are utilized to explore the possible constrains on dark energy models and their relevant physical quantities such as density parameter, pressure and etc., are investigated. As the situation dictates, physical interpretation and visualizations of the results obtained are performed.

Keywords: phantom scalar field , big rip, anti-big rip, general relativity

Introduction

Cosmological models have developed with complex potentials and have shown that they are rather convenient for the description of the so called phantom cosmology, including such an enigmatic phenomenon. Phantom energy is a hypothetical form of dark energy satisfying the equation of state with $\omega < -1$. It possesses negative kinetic energy, and predicts expansion of the universe in excess of that predicted by a cosmological constant, which leads to a Big Rip. To obtain $\omega < -1$, phantom field with a negative kinetic term may be a simplest implementing and can be regarded as one of interesting possibilities describing dark energy.

All these models of scalar fields lead to the equation of state parameter ω greater than or equal to minus one. It is therefore important to look for theoretical possibilities to describe dark energy with $\omega < -1$ called phantom energy. Phantom thermodynamic leads to a negative entropy (or negative temperature) and the energy density increases to infinity in a finite time, at which point the size of the Universe blows up in a finite time. This is known as the Big Rip. As mentioned above the equation of state parameter with super negative values leads to Big Rip which can be avoided in a particular class of models. Phantom states are unphysical states since they have they have a negative kinetic energy and therefore these states roll up the potential. This process will go on to infinity, unless the state reaches a maximum of its

^{1.} Lecturer, Department of Physics, University of West Yangon.

^{2.} Retired Pro-rector (Admin), International Theravada Buddhist Missionary University, Yangon.

potential. If the phantom potential has no maximum, the phantom energy is rolling up to infinity which leads to a curvature of the universe growing to infinity in a finite time. The phantom fluid will rip everything apart. The phantom energy becomes the dominant force that will overrule all known fundamental forces. This scenario is called the Big Rip. This Big Rip singularity can be avoided if the potential has a maximum.

The physical properties of phantom energy are rather weird as they include violation of the dominant energy condition and increasing energy density with the universe expands in a super accelerated fashion, so as the big rip and the possibility for a big trip. The energy density of phantom energy increases with time. The phantom energy density becomes infinite in finite time, which will rip apart the universe. By assuming a particular relation between the time derivative of the phantom field and the Hubble function, an exact solution of the model is constructed. The scale factor 'a' and the Hubble parameter 'H' reach infinity in finite time and the universe ends in an explosive 'big rip', a final singularity in which the universe is destroyed in a finite proper time by excessive expansion. Comparing such model with the current cosmological observations shows that its predictions are consistent with all astrophysical observations.

The exact solution for a phantom scalar field with an exponential potential

The dynamics of the cosmological evolution is characterized by the Hubble variable

$$h = \frac{\dot{a}}{a}$$

Where *a* is the cosmological radius of the universe.

Using the exponential scalar potential energy density:

$$V(\phi) = V_0 e^{\lambda \phi}$$

The parameter λ will ultimately determine the resulting cosmology of the system. It will determine whether or not the system is acceleration and what species will be dominant at a particular time.

Power law is designed to self- consistently solve for the evolution of scalar fields and the scale factor in an expanding universe. In some cases, however, it may wish to solve for the behavior of a set of fields in a universe dominated by other forms of energy, e.g. pure matter or radiation. Exact solution of the field equations are obtained by the assumption of power-law form of the scale factor.

In standard cosmology, these results, when combined with the latest CMB data and clustering estimates, are used to make out a case for a universe in which accelerated expansion is fueled by a self-interacting, unclustered fluid, with high negative pressure, collectively known as dark energy, the simplest and the most favoured candidate being the cosmological constant Λ . Such a discrepancy between theoretical expectations and empirical observations constitute a fundamental problem at interface of astrophysics, cosmology and particle physics.

Also using a power law for the scale factor a, as well as the following ansatz for the scalar field:

$$a = a_0 t^k$$

Suppose that the scalar field has a time dependence,

$$\phi(t) = \phi_0 \ln(t) + \phi_1$$

The Hubble parameter can be written, thus

$$H = \frac{\dot{a}}{a} = \frac{k}{t}$$

Also, rewriting the scalar potential:

$$V = V_0 t^{\lambda \phi_0} e^{\lambda \phi_1}$$

Thus, computing the elements of the Klein-Gordon equations:

$$\dot{\phi} = \frac{\phi_0}{t}$$
$$\ddot{\phi} = -\frac{\phi_0}{t^2}$$

Klein-Gordon equation acquires the form,

$$\ddot{\phi} + 3\frac{\dot{a}}{a}\dot{\phi} + \lambda V_0 e^{\lambda\phi} = 0$$

$$-\frac{\phi_0}{t^2} = -3\left(\frac{k}{t}\right)\frac{\phi_0}{t} - V_0\lambda t^{\lambda\phi_0} e^{\lambda\phi_1}$$
(1)

But, $\phi_0 = -\frac{2}{\lambda}$

$$-\frac{2}{\lambda}\frac{(3k-1)}{t^2} + \frac{\lambda V_0 e^{\lambda \phi_1}}{t^{-\lambda(-\frac{2}{\lambda})}} = 0$$
$$\frac{6k}{\lambda^2} = -\frac{2}{\lambda^2} + V_0 e^{\lambda \phi_1}$$
(2)

Considering the phantom scalar field with a negative kinetic term, we shall have the following Friedmann equation,

$$\frac{\dot{a}^2}{a^2} = -\frac{\dot{\phi}^2}{2} + V_0 e^{\lambda\phi} \tag{3}$$

The Friedmann equation gives now

$$\frac{\dot{a}^{2}}{a^{2}} = -\frac{\dot{\phi}^{2}}{2} + V_{0}e^{\lambda\phi}$$

$$\left(\frac{k}{t}\right)^{2} = -\frac{\phi_{0}^{2}}{2t^{2}} + V_{0}t^{\lambda\phi_{0}}e^{\lambda\phi_{1}}$$

$$k^{2} = -\frac{2}{\lambda^{2}} + V_{0}e^{\lambda\phi_{1}}$$
(4)

Combining eqn (2) and eqn (4),

$$k^{2} = \frac{6k}{\lambda^{2}}$$

$$|\lambda| < 3\sqrt{2}$$
(5)

Thus, to solve the equation, we can have $k = \frac{1}{3}$, which is the law of expansion of the universe filled with stiff matter or massless scalar field, which in turn, means that $V_0 = 0$.

Substituting eqn. (5) into the relation eqn. (4),



Figure 1: Variation of scalar field ϕ_1 with λ

The particular exact solution for the phantom case

We shall look for the solution of the phantom scalar field, which depends logarithmically on the cosmic time t, while the scale factor undergoes a power-law expansion (or contraction).

The explicit form of the exact particular solution,

$$\phi(t) = \phi_0 \ln t + \phi_1$$

If we would like to consider an expanding universe, then the solution will be,

$$\phi(t) = -\frac{2}{\lambda} \ln(-t) + \frac{1}{\lambda} ln \left[\frac{2(18+\lambda^2)}{\lambda^4 V_0} \right]$$
(7)

where t is running from $-\infty$ to 0. The Hubble parameter is now

$$h(t) = \frac{\dot{a}}{a} = \frac{k}{-t}$$
$$= -\frac{6}{\lambda^2 t}$$
(8)

Thus, the formulae (7) and (8) describe a cosmological evolution which begins at $t = -\infty$ and ends at t = 0, encountering a Big Rip singularity. However, another particular solution describes a cosmological evolution which begins at t = 0 and ends at $t = \infty$, phantom field leads the universe to accelerate its expansion.



Figure 2: 3D variation of $\phi(t)$ with the time t and λ



Figure 3: Contour profile of scalar field $\phi(t)$

The general exact solution for the phantom case

We shall introduce the now variables v and u, such that

$$a^3 = e^{\nu + u} \tag{9}$$

$$\phi = A(v - u) \tag{10}$$

$$A = \frac{\sqrt{2}}{3} \tag{11}$$

where *A* is a coefficient to be defined.

The Friedmann equation is

$$\frac{\dot{a}^2}{a^2} = -\frac{\dot{\phi}^2}{2} + V_0 e^{\lambda\phi}$$

However, because of the negative sign of the kinetic term in the right-hand side of the Friedmann equation,

$$a^{2} = (e^{\nu+u})^{\frac{2}{3}}, \quad \dot{a}^{2} = \frac{1}{9}(\dot{\nu}+\dot{u})^{2}(e^{\nu+u})^{2/3}, \ \dot{\phi}^{2} = A^{2}(\dot{\nu}-\dot{u})^{2}$$

(12)

We get, $\dot{u}^2 + \dot{v}^2 = \frac{9}{2} V_0 e^{\lambda \phi}$

It is convenient now to introduce a complex variable

$$z \equiv \frac{1}{\sqrt{2}}(v + iu), \, \bar{z} \equiv \frac{1}{\sqrt{2}}(v - iu)$$
(13)

Now eqn. (12) looks like,
$$\dot{z} = \frac{9}{4} V_0 e^{\lambda \phi}$$
 (14)

where "bar" stands for the complex conjugation.

However,
$$z' \equiv \frac{1}{\sqrt{2}}(v' + iv')$$
, $\bar{z}' \equiv \frac{1}{\sqrt{2}}(v' - iu')$
We obtain, $z'\bar{z}' = 1$ (15)

Rewriting the Klein-Gordon equation,

$$\ddot{\phi} + 3\frac{\dot{a}}{a}\dot{\phi} - \lambda V_0 e^{\lambda\phi} = 0$$

and taking into account the above relation (15) we come to

$$z'' + \frac{\sqrt{2}(1-i)}{2} \left[{z'}^2 \left(1 + \frac{\sqrt{2}\lambda i}{6} \right) - i - \frac{\sqrt{2}\lambda}{6} \right] = 0$$
(16)

Introducing the function f such that

$$z' \equiv \frac{1}{\alpha} \frac{f'}{f} \tag{17}$$

where,

$$\alpha = \frac{\sqrt{2}(1-i)}{2} \left(1 + \frac{\sqrt{2}\lambda i}{6}\right)$$
(18)

From eqn.(16),

$$z'' + \left(1 + \frac{\sqrt{2}\lambda}{6}\right)z'^2 + \left(\frac{\sqrt{2}\lambda}{6} - 1\right) = 0$$

Introducing a new variable, x = z'

Now, the Klein-Gordon equation is

$$x' + \left(1 + \frac{\sqrt{2\lambda}}{6}\right)x^2 + \left(\frac{\sqrt{2\lambda}}{6} - 1\right) = 0$$

$$x = \frac{1}{\left(1 + \frac{\sqrt{2\lambda}}{6}\right)}\frac{f'}{f}$$
(19)

Where,

$$\chi' = \frac{1}{(1+\frac{\sqrt{2}\lambda}{6})} \left[\frac{ff''-f'^2}{f^2} \right]$$

Differentiating with respect to time and the value of x and x', eqn.(19) yields

$$f^{\prime\prime} - \left(1 + \frac{\lambda^2}{18}\right)f = 0$$

The auxiliary function f satisfies the following equation,

$$f'' - \bar{\kappa}^2 f = 0 \tag{20}$$
$$\bar{k} \equiv \sqrt{1 + \frac{\lambda^2}{18}}$$

where,

The general solution of eqn. (20) is

$$f'' = \left(1 + \frac{\lambda^2}{18}\right) f$$

$$f'' = \left(1 + \frac{\lambda^2}{18}\right) f$$
(21)

We have defined $f = Fe^{\overline{\kappa}\tau} + Ge^{-\overline{\kappa}\tau}$ (21)

(See Appendix)

Using eqn.(17),
$$z' = \frac{1}{(1+\frac{\sqrt{2}\lambda}{6})} \frac{f'}{f}$$
$$\int dz = \frac{1}{(1+\frac{\sqrt{2}\lambda}{6})} \int \frac{df}{f}$$
$$z = \frac{1}{(1+\frac{\sqrt{2}\lambda}{6})} lnf + z_0$$
$$z = \frac{1}{(1+\frac{\sqrt{2}\lambda}{6})} ln(Fe^{\overline{\kappa}\tau} + Ge^{-\overline{\kappa}\tau}) + z_0$$
(22)

Using the relation eqn.(22) we can analogously find

$$\bar{z} = \frac{1}{(1 - \frac{\sqrt{2\lambda}}{6})} \ln(F e^{\bar{\kappa}\tau} - G e^{-\bar{\kappa}\tau}) + \bar{z}_0$$
(23)

$$\phi = A(z - \bar{z}), \ A = \frac{\sqrt{2}}{3}$$

Substituting eqn.(22) and eqn.(23),

$$\begin{split} \phi(\tau) &= \frac{\sqrt{2}}{3} \Biggl[\frac{1}{(1 + \frac{\sqrt{2}\lambda}{6})} \ln(Fe^{\bar{\kappa}\tau} + Ge^{-\bar{\kappa}\tau}) + z_0 - \frac{1}{(1 - \frac{\sqrt{2}\lambda}{6})} \ln(Fe^{\bar{\kappa}\tau} - Ge^{-\bar{\kappa}\tau}) + \bar{z}_0 \Biggr] \\ \phi(\tau) &= \frac{\sqrt{2}}{3} \Biggl[(z_0 + \bar{z}_0) + \frac{1}{(1 + \frac{\sqrt{2}\lambda}{6})} \ln(Fe^{\bar{\kappa}\tau} + Ge^{-\bar{\kappa}\tau}) - \frac{1}{(1 - \frac{\sqrt{2}\lambda}{6})} \ln(Fe^{\bar{\kappa}\tau} - Ge^{-\bar{\kappa}\tau}) \Biggr] \end{split}$$



Figure 4: The spherical plot profile of field function *z*



Figure 5: The spherical plot profile of field function \bar{z}

First, the case G = 0, $F \neq 0$ gives the first particular exact solution (eqn. 7) as it should be and in complete analogy with the hyperbolic case. We get,

$$\frac{\sqrt{2}}{3}(z_0 - \bar{z}_0) = -\frac{2\lambda}{9\bar{\kappa}^2} \ln|f|$$

The case F = 0, while $G \neq 0$ gives the second particular exact solution, describing an infinite contraction of the universe, which begins at the anti-Big Rip singularity.

Now, we consider the case when both the constants F and G are different from zero.We can choose one of these constants, say F = 1 while G = i.

$$\begin{split} \phi(\tau) &= -\frac{\sqrt{2}}{3}(z_0 - \bar{z}_0) + \frac{2\sqrt{2}}{6 + \sqrt{2}\lambda}\ln(1 + ie^{-2\bar{\kappa}\tau}) - \frac{2\sqrt{2}}{6 - \sqrt{2}\lambda}\ln(1 - ie^{-2\bar{\kappa}\tau}) \\ \phi(\tau) &= \frac{2\lambda}{9\bar{\kappa}^2}\ln|f| + \ln(1 + ie^{-2\bar{\kappa}\tau})\frac{36\sqrt{2}}{3(18 - \lambda^2)} + const \\ &= \frac{2\lambda}{9\bar{\kappa}^2}\ln|f| - \ln(1 + ie^{-2\bar{\kappa}\tau})\frac{2\sqrt{2}}{3\bar{\kappa}^2} + const \end{split}$$

Now, we can find the expression for the scalar field

$$\phi(\tau) = \frac{2\lambda}{9\bar{\kappa}^2} \ln|f| - \frac{2\sqrt{2}}{3\bar{\kappa}^2} \arg f + const$$
(24)

When $\tau \to -\infty$ the field $\phi \to +\infty$, while when $\tau \to +\infty$ the field $\phi \to +\infty$ again. Thus, the beginning and the end of the cosmological evolution are characterized by a positive infinite value of the scalar field and, hence by the positive infinite value of the potential *V*.

The complete cosmological evolution involves a finite period of the cosmic time t. This solution beginning from "anti-Big Rip" singularity and ending in the Big Rip singularity, passing through the point of minimal contraction was not considered in this paper devoted to the study of phantom solutions with exponential potentials.

In figure (7) we represent two particular exact solution and a typical example of general solution for the phantom case.



Figure 6: 3D variation of ϕ (τ) with f and λ



Figure 7: The phase space diagram $\dot{\phi}$, π , where π stays for the velocity $\pi = \dot{\phi}$. Two straight line trajectories describe two particular solutions, corresponding to the expanding and contracting universe. The curve line represents a trajectory, belonging to the family of those evolving from the anti-Big Rip singularity to the Big Rip singularity, passing through the point of minimal contraction of the universe.

Results and Concluding Remarks

Attempts have been made to describe the general cosmological solution with an exponential in contrast to the "old" particular solution for a phantom scalar field and construct the general solution for piecewise exponential potential with cusps. One can say that these finite time evolutions represent the phantom counterpart of the well-known cosmological evolutions, which begin in the Big Bang singularity reach the point of maximal expansion and then have a stage of contraction culminating in the Big Crunch singularity. The contribution of phantom field leads the universe to reach the critical energy and to accelerate its expansion. The simplest explanation for the phantom dark energy is provided by a scalar field with a negative kinetic energy. The exact solution of the Friedmann and Klein Gordon equations are derived by assuming a particular relation between the time derivative of the phantom field and the Hubble function and then determine the evolution of the expansion scale factor and the potential from it. Our detailed analysis shows that in the model under consideration the phantom field can be an excellent candidate for dark energy.

Acknowledgements

I wish to express my genuine thanks Dr Khin Mya Mya Soe, Professor & Head, Department of Physics, East Yangon University, for her kind permission to carry out this research. I would like to express thankful to Dr Thet Naing, Professor, Department of Physics, East Yangon University, for his help and guidance with this research. Special thanks are due to my Supervisor Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her Supervisions and guidance throughout the entire course of this paper.I am also greatly indebted to Co-supervisor Dr Thant Zin Naing, Pro-Rector (Retired), International Theravā da Buddhist Missionary University, for his close guidance and supervision throughout the whole paper.

References

- Andrianov. A.A, Cannata.F, Kamenshchik.A.Y and Regoli.D, (2010), 'Phantom Cosmology Based On PT Symmetry', Int. J. Mod. Phys. D 19 97.
- Cai. R.G and Wang.A, (2005), 'Cosmology With Interaction Between Phantom Dark Energy and Dark Matter and the coincidence problem', JCAP 0503 002 [hepth/0411025].
- Caldwell. R.R, Kamionkowski.M and Weinberg.N.N, (2003), 'Phantom Energy and Cosmic Doomsday', Phys. Rev. let. 91071301 [astro-ph/0302506].
- Cannata. F. and Kamenshchik.A.Yu, (2007), 'Networks of Cosmological Histories, Crossing of the Phantom Divide Line and Potentials with Cusps', Int. J. Mod. Phys. D 16 1683 [gr-qc/0603129].

Appendix

The exact solution for a phantom scalar field with an exponential potential The Friedmann equation is

 $\frac{\dot{a}^{2}}{a^{2}} = -\frac{\dot{\phi}^{2}}{2} + V_{0}e^{\lambda\phi}$ (3) $a^{3} = e^{\nu+u}$ $a^{2} = (e^{\nu+u})^{\frac{2}{3}}$ $\dot{a}^{2} = \frac{1}{9}(\dot{\nu} + \dot{u})^{2}(e^{\nu+u})^{\frac{2}{3}}$ $\frac{\dot{a}^{2}}{a^{2}} = \frac{1}{9}(\dot{\nu} + \dot{u})^{2}$ $\dot{\phi}^{2} = A^{2}(\dot{\nu} - \dot{u})^{2}$

Now, eqn.(3) becomes

From eqn.(9),

$$\therefore \frac{1}{9}(\dot{u}^2 + \dot{v}^2 + 2\dot{u}\dot{v}) = -\frac{A^2}{2}(\dot{u}^2 + \dot{v}^2 - 2\dot{u}\dot{v}) + V_0 e^{\lambda\phi}$$

The Friedmann equation (3) has now the form

$$\frac{1}{9}(\dot{u}^2 + \dot{v}^2 + 2\dot{u}\dot{v}) = -\frac{1}{9}(\dot{u}^2 + \dot{v}^2 - 2\dot{u}\dot{v}) + V_0 e^{\lambda\phi}$$
$$\dot{u}^2 + \dot{v}^2 = \frac{9}{2}V_0 e^{\lambda\phi}$$
(12)

It is convenient now to introduce a complex variable

$$z \equiv \frac{1}{\sqrt{2}}(v + iu), \bar{z} \equiv \frac{1}{\sqrt{2}}(v - iu)$$
(13)

From eqn.(12),

$$\frac{1}{2}(\dot{u}^{2}+\dot{v}^{2}) = \frac{9}{4}V_{0}e^{\lambda\phi}$$
$$\frac{1}{\sqrt{2}}(\dot{v}+i\dot{u})\frac{1}{\sqrt{2}}(\dot{v}-i\dot{u}) = \frac{9}{4}V_{0}e^{\lambda\phi}$$
$$\dot{z} = \frac{1}{\sqrt{2}}(\dot{v}+i\dot{u})$$

$$\dot{\bar{z}} = \frac{1}{\sqrt{2}} (\dot{v} - i\dot{u})$$

$$\dot{z}\dot{\bar{z}} = \frac{1}{2} (\dot{v}^2 + \dot{u}^2)$$

$$= \frac{1}{2} \times \frac{9}{2} V_0 e^{\lambda \phi}$$

$$\dot{z} \, \dot{\bar{z}} = \frac{9}{2} V_0 e^{\lambda \phi}$$
(14)

Now eqn. (12) looks like, $\dot{z} \, \dot{\overline{z}} = \frac{9}{4} V_0 e^{\lambda \phi}$

Another complex variable, $z' = \frac{1}{\sqrt{2}}(v' + iu')$

$$\bar{z}' = \frac{1}{\sqrt{2}}(v' - iu')$$

(15)

(18)

We obtain, $z'\bar{z}' = 1$

where,

Introducing the function f such that

$$z' \equiv \frac{1}{\alpha} \frac{f'}{f} \tag{17}$$

 $\alpha = \frac{\sqrt{2}(1-i)}{2} \left(1 + \frac{\sqrt{2}\lambda i}{6}\right)$

Now, substituting eqn.(15) and eqn.(18) into eqn.(16).We get,

$$z^{\prime\prime} + \left(1 + \frac{\sqrt{2}\lambda}{6}\right)z^{\prime 2} + \left(\frac{\sqrt{2}\lambda}{6} - 1\right) = 0$$

Introducing a new variable, x = z'

$$\therefore x' + \left(1 + \frac{\sqrt{2\lambda}}{6}\right)x^2 + \left(\frac{\sqrt{2\lambda}}{6} - 1\right) = 0$$
(19)

This Klein-Gordon equation can be satisfied the Raccati form;

$$x = \frac{1}{(1 + \frac{\sqrt{2}\lambda}{6})} \frac{f'}{f}$$
$$x' = \frac{1}{(1 + \frac{\sqrt{2}\lambda}{6})} \left[\frac{ff'' - f'^2}{f^2}\right]$$

Substituting into eqn.(19),

$$\frac{1}{(1+\frac{\sqrt{2\lambda}}{6})} \left[\frac{ff''-f'^2}{f^2} \right] + \frac{(1+\frac{\sqrt{2\lambda}}{6})}{(1+\frac{\sqrt{2\lambda}}{6})^2} \frac{f'^2}{f^2} + \left(\frac{\sqrt{2\lambda}}{6} - 1 \right) = 0$$

$$\frac{1}{(1+\frac{\sqrt{2\lambda}}{6})}\frac{f''}{f} - \frac{1}{\left(1+\frac{\sqrt{2\lambda}}{6}\right)}\frac{f'^2}{f^2} + \frac{1}{\left(1+\frac{\sqrt{2\lambda}}{6}\right)}\frac{f''^2}{f^2} + \left(\frac{\sqrt{2\lambda}}{6} - 1\right) = 0 \quad \left(\times\left(1+\frac{\sqrt{2\lambda}}{6}\right)f\right)$$

$$f'' + \left(\frac{\sqrt{2\lambda}}{6} - \frac{2\lambda^2}{36} - 1\right)\left(1 + \frac{\sqrt{2\lambda}}{6}\right)f = 0$$

$$f'' + \left(\frac{\sqrt{2\lambda}}{6} - \frac{2\lambda^2}{36} - 1 - \frac{\sqrt{2\lambda}}{6}\right)f = 0$$

$$f'' - \left(1 + \frac{\lambda^2}{18}\right)f = 0$$

$$f'' - \left(1 + \frac{\lambda^2}{18}\right)f$$

$$\frac{d^2f}{d\tau^2} = \bar{\kappa}^2 f$$

$$\int \frac{df}{d\tau} = \pm \int \bar{\kappa} f$$

$$\ln f = \pm \bar{\kappa} \tau$$

$$f = \pm e^{\bar{\kappa}\tau}$$

$$f = Fe^{\bar{\kappa}\tau} + Ge^{-\bar{\kappa}\tau} \qquad (21)$$

DYNAMICAL SYSTEMS APPROACH TO FRW MODELS

Hla Hla Maw¹, Thei` Theint Theint Aung² and Thant Zin Naing³

Abstract

Dynamical systems approach to FRW models have been presented. Some techniques of non-linear dynamics have been utilized to find evolution equations. Visualization of stable and unstable points have been performed and a brief discussion for the results obtained has been given.

Keywords : Dynamical systems approach, FRW models, non-linear dynamics.

Introduction

All the dark energy models obey the general form of the equation of statep = $\omega(x(z))\rho$ in which the coefficient ω is parameterized by the scale factor x or red shift z. It is interesting to some general properties of an evolutional path of such models. For this aim dynamical system methods seem to be a natural method because it offers the possibility of investigating whole space of solutions starting from all admissible initial conditions. The dynamics of the FRW model with dark energy can be represented in the form of two dimensional dynamical systems, $\dot{x} = P(x, y), \dot{y} = Q(x, y)$ where $P, Q \in C^{\infty}$. The phase portraits of the system are organized by critical pointsP $(x_0, y_0) = Q(x_0y_0) = 0$.

Theoretical Background

Dynamical System in General

Any physical or abstract entity whose configuration at any given time can be specified by some set of numbers, system variables, and whose configuration at a later time is uniquely determined by its present and past configurations through a set of rules are often encountered. In continuous-time systems the rules are expressed as equations that specified the time derivatives of the system variables in terms of their current (and possible past) values. In such cases, the system variables are real numbers that varies continuously in time. The continuous-time dynamical system takes the form,

^{1.} Lecturer, Department of Physics, Yangon University of Education.

² Demonstrator, Department of Physics, Bago University.

^{3.} Retired Pro-Rector (Admin), International Theravda Buddhist Missionary University, Yangon.

 $\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t); \mathbf{p}, t)$

The components of vector xare the system variables and the vector f represents function of all the system variables at fixed values of the parameters. In discrete-time systems the rules are expressed as equations giving new values of the system variables as function of the current (and possible past) values. In spatially extended systems, each system variable is a continuous function of spatial position as well as time and the equations of motion take the form of partial differential equations

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{f}(\mathbf{x}, \nabla \mathbf{x}, \nabla \mathbf{x}^2, \dots; \mathbf{p}, \mathbf{t})$$

A set of equations describing a discrete-time dynamical system takes the form,

$$x(t + 1) = F(x(t); p, t)$$

Here the function F directly gives the new x at the next time step, rather than the derivative from which a new x can be calculated. The function F is often referred to as a map that takes the system from one time step to the next. In all cases the evolution of the system is described as a motion instate space of all possible values of the vectorx. A trajectory is a directed path through state space that shows the values of the system variables at successive times.

Linear and Nonlinear Systems

A linear system is one for which any two solutions of the equations of motion can be combined through simple addition to generate a third solution, given appropriate definition of the zeros of the variables. The way to recognize a linear dynamical system is that its equations of motion will involve only polynomial functions degree one in the system variables; there will be no products of different system variables or nontrivial functions of any individual variable. For all types of linear systems, the constraint that the sum of any two solutions also must be a solution has profound consequences. In a linear stable system, all solutions asymptotically approach the fixed point as time progresses. In an unstable system, all solutions that do not starts exactly on the fixed point diverge from it exponentially at long times. The marginal case, in which the variables neither decay to zero nor diverge, occurs primarily in Hamiltonian systems, in which conservation of energy prohibits convergence or divergence of nearby phase space trajectories. In the nonlinear system, the equations of motion include at least one term that contains the square or higher power, a product of system variables (for more complicated functions or them), or some sort of threshold function, so that the addition of two solutions does not yield a valid new solution, no matter how the system variables are defined. All physical systems describable in terms of classical equations of motion are nonlinear. The quantum mechanical theory of atoms and molecules is a linear theory.

Phase Plane Analysis of Dynamical Systems

For understanding the dynamics of linear and nonlinear systems, the description of its behavior in phase space is quite useful. The two independent variables (x, p_x) here $x, y = \dot{x}$, define the space in which the solution moves. For a particle having only one independent variable, the phase space is only two-dimensional and hence it is often referred to as the phase plane. At any time the value of the phase space co-ordinates (x, y) completely defines the state of the system. A given solution to the equations of motion will map out a smooth curve in the phase plane as a function of time. This is called a phase curve or phase trajectory and the motion along it is called the phase flow. Because of the unique properties of solutions to differential equations, different phase space trajectories do not cross each other. A picture made up of sets of phase curves is called a phase portrait.

Classification of Fixed Points

The nature of phase curves will depend on the eigenvalues of the stability matrix λ_1 and λ_2 . However, the form of eigenvectors determines the actual directions of the local phase flow. The different possibilities are discussed in this section.

Case (i): $\lambda_1 < \lambda_2 < 0 - \underline{\mathbf{a}}$ stable node. As the eigenvalues are negative, the local flow decays in both directions determined by D_1 and D_2 into the fixed point, as illustrated in figure (1(a)).

- Case (ii): $\lambda_1 \lambda_2 > 0 -$ an unstable node. The local flow grows exponentially away from the fixed point in both directions, as shown in figure (1(b)).
- Case (iii): $\lambda_1 < 0 < \lambda_2$ –hyperbolic point or saddle point. One direction grows exponentially and the other decays exponentially, as illustrated in figure (1(c)). The incoming and outing directions are often referred to as the stable and unstable manifolds of separatrix, respectively.
- Case (iv): $\lambda_1 = -\alpha + i\beta$, $\lambda_2 = -\alpha i\beta(\alpha, \beta > 0) a$ stable spiral point .Since the two eigenvalues λ_1 and λ_2 have the negative real part $-\alpha$ the flow spirals in toward the fixed points, as shown in figure (1(d)).
- Case (v): $\lambda_1 = \alpha + i\beta$, $\lambda_2 = \alpha i\beta$ an unstable spiral point. Because of the positive real parts, the flow spirals away from the fixed point (figure (1(e))) will be stable equilibrium point.
- Case (vi): $\lambda_1 = i\omega$, $\lambda_2 = -i\omega$ an elliptic point or simply centre. As the two eigenvalues are purely imaginary, the phase curves will be closed ellipses, as shown in figure (1(f)). This will be stable equilibrium point.



Figure 1: Local phase flows for (a) stable star; (b) unstable star; (c) stable improper node; (d) unstable improper node.

The Friedmann-Robertson-Walker Model with Dynamical Dark Energy

The Friedmann-Robertson-Walker model with source in the form of non –interacting dust matter and dark energy which the equation of state is parameterized by $p = \omega(x)\rho$. Then from the conservation condition,

$$\dot{\rho} = -3 H (\rho + p)$$

The FRW dynamics is

$$H^2 = \frac{\rho}{3} - \frac{k}{x^2}$$
, and $\rho = 3 \frac{\dot{x}^2}{x^2} + \frac{3}{x^2}k$

From conservation condition

$$p = -\frac{\dot{\rho} x}{3 \dot{x}} - \rho$$
$$\dot{\rho} = 3 \frac{2 \dot{x} \ddot{x}}{x^2} + 3 x^2 (-2x^{-3} \dot{x}) + 3 k (-2x^{-3} \dot{x})$$
$$p = -2 \frac{\ddot{x}}{x} - \frac{\dot{x}^2}{x^2} - \frac{k}{x^2}$$

Then the basic dynamical equations reduce to

$$\dot{x} = y$$

$$\rho + p = 2 \frac{\rho}{3} - 2 \frac{\ddot{x}}{x}$$
Therefore
$$\ddot{x} = -\frac{1}{6}(\rho + 3p)x$$

then one get

$$\dot{y} = -\frac{1}{6}(\rho(x) + 3p(x))x$$

This equation constitutes a two dimensional autonomous dynamical systems.

The General Properties of the FRW Model

The basic dynamical equations reduce to $\dot{x} = y$ and $\dot{y} = -\frac{1}{6}(\rho + 3p)x$, where $p = \omega \rho$. The dynamics of the FRW model with dark energy can be represented in the form of two dimensional systems,

$$\dot{x} = P(x, y), \quad \dot{y} = Q(x, y)$$

where $P, Q \in C^{\infty}$.

The character (type) of critical points is determined from eigenvalues of the

linearization matrix A:
$$A = \begin{bmatrix} \frac{\partial P}{\partial x} & \frac{\partial P}{\partial y} \\ \frac{\partial Q}{\partial x} & \frac{\partial Q}{\partial y} \end{bmatrix}_{(x_0, y_0)}^{P}$$
 where,
$$\frac{\partial P}{\partial x} = \frac{\partial y}{\partial x} = 0 \text{ and } \frac{\partial P}{\partial y} = \frac{\partial y}{\partial y} = 1$$
$$\frac{\partial Q}{\partial x} = \frac{\partial y}{\partial x} = \frac{\partial}{\partial x} \left(-\frac{1}{6} [\rho(x) + 3\omega\rho(x)]x \right) = -\frac{1}{6} \frac{\partial}{\partial x} [x\rho(x)[1 + 3\omega(x)]]$$
$$\frac{\partial Q}{\partial y} = \frac{\partial y}{\partial y} = \frac{\partial y}{\partial y} \left[-\frac{1}{6} [\rho(x)[1 + 3\omega(x)]x \right] = 0$$
Therefore, one has

$$A = \left[-\frac{1}{6} \frac{\partial}{\partial x} \left(x \rho(x) (1 + 3\omega(x)) \right)_{0}^{1} \right]_{(x_{0}, y_{0})},$$

where x = a is dimensionless scale factor expressed in terms of its present value a_0 . In the eigen problem det $[A - \lambda I] = 0$ then reads $\lambda^2 - \lambda TrA + \det A = 0$. Consequently the sign of determent A determines the type of the critical points that is whether λ is real or complex. It is consequence of the fact that,

$$TrA = 0$$
 and det $A = \frac{1}{6} \frac{\partial}{\partial x} (x\rho(x)(1+3\omega(x)))$.

Then one gets, the critical points of the system can be saddle points if $det(A)_{x_0} > 0$ or centers if $det(A)_{x_0} > 0$ In the first case eigenvalues are real of opposite sign while in the second case they are purely imaginary and conjugated.

Concluding Remarks

The main message of this paper is to note that there exists a systematic methods of classification and investigation the dynamical equation of state in the quite general form, the equation of statep = $\omega(x)\rho$. The FRW models with dynamical dark energy modeled in terms of the equation of statep = $\omega(x(z))\rho$ in which the coefficient ω is parameterized by the scale factor xorz. The advantages of using a complementary description of dynamic as a Hamiltonian flow, the evolution of the model is represented as a motion of unit mass in one –dimensional potential V(a). The properties of potential function V can serve as a toolfor qualitative classification of all evolution paths. The main subject of this paper is presentation how dynamics of the FRW model with dynamical dark energy can be reduced to the form of a two -dimensional dynamical system.

Acknowledgements

I am highly grateful to Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her kind permission to do and her encouragement to carry out this paper.

I would like to thank Professor Dr Aye Aye Thant, Department of Physics, University of Yangon, for her valuable guidance, kind encouragement, valuable help, and support in this paper.

References

Aruldhas, G. (2008) "Classical Mechanics", PHI Learning Private Limited, New Delhi.

- Grobman, D.M.(1962). Topological Classification of Neighborhoods of a Singularity in Nspace, Mat. Sbornik56, no. 98, 77.
- Hartman, P. (1960). On Local Homeomorphisms of Euclidean Spaces, Bol. Soc. Mat. Mexicana (2) 5, 220.

Peacock, J.A.(1999). "Cosmological Physics", CUP, Cambridge.

Perco, L. (1991). "Differential Equations and Dynamical System", Springer-Verlag, New York.

THEORETICAL AND NUMERICAL ASPECTS OF GRAVITATIONAL WAVES

Nyein Thida¹, Hla Hla Maw²

Abstract

It has been attempted to give a brief description of gravitational waves and its underlying physics for both theoretical and numerical aspects. First of all, the theoretical background of long sought gravitational waves (GWs) and its related connection to astrophysics and cosmology have been given in detail. Then, the accelerating charge, accelerating mass and amplitude of GWs are theoretically and numerically investigated within the framework of general relativity, classical mechanics and statistical mechanics points of view.

Keywords: gravitational waves, general relativity, dipole and quadrupole moments.

Introduction

Gravitational waves (GWs) are generated by accelerated masses, that propagate as waves outward from their source at the speed of light. They were predicted by Albert Einsteinin 1916on the basis of his general theory of relativity. Gravitational waves transport energy as gravitational radiation, a form of radiant energy similar to electromagnetic radiation. Gravitational wave astronomy is a branch of observational astronomy that uses gravitational waves to collect observational data about sources of detectable gravitational waves such as binary star systems composed of white dwarfs, neutron stars, black holes and events such as supernovae and the formation of the early universe shortly after the Big Bang.

On 11 February 2016, the LIGO and Virgo Scientific Collaboration announced they had made the first observation of gravitational waves. The observation was made five months earlier, on 14 September 2015, using the Advanced LIGO detectors. The gravitational waves originated from a pair of merging black holes. After the initial announcement the LIGO instruments detected two more confirmed, and one potential, gravitational wave events. In August 2017, the two LIGO instruments and the Virgo instrument observed a

¹ Dr, Associate Professor, Department of Physics, University of Yangon

^{2.} Lecturer, Department of Physics, University of Yangon.

fourth gravitational wave from merging black holes, and a fifth gravitational wave from abinary neutron starmerger. Several other gravitational wave detectors are planned or under construction.

penetrate regions Gravitational waves can of space that electromagnetic waves cannot. They are able to allow the observation of the merger of black holes and possibly other exotic objects in the distant Universe. Such systems cannot be observed with more traditional means such as optical telescopes or radio telescopes, and so gravitational wave astronomy gives newinsights into the working of the Universe. In principle, gravitational waves could exist at any frequency. However, very low frequency waves would be impossible to detect and there is no credible source for detectable waves of very high frequency. Stephen Hawking and Werner Israel list different frequency bands for gravitational waves that could plausibly be detected, ranging from 10^{-7} Hz up to 10^{11} Hz.

Gravitational waves have two important and unique properties. First, there is no need for any type of matter to be present nearby in order for the waves to be generated by a binary system of uncharged black holes, which would emit no electromagnetic radiation. Second, gravitational waves can pass through any intervening matter without being scattered significantly. Whereas light from distant stars may be blocked out by interstellar dust, for example, gravitational waves will pass through essentially unimpeded. These two features allow gravitational waves to carry information about astronomical phenomena heretofore never observed by humans, and as such represent a revolution in astrophysics.

Effect of Gravitational Waves on Free Particles

To investigate the geodesic equations for the trajectories of material particles and photons in a nearly flat space time, during to the passage of a gravitational wave, one need to study the following.

Proper Distance Between Test Particles

The amplitude of the metric perturbation is described by just two independent constants, A_{xx} and A_{xy} . The physical significance of these constants by examining the effect of the gravitational wave on a free particle,

in an initially wave-free region of space time. The free particle's trajectory satisfies the geodesic equation

$$\frac{dU^{\beta}}{d\tau} + \Gamma^{\beta}_{\mu\nu}U^{\mu}U^{\nu} = 0$$
 (1)

where τ is the proper time. The particle is initially at rest, i.e. initially $U^{\beta} = \delta_t^{\beta}$.

Thus, the initial acceleration of the particle is

$$\left(\frac{dU^{\beta}}{d\tau}\right)_{0} = -\Gamma_{tt}^{\beta} = -\frac{1}{2}\eta^{\alpha\beta}(h_{\alpha t,t} + h_{t\alpha\alpha}, -h_{tt,\alpha})$$

$$A_{t} = 0 \Rightarrow h_{\alpha t} = 0$$
(2)

However,

Also, recall that $h = \overline{h} = 0$. Therefore it follows that $h_t = 0$ for all α which in turn implies that $\left(\frac{dU^{\beta}}{d\tau}\right)_0 = 0$ (3)

Hence a free particle, initially at rest, will remain at rest indefinitely. However, 'being at rest' in this context simply means that the coordinates of the particle do not change. As the gravitational wave passes, this coordinate system adjusts itself to the ripples in the space time, so that any particles remain 'attached' to their initial coordinate positions. Coordinates are merely frame-dependent labels, however, and do not directly convey any invariant geometrical information about the space time.^[5]

The proper distance between the particles is then given by

$$\Delta l = \int \left| g_{\alpha\beta} dx^{\alpha} dx^{\beta} \right|^{\frac{1}{2}}$$
(4)

$$\Delta l = \int_{0}^{\varepsilon} |g_{XX}|^{\frac{1}{2}} \cong \sqrt{g_{XX}(x=0)} \in$$
(5)

$$g_{XX}(x=0) = \eta_{XX} + h_{XX}^{(TT)}(x=0)$$
(6)

Since $h_{xx}^{(TT)}(x = 0)$ in general is not constant, it follows that the proper distance between the particles will change as the gravitational wave passes. It is essentially this change in the proper distance between test particles which gravitational wave detectors attempt to measure.

Geodesic Deviation of Test Particles

The study of the behaviour of test particles are more formally using the idea of geodesic deviation. By defining the vector ξ^{α} which connects the two particles and for a weak gravitational field, taking proper time approximately equal to coordinate time is

$$\frac{\partial^2 \xi^{\alpha}}{\partial t^2} = R^{\alpha}_{\mu\nu\beta} U^{\mu} U^{\nu} \xi^{\beta}$$
(7)

where U^{μ} are the components of the four-velocity of the two particles. Since the particles are initially at rest, then $U^{\mu} = (1,0,0,0)T$

and $\boldsymbol{\xi}^{\boldsymbol{\beta}} = (\boldsymbol{0}, \boldsymbol{\epsilon}, \boldsymbol{0}, \boldsymbol{0})^T$

then simplifies to

$$\frac{\partial^2 \xi^{\alpha}}{\partial t^2} = \in R^{\alpha}_{ttx} = - \in R^{\alpha}_{txt}$$
(8)

Hence, two particles initially separated by in the x-direction, have a geodesic deviation vector which obeys the differential equations. Similarly, it is straightforward to show that two particles initially separated by in the y-direction, have a geodesic deviation vector which obeys the differential equations.

Ring of Test Particles: Polarisation of Gravitational Waves

To consider the geodesic deviation of two particles, one at the origin and the other initially at coordinates $x = \epsilon \cos \theta$, $y = \epsilon \sin \theta$ and z = 0, i.e. in the *x*-*y* plane as a gravitational wave propagates in the *z*-direction. ξ^{x} and ξ^{y} obey the differential equations

$$\frac{\partial^2}{\partial t^2} \xi^x = \frac{1}{2} \in \cos\theta \frac{\partial^2}{\partial t^2} h_{xx}^{(TT)} + \frac{1}{2} \in \sin\theta \frac{\partial^2}{\partial t^2} h_{xy}^{(TT)}$$
(9)

and
$$\frac{\partial^2}{\partial t^2} \xi^y = \frac{1}{2} \epsilon \cos\theta \frac{\partial^2}{\partial t^2} h_{xy}^{(TT)} - \frac{1}{2} \epsilon \sin\theta \frac{\partial^2}{\partial t^2} h_{xx}^{(TT)}$$
 (10)

We can identify the solution

$$\xi^{x} = \epsilon \cos\theta + \frac{1}{2} \epsilon \cos\theta A_{xx}^{(TT)} \cos\omega t + \frac{1}{2} \epsilon \sin\theta A_{xy}^{(TT)} \cos\omega t$$
(11)

and
$$\xi^{x} = \epsilon \sin \theta + \frac{1}{2} \epsilon \cos \theta A_{xy}^{(TT)} \cos \omega t - \frac{1}{2} \epsilon \sin \theta A_{xx}^{(TT)} \cos \omega t$$
 (12)

 θ varies between 0 and 2π . An initially circular ring of test particles in the xy plane, initially equidistant from the origin and the metric perturbation has $A_{xx}^{(TT)} \neq 0$ and $A_{xy}^{(TT)} = 0$. In this case the solution for ξ^x and ξ^y reduces to

$$\xi^{x} = \epsilon \cos \theta \left(1 + \frac{1}{2} A_{xx}^{(TT)} \cos \omega t \right)$$

$$\xi^{y} = \epsilon \sin \theta \left(1 - \frac{1}{2} A_{xx}^{(TT)} \cos \omega t \right)$$
(13)

$$\xi^{\gamma} = \epsilon \sin \theta \left(1 - \frac{1}{2} A_{xx}^{\gamma} \cos \omega t \right)$$
(14)

In the case of the metric perturbation has $A_{xy}^{(TT)} \neq 0$ and $A_{xx}^{(TT)} = 0$, the solutions for ξ^x and ξ^y reduce to

$$\xi^{x} = \epsilon \cos \theta + \frac{1}{2} \epsilon \sin \theta A_{xy}^{(\text{TT})} \cos \omega t$$
(15)

$$\xi^{y} = \epsilon \sin \theta + \frac{1}{2} \epsilon \cos \theta A_{xy}^{(\text{TT})} \cos \omega t$$
(16)

To understand the relationship between these solutions and those for $A_{xx}^{(TT)} = 0$, we define new coordinate axes x'and y' by rotating the x and y axes through an angle of $-\pi/4$, so that

$$x' = \frac{1}{\sqrt{2}} (x - y)$$
(17)

$$y' = \frac{1}{\sqrt{2}} \left(x + y \right) \tag{18}$$

If we write the solutions for $A_{xy}^{(TT)} \neq 0$ in terms of the new coordinates x' and y' after some algebra we find that

$$\xi'^{x} = \in \cos\left(\theta + \frac{\pi}{4}\right) + \frac{1}{2} \in \sin\theta\left(\theta + \frac{\pi}{4}\right) A_{xy}^{(\text{TT})} \cos\omega t$$
(19)

and
$$\xi'^{y} = \epsilon \sin \left(\theta + \frac{\pi}{4}\right) + \frac{1}{2} \epsilon \sin \theta \left(\theta + \frac{\pi}{4}\right) A_{xy}^{(TT)} \cos \omega t$$
 (20)



Figure 1: Parametric Plot for the interactive relation between \boldsymbol{x}' and \boldsymbol{y}'



Figure 2: Contour Plot for Gravitational wave of the new coordinate x' and y' $A_{xx}^{(TT)} = 1$



Figure 3: Contour plot for Gravitational waves of the new coordinate x' and $y' A_{xy}^{(TT)} = 1$

The Production of Gravitational Waves

The reasons why gravitational radiation is quadrupolar to lowest order, and we estimate the amplitude of the gravitational wave signal from binary neutron star system.

The Quadrupolar Nature of Gravitational Waves

The nature of gravitational radiation by drawing analogies with the formulae that describe electromagnetic radiation. This approach is crude at best since the electromagnetic field is a vector field while the gravitational field is a tensor field, but it is good enough for our present purposes. Essentially, we will take familiar electromagnetic radiation formulae and simply replace the terms which involve the Coulomb force by their gravitational analogues from Newtonian theory⁻

Electric and Magnetic Dipoles

In electromagnetic theory, the dominant form of radiation from a moving charge or charges is electric dipole radiation. For a single particle (e.g. an electron) of charge e with acceleration a and dipole moment changing as $d = e \ddot{x} = ea$, the power output or luminosity is given by

$$L_{\text{electric dipole}} \propto e^2 a^2$$
 (23)

For a general distribution of charges, with net dipole moment d, the luminosity is

$$L_{\text{electric dipole}} \propto e^2 \ddot{d}^2$$
 (24)

The next strongest types of electromagnetic radiation are magnetic dipole and electric quadrupole radiation. For a general distribution of charges, the luminosity arising from magnetic dipole radiation is proportional to the second time derivative of the magnetic dipole moment, i.e.

$$L_{\text{magnetic dipole}} \propto \ddot{\mu}$$
 (25)

where μ is given by a sum (or integral) over a distribution of charges:-

$$\mu = \sum_{q_i} (\text{ position of } q_i) \times (\text{current due to } q_i)$$
(26)

Gravitational Analogues

The gravitational analogue of the electric dipole moment is the mass dipole moment d summed over a distribution of particles, $\{Ai\}$

$$d = \sum_{A_i} (m_i x_i) \tag{27}$$

where m_i is the rest mass and x_i is the position of particle A_i .

The luminosity of gravitational 'mass dipole' radiation should be proportional to the second time derivative of d. However, the first time derivative of d is

$$\dot{\mathbf{d}} = \sum_{\mathbf{A}:} (\mathbf{x}_i) \dot{\mathbf{x}}_i = \mathbf{P}$$
(28)

where p is the total linear momentum of the system. Since the total momentum is conserved, it follows that the gravitational 'mass dipole' luminosity is zero i.e there can be no mass dipole radiation from any source. Similarly, the gravitational analogue of the magnetic dipole moment is

$$\mu = \sum_{A_i} (x_i) \times (m_i v_i) \equiv J$$
(29)

where J is the total angular momentum of the system. Since the total angular momentum is also conserved, again it follows that the gravitational analogue of magnetic dipole radiation must have zero luminosity. Hence there can be no dipole radiation of any sort from a gravitational source. The simplest form of gravitational radiation which has non-zero luminosity is, therefore, quadrupolar.

Example: ABinary Neutron Star System

Finally, the example of the gravitational wave signature of a particular astrophysical system: a binary neutron star. In general it can be called slow motion approximation for a weak metric perturbation $h_{\mu}v << 1$ then for a source at distance r

$$h_{\mu\nu} = \frac{2G}{c^4 r} \quad \ddot{\mathbf{I}}_{\mu\nu} \tag{30}$$

Where $I_{\mu\nu}$ is the reduced quadrupole moment defined as

$$I_{\mu\nu} = \int \rho(\vec{r}) (x_{\mu} x_{\nu} - \frac{1}{3} \delta_{\mu\nu} r^2) dV$$
(31)

Consider a binary neutron star system consisting of two stars both of Schwarzschild mass M, in a circular orbit of coordinate radius R and orbital frequency f. For simplicity we define our coordinate system so that the orbital plane of the pulsars lies in the x-y plane, and at coordinate time t = 0, the two pulsars lie along the x-axis.

$$I_{xx} = 2MR^2 [\cos^2(2\pi ft) - \frac{1}{3}]$$
(32)

$$I_{yy} = 2MR^2 [\sin^2(2\pi f t) - \frac{1}{3}]$$
(33)

$$I_{xy} = I_{yx} = 2MR^2 \left[\cos(2\pi ft) \sin(2\pi ft) \right]$$
(34)

From equation no (30) and (32) - (34) it then follows that

$$h_{xx} = -h_{yy} = h\cos(4\pi f t) \tag{35}$$

and

$$h_{xy} = h_{yx} = -hsin(4\pi ft) \tag{36}$$

where the amplitude term h is given by

$$h = \frac{32\pi^2 GMR^2 f^2}{c^4 r}$$
(37)

The binary system emits gravitational waves at twice the orbital frequency of the neutron stars. Suppose we take M equal to the Chandrasekhar mass, $M \sim 1.4M$ solar = $2.78 \times 10^{30} kg$. We can then evaluate the constants in(37) and express h in more convenient units as

$$h = 2.3 \times 10^{-28} \frac{\text{R}^{2}[\text{km}]\text{f}^{2}[\text{Hz}]}{\text{r}[\text{Mpc}]}$$
 (38)

If we take R = 20km, say, f = 1000Hz (which is approximately the orbital frequency that Newtonian gravity would predict) and r = 15Mpc (corresponding to a binary system in e.g. the Virgo cluster), then we find that

 $h \sim 6 \times 10^{-21}$. Thus we see that the signal produced by a typical gravitational wave source places extreme demands upon detector technology.

Concluding Remarks

The direct detection of GWs by LIGO initiates a new era of GW astronomy and GW cosmology. The GW physics is not only related to gravitational physics, but also closely related to particle physics, cosmology and astrophysics. The GWs provide us a new powerful tool to reveal various secrets of the nature. Indeed, a lot of relevant papers have appeared since the announcement of the direct detection of GWs. In this paper, we have briefly introduced three kinds of GW sources and relevant physics. The GWs are produced during inflation and preheating in the early Universe, from cosmic PTs and dynamics of compact binary systems, (Binary Black Holes and Binary Neutron Stars, etc,...) respectively. We also have discussed in a simple way the GWs as standard siren in the evolution of the Universe.

Acknowledgements

I would like to thank Dr Khin KhinWin, Professor and Head, Department of Physics, University of Yangon, for her kind permission and encouragements to carry out this work.

I would like to express my gratitude to Professor Dr Aye Aye Thant, Professor, Department of Physics, University of Yangon, for her encouragements to undertake this research paper.

Special thanks are due to Professor, Dr Thant Zin Naing, Retired Pro-Rector (Admin), International Theravāda Buddhist Missionary University, for his valuable guidance and helpful advice to carry out this work.

References

- A. Einstein, Approximative Integration of the Field Equations of Gravitation, Sitzungsber. Preuss. Akad. Wiss. Berlin (Math. Phys.) 1916 (1916) 688–696.
- A. H. Guth, (1981), "The Inflationary Universe: A Possible Solution to the Horizon and Flatness Problems", Phys. Rev. D23, 347–356.
- A. D. Linde, (1982), "A New Inflationary Universe Scenario: A Possible Solution of the Horizon, Flatness, Homogeneity, Isotropy and Primordial Monopole Problems", Phys. Lett. B108, 389–393.
- B. P. Abbott et al., (2016) Virgo, LIGO Scientific collaboration "Observation of Gravitational Waves from a Binary Black Hole Merger", Phys. Rev. Lett.116,061102, [1602.03837].
- B. P. Abbott et al., Virgo, LIGO Scientific collaborationGW151226: Observation of Gravitational Waves from a 22-Solar-Mass Binary Black Hole Coalescence, Phys. Rev. Lett. 116 (2016) 241103, [1606.04855].
- H. Bondi, Plane gravitational waves in general relativity, Nature 179 (1957) 1072-1073.
- P. R. Saulson, Josh Goldberg and the physical reality of gravitational waves, Gen. Rel. Grav. 43 (2011) 3289–3299.

AN ANALYSIS OF NUMERICAL HYDRODYNAMICS FOR SPHERICALLY SYMMETRIC SPACETIMES

Yee May Thwin¹, Zaw Myint²

Abstract

The interesting features of numerical hydrodynamics for spherically symmetric spacetimes has been presented in the context of general relativity. Some distinct results are visualized and physical interpretations have been given.

Keywords: numerical hydrodynamics, spherically symmetric spacetimes

Introduction

The description of important areas of modern astronomy, such as highenergy astrophysics or gravitational wave astronomy requires general relativity. Einstein's theory of gravitation plays a major role in astrophysical scenarios involving compact objects such as neutron stars and black holes. High-energy radiation is often emitted in regions of strong gravitational fields near such compact objects. The production of relativistic radio jets in active galactic nuclei, explained by either hydrodynamic or electromagnetic mechanisms, involves rotating supermassive black holes. The discovery kHz quasi-periodic oscillations in low-mass X-ray binaries extended the frequency range over which these oscillations occur into timescales associated with the relativistic, innermost regions of accretion disks. A relativistic description is also necessary in scenarios involving explosive collapse of very massive stars to black hole, or during the last phases of the coalescence and merge of neutron star binaries and neutron-star-black-hole binaries. These catastrophic events are believed to occur at the central engine of the most highly energetic events in nature, gamma-ray bursts (GRBs). Astronomers have long been scrutinizing these systems using the complete frequency range of the electromagnetic spectrum. Nowadays, they are the main targets of groundbased laser interferometers of gravitational radiation. The direct detection of these elusive ripples in the curvature of space time, and the wealth of new information that could be extracted from them, is one of the driving motivations of present-day research in relativistic astrophysics.

^{1.} Lecturer, Department of Physics, University of Yangon, Myanmar

² Assistant Lecturer, Department of Physics, East Yangon University, Myanmar

An accurate description of relativistic flows with strong shocks is nowadays demanded for the study of a large number of important problems in physics and astrophysics. Ultra relativistic flows are found not only in extragalactic jets (Begelman, Blandford, & Rees 1984; see also Marti et al. 1997 for an up-to-date bibliography) but also in high-energy heavy-ion collisions (Clare & Strottman 1986). General relativistic effects caused by the presence of strong gravitational fields appear connected to extremely fast flows in different astrophysical scenarios, e.g., accreting compact objects, stellar collapse, and coalescing compact binaries (Shapiro & Teukolsky 1983; Thorne 1987; Bonazzola & Marck 1994). In recent years, much effort has been addressed to developing accurate numerical algorithms able to solve the equations of general relativistic hydrodynamics in the extreme conditions described above. The main conclusion that has emerged is that modern algorithms exploiting the hyperbolic (and conservative) character of the system of equations are by far more accurate at describing relativistic flows than traditional finite-difference upwind techniques with artificial viscosity (introduced by Wilson 1972,1979). Wilsons work marked further developments for the integration of the relativistic hydrodynamics system of equations(Piran 1983; Stark & Piran 1987; Nakamura et al. 1980; Nakamura 1981; Nakamura & Sato 1982; Centrella & Wilson 1984; Hawley, Smarr, & Wilson 1984a, 1984b; Evans 1986). However, the procedure seems to break down for relativistic flows with high Lorentz factors, for which large numerical inaccuracies and instabilities are obtained (Norman & Winkler 1986). Totake advantage of the conservation properties of the system, modern algorithms are written in conservation form, in the sense that the variation of the mean values of the conserved quantities within the numerical cells is given, in the absence of sources, by the fluxes across the cell boundaries. Furthermore, the hyperbolic character of the system of equations allows one to obtain these fluxes from solutions of discontinuous initial problems (i.e., Riemann problems) between neighboring numerical cells. In this way, physical discontinuities appearing in the flow are treated consistently (the shock-capturing property).

The use of Riemann solutions in numerical codes comes from the idea of Godunov (1959), who first introduced them in classical fluid dynamics, but it was not until the late seventies when, thanks to the development of new

cell-reconstruction procedures (van Leer 1979; Colella & Woodward 1984a, 1984b; Marquina 1994), high-resolution shock-capturing (HRSC)techniques were recognized as the most effective way to describe complex flows accurately. Since then, efficient Riemann solvers based on exact or approximate solutions of the initial-value problem have been developed. A general approach, followed here, is to obtain the fluxes from the solution of a linearized form of the original system of equations (the local characteristic approach). This solution can be obtained exactly by writing the system in terms of the so-called characteristic variables. In terms of these variables, which are obtained by projection of the original variables onto the right eigenvectors of the Jacobian matrices, the system decouples into a set of scalar advection equations, the eigenvalues of the Jacobian matrices being the advection velocities (characteristic speeds). Intrinsic to this approach is the spectral decomposition of the Jacobian matrices of the partial derivative system of equations.

Equations of General Relativistic Hydrodynamics as a System of Conservation Laws

The equations that describe the evolution of a relativistic fluid are local conservation laws: the local conservation of baryon number,

$$\nabla . J = 0$$

and the local conservation of energy-momentum,

$$\nabla \cdot T = 0$$

where ∇ . stands for the covariant divergence. If $\{\partial_t, \partial_i\}$ define the coordinate basis of 4-vectors that are tangents to the corresponding coordinate curves, then the vector *J*-the current of rest mass - and the bilinear form T - the energy-momentum tensor have the components

$$J^{\mu} = \rho u^{\mu}, \ J^{\mu\nu} = \rho h u^{\mu} u^{\nu} + p g^{\mu\nu}$$

 ρ being the rest-mass density, p the pressure, and h the specific enthalpy, defined by $\rho h = 1 + \varepsilon + \frac{p}{\rho}$ where ε is the specific internal energy. Here u^{μ} is the 4-velocity of the fluid, and $g_{\mu\nu}$ defines the metric of the spacetime *M*in which the fluid evolves.

Throughout this paper, Greek (Latin) indices run from 0 to3 (1 to 3)or, alternatively, they stand for the general coordinates $\{t, x, y, z\}(\{x, y, z\})$ -and geometrized units are used(c=G=1). An equation of state p=p (ρ , ε), as usual, closes the system.

A very important quantity derived from the equation of state is the local sound velocity, c_s :

$$hc_s^2 = \chi + \left(\frac{p}{\rho^2}\right)\kappa$$
,

with $\chi = \frac{\partial p}{\partial \rho}|_{\varepsilon}$ and $\kappa = \frac{\partial p}{\partial \varepsilon}|_{\rho}$. Let \mathcal{M} be a general spacetime, described by the four-dimensional metric tensor $g_{\mu\nu}$.



Figure 1: The variation of the local sound velocity c_s with ρ and ϵ



Figure 2: The variation of the local sound velocity c_s with ρ and ϵ

According to the $\{3+1\}$ formalism the metric is split into the objects $\alpha(lapse)$, β^i (shift), and γ_{ij} , keepingthe line element in the form

$$ds^{2} = -(\alpha^{2} - \beta_{i}\beta^{i})dt^{2} + 2\beta_{i}dx^{i}dt + \gamma_{i} + dx^{i}dx^{j}$$

If *n* is a unit timelike vector field normal to the spacelike hyper surfaces Σ_t (t=const), then, by definition of α and β^i ,

$$\partial_t = \alpha n + \beta^i \partial_i$$

with $n \cdot \partial_i = 0$ for all i.

Observers \mathcal{O}_E at rest in the slice Σ_t , i.e., those having *n* as 4-velocity measure the following velocity of the fluid:

$$\upsilon_i = \frac{u \cdot \partial_i}{-u \cdot n},$$

where the contravariant components $v^i = \gamma^{ij} v_j$ are

$$\upsilon^i = \frac{u^i}{\alpha u^i} + \frac{\beta^i}{\alpha}$$

and the denominator. In equation is the Lorentz factor $W \equiv -u \cdot n = \alpha u^t$ which satisfies $W = (1 - v^2)^{-1/2}$ with $\gamma_{ij} v^i v^j$.

Let us define a basis adapted to the observer \mathcal{O}_E

$$e_{(\mu)} = \{n, \partial_i\},\$$

and the following five 4-vectors $\mathcal{D}_{(A)}$:

$$D_{(A)} = \{T(e_{(\gamma)}, .), J\}, A=0,...,4.$$

Hence the above system of equations (1) and (2) can be written

$$\nabla . D_{(A)} = s_{(A)}$$

The five quantities $s_{(A)}$ on the right-hand side of sources are equation the

$$s_{(A)} = T^{\mu\nu} \nabla_{\mu} e$$
$$s_{(A)} = \{T^{\mu\nu} \overline{\nabla}_{\mu} e_{(\gamma)\nu}, 0\}, \quad \nabla_{\mu} e_{(\mu)\nu} = \frac{\partial e_{(\gamma)\nu}}{\partial \chi^{\mu}} - \Gamma^{\delta}_{\nu\mu} e_{(\gamma)\delta},$$

where the quantities $\Gamma^{\mu}_{\beta\nu}$ are the Christoffel symbols and

$$e_{(0)\nu} = -\alpha \delta_{0\nu}, \qquad e_{(k)\nu} = g_{k\nu} = (\beta_k, \gamma_{kj}) .$$

Taking into account those quantities that are directly measured by \mathcal{O}_E i.e., the rest-mass density (*D*), the momentum density in the *j*-direction (*S_j*), and the total energy density (*E*), we can display them in terms of the primitive variables

$$w = (\rho, v_{i}, \varepsilon)^{\mathrm{T}}$$

by the following relations :

$$D \equiv -J.n = \rho W, S_j \equiv -T(n, e_{(j)}) = \rho h W^2 v_j, E \equiv -T(n, n) = \rho h W^2 - p.$$

Putting together all the above relations, the fundamental system to be considered for numerical applications is

$$\frac{1}{\sqrt{-g}}\left[\frac{\partial\sqrt{\gamma}F^{0}(w)}{\partial x^{0}}+\frac{\partial\sqrt{-g}F^{i}(w)}{\partial x^{i}}\right]=s(w),$$

where the quantities $F^{\alpha}(w)$ are

$$F^{0}(w) = (D, S_{j}, \tau)^{T}$$

$$F^{i}(w) = \left[D\left(\upsilon^{i} - \frac{\beta^{i}}{\alpha}\right), S_{j}\left(\upsilon^{i} - \frac{\beta^{i}}{\alpha}\right) + p\delta_{j}^{i}, \tau\left(\upsilon^{i} - \frac{\beta^{i}}{\alpha}\right) \right]^{T} + p\upsilon^{i}$$

and the corresponding sources s(w) are

$$s(w) = \left[0, T^{\mu\nu}\left(\frac{\partial g_{\nu j}}{\partial \chi^{\mu}} - \Gamma^{\delta}_{\nu\mu}g_{\delta j}\right), \alpha\left(T^{\mu 0}\frac{\partial \ln \alpha}{\partial \chi^{\mu}} - T^{\mu\nu}\Gamma^{0}_{\nu\mu}\right)\right]^{T},$$

 τ being $\tau \equiv E - D$; that is, the total energy density minus the rest-mass density, $g \equiv \det g_{\mu\nu}$ is such that

$$\sqrt{-g} \equiv \alpha \sqrt{\gamma} , \qquad \gamma \equiv \det \gamma_{ij} ,$$

and "det" stands for the determinant of the corresponding matrix. The quantities F^{α} have been expressed in terms of the physical quantities measured by \mathcal{O}_E which are the conserved variables. It is worthwhile, for numerical purposes, to point out, that the sources do not contain any differential operator acting on the components of w, which is a fundamental condition for preserving, numerically, the hyperbolic character of the system.

Concluding remarks

It has been presented that the most fundamental elements of the mathematical structure of multidimensional general relativistic hydrodynamics as a hyperbolic system of conservation laws. The analysis acquires an outstanding relevance in the context of numerical relativistic astrophysics. This study has been carried out in terms of the $\{3+1\}$ formalism, which is well suited for the solution of the Einstein field equations. The

spectral decomposition of the Jacobian matrices of the system, necessary to build up a Riemann solver and for taking advantage of the local characteristic approach, have been explicitly derived.

Acknowledgements

I would like to thank Dr Khin Khin Win, Professor and Head, Department of Physics, University of Yangon, for her kind permission and encouragements to carry out this work.

I would like to thank my respected Dr Aye Aye Thant, Professor, Department of Physics, University of Yangon, for her encouragements to carry out this work.

Special thanks are due to Professor, Dr Thant Zin Naing, Retired Pro-rector(Admin), International Theravā da Buddhist Missionary University, for his valuable guidance and helpful advice to carry out this work.

References

- Freying, B., Steffen, M., Ludwig, H.G., et al.(2012), Journal of Computational Physics, 231,919
- Papadopoulos, P. and Font, J. A. Relativistic Hydrodynamics around Black Holes and Horizon Adapted Coordinate Systems. arXiv. (1998).
- Radice, D., and Rezzolla, L., Discontinuous Galerk in Methods for General Relativistic Hydrodynamics: Formulation and Application to Spherical Symmetric Spacetimes, Phys. Rev. D 84, 024010 (2011)
- Radice, D., and Rezzolla, L., THC: a New High-Order Finite-Difference High- Resolution Shock-Capturing Code for Special-Relativistic Hydrodynamics, A&A547, A26 (2012)
- Rossmanith, J. A. High-Order Residual Distribution Schemes for Steady 1D Relativistic Hydrodynamics. Hyperbolic Problems: Theory, Numerics, and Applications (2006)

SIMPLE SIMULATIONS OF MASSLESS SCALAR FIELD MINIMALLY COUPLED TO GRAVITATIONAL FIELD

Naing Naing Wint Htoon¹, Thant Zin Naing²

Abstract

Simple simulations have been implemented for Massless Scalar Field Minimally Coupled to Gravitational Field within the framework of general relativity and astrophysics. Distinct features of 1-D Einstein-Klein-Gordon (EKD) system have been utilized and interesting simulations for physical properties have been carried out.

Keywords: Massless scalar field, 1-D Einstein-Klein-Gordon system

Introduction

Black hole spacetimes are spacetimes possessing remarkable properties. The four laws of black hole mechanics and their relation to the familiar thermodynamical ones suggest a deep connection between gravity, quantum physics, and thermodynamics a connection that despite persistent efforts still has not been fully understood (Alan R. Parry,2012). If the Cosmic Censorship Hypothesis (V. F. Mukhanov, 2000) holds true.

Black hole spacetime is not an exclusive property of the vacuo or electrovacuo Einstein's equations. Einstein's gravity coupled to scalar or other fields admits called hairy family of black holes. However, here matters are not yet on a firm state as for the vacuum or electrovacuum case. Even though a number of uniqueness theorems for particular field configurations have been established,(R.Dave,1998), their classification is for the moment open and mathematically challenging problems are likely to persist for some time . The absence of black hole states within the Einstein- Maxwell system possessing an ergoregion disconnected from the event horizon has been settled only relatively recently with the work of Sudarsky and Wald.

In this work we shall assume that the external matter is endowed with a scalar charge distribution so that the same spacetime region is permeated by a massless scalar field Φ obeying the Einstein-Klein-Gordon equations. We shall show that such a region can be described by a spacetime (M, g, Φ) with

^{1.} Dr, Lecturer, Department of Physics, University of Yangon, Myanmar.

^{2.} Retired Pro-Rector (Admin), International Theravā da Buddhist Missionary University, Yangon.

 (g, Φ) particular static axisymmetric solutions of the Einstein-Klein-Gordon system admitting an isometric extension into a larger manifold (M', g', Φ') possessing a regular $R \times S^2$ bifurcating Killing horizon. This bifurcating regular Killing horizon may be elevated to the status of an event horizon and thus (M', g', Φ') may be interpreted as representing the spacetime near the

event horizon of a distorted black hole of the Einstein-Klein-Gordon system. In this work we construct two families of such solutions characterized by an infinite set of parameters interpreted as describing the structure of the perturbing distribution of matter as well as the structure of the scalar charge distribution responsible for the field Φ .

Static-Axisymmetric Solutions of the Einstein-Klein-Gordon **Equations, Admitting a Bifurcating Killing Horizon**

The Einstein-Klein-Gordon minimally coupled to gravity field equations on a spacetime M are described by

$$G_{\mu\nu} = k(\nabla_{\mu}\Phi\nabla_{\nu}\Phi - \frac{1}{2}g_{\mu\nu}\nabla^{\sigma}\Phi\nabla_{\sigma}\Phi), \qquad (1)$$
$$\nabla_{\mu}\nabla_{\nu}\Phi = 0 \qquad (2)$$

For any nonsingular, minimally C^2 solution (g, Φ) of the above equations admitting two hyper surfaces orthogonal, commuting, and orthogonal Killing vector fields, a timelike one ξ_i and a spacelike ξ_{φ} chart (t, φ, x^1, x^2) can be constructed so that $\xi_t = \frac{\partial}{\partial t}$, $\xi_{\varphi} = \frac{\partial}{\partial \varphi}$, and g takes the Weyl canonical form:

$$g = -e^{2U}dt^{2} + r^{2}e^{-2U}d\varphi^{2} + e^{2(V-U)}(dr^{2} + dz^{2}), \qquad (3)$$

where U = U(r, z), V = V(r, z), and points on the manifold where r=0 define the symmetry axis associated with the rotational Killing field ξ_{φ} . Relative to this local chart, equations (1) and (2) implies that U = U(r, z), $\Phi(r, z)$ and V = V(r, z), satisfy

$$\frac{\partial^2 U}{\partial r^2} + \frac{\partial^2 U}{\partial z^2} + \frac{1}{r} \frac{\partial U}{\partial r} = 0, \qquad (4)$$

$$\frac{\partial^2 \Phi}{\partial r^2} + \frac{\partial^2 \Phi}{\partial z^2} + \frac{1}{r} \frac{\partial \Phi}{\partial r} = 0,$$
(5)

$$\frac{\partial V}{\partial r} = r \left\{ \left(\frac{\partial U}{\partial r} \right)^2 + \left(\frac{\partial U}{\partial z} \right)^2 + \frac{k}{2} \left[\left(\frac{\partial \Phi}{\partial r} \right)^2 - \left(\frac{\partial \Phi}{\partial z} \right)^2 \right] \right\}, \quad (6)$$

$$\frac{\partial V}{\partial r} = r \left[2 \frac{\partial U}{\partial r} \frac{\partial U}{\partial r} + k \frac{\partial \Phi}{\partial r} \frac{\partial \Phi}{\partial r} \right] \quad (7)$$

$$\frac{\partial V}{\partial z} = r \left[2 \frac{\partial U}{\partial r} \frac{\partial U}{\partial z} + k \frac{\partial \Phi}{\partial r} \frac{\partial \Phi}{\partial z} \right].$$
(7)

Equations (4) and (5) are recognized as the Laplace equations on Euclidean \mathbb{R}^3 equipped with cylindrical coordinates $\Phi(r, z)$ and once a choice of the harmonic functions (U, Φ) has been made, equations (6) and (7) determine V via quadratures. The integrability conditions for the existence of V are satisfied by virtue of equations (4) and (5).

Our goal is to construct solutions of equations (4) and (7) so that the resulting (g, Φ) admits an extension possessing a regular bifurcating Killing horizon. In order to identify such solution we consider an open subset $S = \{(r, z, \Phi) | r < a, z < b, ab \neq 0\}$ containing the origin of the Euclidean three space, where (r, z, Φ) are standard cylindrical coordinates and (a, b) arbitrary for the moment parameters. We then consider the product manifold $M \times R \times S$ and for any triplet (U, V, Φ) satisfying equations (4), (7) on *S*, we take their lifts on $M \times R \times S$. In view of equation (3) they define a static-axisymmetric metric *g* and a scalar field on $M \times R \times S$, satisfying the covariant equations (1) and (2). At first we require that the solutions (U, V, Φ) of equations(4) and (7) must be chosen so that the resulting (g, Φ) on $M = R \times S$ on (U, V, Φ) would satisfy the following:

(α) elementary flatness holds true on any point of the axis;

 (β) the spacetime $(R \times S, g, \Phi)$ is singularity free.

A point of departure for the specification of such a triplet is the observation that any regular axisymmetric harmonic functions, say, standing for field Φ on *S* can be represented in the form:

$$\Phi(r,z) \coloneqq \sum_{l=0}^{\infty} \alpha_l (r^2 + z^2)^{l/2} P_l \left(\frac{z}{\sqrt{r^2 + z^2}} \right), \tag{8}$$

where α_l , l = 0,1,... are arbitrary constants while P_l stands for the Legendre polynomials. We begin applying the above procedure by taking Φ as above and choosing for U the trivial harmonic function $U \equiv 0$. Despite this special choice, the function V resulting from the integration of equations (6) and (7) is rather complicated. For simplicity we shall employ hereafter a truncated version of equation (8) described by

$$\Phi(r,z) = \alpha_0 + \alpha_1 z + \alpha_2 (2z^2 - r^2).$$
(9)

Making use of this $\Phi(r, z)$, the integration of equations (6) and (7) combined with $U \equiv 0$ yields

$$V(r,z) = \frac{1}{4}kr^{2}[2\alpha_{2}^{2}r^{2} - (4\alpha_{2}z + \alpha_{1})^{2}] + V_{0}.$$
 (10)

By setting $V_0 = 0$ it follows immediately that V(r, z) is vanishing on the entire *z* axis. The so-constructed $U(r, z) \equiv 0$ combined with the metric

$$g = -dt^{2} + r^{2}d\phi^{2} + e^{2V(r,z)}(dr^{2} + dz^{2}).$$
 (11)

which is a static, axially symmetric metric admitting $\frac{\partial}{\partial t}$ as a timelike Killing vector field possessing complete orbits, commuting with the axial Killing field $\frac{\partial}{\partial \varphi}$, and both fields are hypersurface orthogonal. By virtue of the fact that V(r=0,z)=0 it is regular on the axis and moreover it can be checked directly that this g combined with described by equation (9) satisfies the covariant equations (1) and (2). A computation of the scalar invariants $R^{\alpha\beta\gamma\delta}R_{\alpha\beta\gamma\delta}$, $C^{\alpha\beta\gamma\delta}C_{\alpha\beta\gamma\delta}$, $R^{\alpha\beta}R_{\alpha\beta}$, and R yields

$$R^{\mu\nu\sigma\tau}R_{\mu\nu\sigma\tau} = 4C^{\mu\nu\sigma\tau}C_{\mu\nu\sigma\tau} = 3R^{\mu\nu}R_{\mu\nu} = 3R^2$$
(12)

$$R = [4\alpha_2^2(r^2 + 4z^2) + 8\alpha_1\alpha_2 z + \alpha_1^2]e^{f(r,z)},$$
(13)

$$f(r,z) = \frac{1}{2}kr^{2}[2\alpha_{2}^{2}(8z^{2}-r^{2})+\alpha_{1}(8\alpha_{2}z+\alpha_{1})],$$

indicating a regular geometry on any point on $M = R \times S$. Extending the coordinates (r, z) over the entire plane, the resulting spacetime $(M = R \times R^3, g, \Phi)$ fails to be asymptotically flat and thus equations (9) and (11) appear to be of limited utility. However, by appealing to the partial linearity afforded by equations (4) and (7), they can used as a seed for the construction of more interesting families of staticaxisymmetric solutions of equations(1) and (2). In that regard we recall that the positive mass Schwarzschild metric in Weyl coordinates e(3) is described by

$$U_{BH} = \frac{1}{2} \ln \left(\frac{R_{+} + R_{-} - 2m}{R_{+} + R_{-} + 2m} \right)$$

$$V_{BH} = \frac{1}{2} \ln \left(\frac{(R_{+} + R_{-})^{2} - 4m^{2}}{4R_{+}R_{-}} \right)$$

$$R_{\pm}^{2} = r^{2} + (z \pm m)^{2},$$
(14)



Figure 1: Occupied Acceleration Kick of the Universe



Figure 2: Formal development profile of *a* in terms of pressure and energy density ρ^*

Concluding Remarks

To make this discussion precise, we need a model for the regular matter. In order to study stability questions, we need to know how the regular matter distribution changes as the wave dark matter distribution changes, and vice versa. For example, a relatively simple way to model regular matter is with another scalar field. There are others ways to model regular matter which we do not discuss here. We caution the reader that this second scalar field is only a practical device for approximately modeling the regular baryonic matter namely the gas, dust, and stars in a galaxy. In no way are we suggesting a second scalar field should exist physically. Furthermore, the parameters of this second scalar field are chosen simply to fit the regular matter distribution of a galaxy as well as possible.

Acknowledgements

I would like to thank Dr Khin Khin Win, Professor and Head, Department of Physics, University of Yangon, for her kind permission and encouragements to carry out this work.

I would like to express my gratitude to Professor Dr Aye Aye Thant, Professor, Department of Physics, University of Yangon, for her kind permission and encouragements to undertake this research paper.

Special thanks are due to Professor, Dr Thant Zin Naing, Retired Pro-Rector(Admin), International Theravā da Buddhist Missionary University, for his valuable guidance and helpful advice to carry out this work.

References

- Alan R. Parry., (2012) "Wave Dark Matter and Dwarf Spheroidal Galaxies". Ph.D.Duke University, arXiv:1311.6087 [gr-gc].
- C.Armendariz- Picon, V. F. Mukhanov and P.J. Steinhardt, (2000), "A Dynamical Solution to the Problem of a Small Cosmological Constant and Phys". Rev. Lett. 85, 4438 [arXiv: astro-phy/004134].
- R. R. Caldwell, R. Dave and P.J. Steinhardt, (1998) ,Phys. Rev.Lett. 80 ,1582 [astro-ph/ 9708069].
- S. Chandrasekhar, (1983), "The Mathematical Theory of Black Holes" ,Clarendon Press, Oxford.
- V. Moncrief, O. Rinne, (2009), "Regularity of the Einstein Equations at Future Null Infinity", Class. Quantum Grav. 26 125010.

SIMPLE ASTROPHYSICAL SIMULATIONS FOR COLLISIONLESS STELLAR SYSTEMS

Zaw Shin¹, Min Thaw Tar²

Abstract

Simple astrophysical simulations for stellar systems which are assumed to be collision less have been studied using N-body simulation techniques. Physical entities such as potential-density pair profiles for the dark halo and stellar bulge have been simulated and some interesting remarks are given.

Keywords: collision less stellar systems, N-body simulation, stellar disk, dark halo, stellar budge

Introduction

The underlying dynamics relevant in the astrophysical context for a system of N particles interacting gravitationally is typically Newton's law plus, in case, an external potential field (see however below for a discussion of N-body simulations in general relativity). The force F_i acting on particle i of mass m_i is:

$$\bar{\mathbf{F}}_{i} = -\sum_{j \neq i} \frac{\mathbf{Gm}_{i} \mathbf{m}_{j} (\bar{\mathbf{r}}_{i} - \bar{\mathbf{r}}_{j})}{\left| \bar{\mathbf{r}}_{i} - \bar{\mathbf{r}}_{j} \right|^{3}} - \bar{\nabla} \boldsymbol{\phi}_{ext} (\bar{\mathbf{r}}_{i})$$

$$\tag{1}$$

Where $G = 6.673 \times 10^{-11} \text{m}^3 \text{kg}^{-1} \text{s}^{-2} \text{is the gravitational constant, and } \phi_{\text{ext}} \text{ is the external potential.}$ The problem is thus a set of non-linear second order ordinary differential equations relating the acceleration $\frac{\partial^2 \bar{r}_i}{\partial t^2} = \frac{\bar{F}_i}{m_i}$ with the position of all the particles in the system. Once a set of initial condition is specified (for example the initial positions r_i and velocities $\bar{v}_i = \frac{\partial r_i}{\partial t}$ of all particles) it exists a unique solution, analytical only for up to two bodies, while larger N require numerical integration (e.g. see Press et al. 2007). However special care must be employed to ensure both accuracy and efficiency. In fact, the gravitational force (eq.1) presents a singularity when

¹ Dr, Lecturer, Department of Physics, Mandalar Degree College

² PhD Candidate, Department of Physics, University of Yangon

the distance of two particles approaches 0, which can lead to arbitrarily large relative velocities. In depend on the specific choice of initial conditions. In contrast, all singularities in linear ordinary differential equations are independent of initial conditions and thus easier to treat. Therefore constant time step methods are unable to guarantee a given accuracy in the case of gravitational dynamics and lead to unphysical accelerations during close encounters, which in turn may create unbound stars.

A shared adaptive time step scheme can correctly follow a close encounter, but the price is paid in terms of efficiency as all the other particles of the system are evolved on the timescale of the encounter, which may be several orders of magnitude smaller than the global timescale, resulting essentially in a freezing of the system. The singularity may be avoided by introducing a smoothing length in Eq. 1 (e.g. see Aarseth 1963), that is by modifying the gravitational interaction at small scales. For example:

$$\vec{F}_{i} = -\sum_{j \neq i} \frac{Gm_{i}m_{j}(\vec{r}_{i} - \vec{r}_{j})}{\left\{ \left| \vec{r}_{i} - \vec{r}_{j} \right|^{2} + \epsilon^{2} \right\}^{3/2}}$$
(2)

where $\epsilon > 0$ is the softening, or smoothing length, that is a typical distance below which the gravitational interaction is suppressed. To minimize the force errors and the global impact of the softening for distances larger than ϵ , finite size kernels that ensure continuous derivatives of the force may be employed (e.g., see Dehnen 2001). This strategy effectively suppresses binary formation and strong gravitational interactions, but at the price of altering the dynamics of the system.



Figure 1: The 3D Plot of Gravitational Force against distance



Figure 2: Snapshot - profiles of the evolution of \in for Gravitational force F

Timescales, Equilibrium and Collisionality

A system of N particles interacting gravitationally with total mass M and a reference dimension R (for example the radius containing half of the total mass) reaches a dynamic equilibrium state on a timescale comparable to a few times the typical time (T_{cr}) needed for a particle to cross the system $(T_{cr} \approx 1/\sqrt{GM/R^3})$. This is the response time needed to settle down to virial equilibrium, that is 2K/|W|=1, where K is the kinetic energy of the system $K = 1/2\sum_{i=1,N} m_i |\bar{v}_i|^2$, and W is its potential energy: $W = -1/2\sum_{i\neq j} Gm_i m_j / |\bar{r}_i - \bar{r}_j|^2$ (assuming no external field). If the system is initially out of equilibrium, this is reached through mixing in phase space due to fluctuations of the gravitational potential, a process called violent relaxation.

Once the system is in dynamic equilibrium a long term evolution is possible, driven by two-body relaxation. Energy is slowly exchanged between particles and the system tends to evolve toward thermodynamic equilibrium and energy equipartition. The timescale (T_{rel}) for this process depends on the number of particles and on the geometry of the system: $T_{rel} \propto N/\log(0.11N)T_{cr}$. N-body systems such as galaxies and dark matter halos have a relaxation time much longer than the life of the Universe and are thus considered collision less systems. Smaller systems, such as globular and open clusters, are instead collisional, as the relaxation time is shorter than their age. Two body relaxation is also suppressed when one particle in the system dominates the gravitational potential, such as in the case of solar system dynamics, where planets are essentially quasi-test particles. Close encounters between three or more particles not only contribute to energy exchange, but can also lead to the formation of bound subsystems (mainly binaries). The formation and evolution of a binary population is best followed through direct, unsoftened, N-body techniques. A self-gravitating N-body system made of single particles has a negative specific heat, that is it increases its kinetic energy as a result of energy losses. This is a consequence of the virial theorem and qualitatively it is analogous to the acceleration of a Earth artificial satellite in presence of atmospheric drag. A negative specific heat system is thermodynamically unstable and over the two body relaxation timescale it evolves toward a gravothermal collapse, creating a core-halo structure, where the core progressively increases its concentration, fueling an overall halo expansion. The collapse is eventually halted once three body interactions lead to the formation of binaries. The so called core collapsed globular clusters" are considered to be formed as a result of this mechanism.

Methods for cosmological N-body simulations

Cosmological N-body simulations play an important role in modern cosmology by providing vital information regarding the evolution of the dark matter: its clustering and motion, about properties of dark matter halos. The simulations are instrumental for the transition of the theoretical cosmology from an inspiring but speculative part of astronomy to the modern precision cosmology. In spite of more than 50 years of development, N-body methods are still a thriving field with invention of more powerful methods providing more accurate theoretical predictions.

Dark matter is important component of universe. All observational evidence indicates that it dominates dynamics of normal and dwarf galaxies clusters and groups of galaxies. At high red shifts it provided the force that drove the formation of first galaxies and quasars. The observed large filaments and giant voids all can be understood and explained if we combine the dynamics of dark matter with the predictions of the inflation model on the spectrum of primordial fluctuations.

The dark matter is likely made of particles that other than the gravity force do mot couple with the other matter. There may be some channel of interactions between dark matter particles resulting in annihilation and production of normal particles. However, even if present (no observational evidence so far), this channel is weak and the dark matter is (mostly) preserved over the evolution of the Universe.

How this dark matter evolves and how it forms different structures and objects was an active field of research for a very long time. The first (Somewhat) realistic N-body simulation collapse of a cloud of 300 self-interacting particles was done by P.J.E. Peebles Peebles (1970). Remember that at that time of the dawn of cosmology, there was no dark matter, the hot gas x-ray in clusters had not been yet discovered (it was discovered in 1971), there were no voids or superclusters. So the first N-body simulation had indicated that the force of gravity alone may be responsible for the formation of clusters of galaxies, which was a big step forward. It also discovered a problem the density profile in the model was not right: too steep. The Solution for this problem was continuous mass accretion on the forming cluster instead of a one-time event of collapse (Gunn & Gott 1972)

From that moment the simulations took off. Larger and larger numbers of particles were used as new codes and new computers became available. For some time it looked almost like a sport: whose simulation has more "muscle". The pace has slowed down in recent years mostly because it became more difficult to analyse the simulations and to make the results accessible to the larger community. Development of numerical methods was crucial for advances in N-body simulations. At the beginning direct summation technique was used to run the simulations (Peebles1970;White 1976; Aarseth et al. 1979). At that time slower processors, no parallel computing it was difficult to make simulations with more than just a few thousand particles.

The main motivation at that time was to develop new computational methods. The number of operations in the direct summation method scales as $\propto N^2$, where N is the number of particles. So, one quickly ran out of available cpu. However, now the situation is different: processors are much faster and the number of cores on a workstation can be significant. A simulation with N = $10^5 - 10^6$ is relatively fast(from few hours to few days). Such simulations can be very useful for testing different ideas and for small runs. It is also very easy to modify the code because everything is very

transparent. For example, one can add external tidal force or modify the law of gravity. It is also a great tool for training students: a simple parallel pairwise summation code can be written in few hours. Particle-Mesh method a big step forward with cpu scaling $\propto N^2$ However, it requires a large 3D mesh for computation of the gravitational potential. The size of a cell in that mesh defines the force resolution, and, if one needs better resolution, the number of cells should be increased. As the result, one may run out of available computer memory. Still, the PM method is very fast and is easy to implement.

Cosmological N-body problem: main equations

In order to derive equations for the cosmological N-body problem, one can start with the equations of general relativity and derive equations of motion of self-gravitating nonrelativistic particles in the expanding Universe. For the case of nonrelativistic matter and the weak-field limit, we simply arrive at the Newtonian equations. There are some limitations with this approach: we cannot treat relativistic particles and we neglect time needed for gravitational perturbations to travel from one point to another effectively treating changes in the gravitational potential as instantaneous. However, these effects are not significant for most applications: velocities are typically well below relativistic and effects of the finite time of gravitational perturbations are small. We start with definitions, proper position r and comoving coordinates x are related:

$$\mathbf{r}(\mathbf{x},\mathbf{t}) = \mathbf{a}(\mathbf{t})\mathbf{x}(\mathbf{t}) \tag{3}$$

where a(t) is the expansion factor. Differentiating eq.(3) overtime, we get velocities:

$$\mathbf{v}(\mathbf{x}, \mathbf{t}) \equiv \dot{\mathbf{r}} = \mathbf{a}\dot{\mathbf{x}} + \dot{\mathbf{a}}\mathbf{x} = \mathbf{H}\mathbf{r} + \mathbf{v}_{\text{pec}}$$
(4)

Here $v_{pec} = a\dot{x}$ is the peculiar velocity and $H = \dot{a}/a$ is the Hubble constant. It is also useful to introduce the specific momentum defined as $p = a^2 \dot{x} = av_{pec}$

In cosmology we deal with a rather specific case of the N-body problem. Here discreteness of matter can be neglected. In general this is not the case with the two-body effects gradually accumulating over time. Systems studied in cosmology such as the nonlinear evolution of dark matter clustering do not suffer from the two-body scattering and can be treated using the collision less Boltzmann equation paired with the Poisson equation for the gravitational potential. In the comoving coordinates the Boltzmann equation describing the evolution of the distribution function f(x, p, t) can be written as:

$$\frac{\partial f}{\partial t} + x \frac{\partial f}{\partial x} - \nabla \phi \frac{\partial f}{\partial p} = 0$$
(5)

where peculiar gravitational potential $\phi(x)$ is related with the normal gravitational potential Φ as $\Phi = 2\pi G\rho_b r^2/3 + \phi$ where the first term is the potential of the background (constant over space) density field ρ_b and the second term is the deviation from the background. Changing coordinates from proper r to comoving x we can write the Poisson equation as:

$$\nabla^2 \phi = 4 \pi G a^2 (\rho(\mathbf{x}) - \rho_b) = 4 \pi G \frac{\Omega_0 \rho_{cr0}}{a} \delta_{dm}(\mathbf{x}, \mathbf{t})$$
(6)

Here $\delta_{dm} \equiv (\rho_{dm} (x, t) - \langle \rho_{dm} \rangle) / \langle \rho_{dm} \rangle$ is the dark matter density contrast. Factors Ω_0 and $\rho_{cr,0}$ are the average matter(dark matter plus baryons) density in the units of the critical density and the critical density all taken at the present moment a = 1.Note that the right hand side of eq.(6) may have a positive or negative sign. This is unusual considering that in a normal Poisson equation the density is always positive. The negative sign of the density term in eq.(6) happens in locations where the density is below the average density of the Universe. While there are no real negative densities in the Poisson equation, the regions with the negative r.h.s. of eq.(6) in comoving coordinates act as if there are. For example, in these regions the peculiar gravitational acceleration points away from the centre of an under dense region resulting in matter being pushed away from the centre. This explains why over time voids (large under dense regions) observed in the large-scale distribution of the dark matter become bigger and more spherical.


Figure 3: Snapshot -profiles of the evolution of ϕ for Gravitational Potential

The collision less Boltzmann equation eq.(5) is a linear first order partial differential equation in the 7-dimensionalspace (x,p, t). It has a formal solution in the form of characteristics: a set of curves that cover the whole space. The characteristics do not intersect and do not touch each other. Along each characteristic the value of the distribution function is preserved. In other words, if at some initial moment t_i we have coordinate x_i , momentum p_i , and phase-space density f_i , then at any later moment t along the characteristic we have $f(x, p, t) = f_i(x_i, p_i, t_i)$. Equations of the characteristics, the Piosson equation, and the Friedmann equation can be written as follows:

$$\frac{\mathrm{dx}}{\mathrm{da}} = \frac{\mathrm{P}}{\mathrm{a}^{3}\mathrm{H}}, \frac{\mathrm{dp}}{\mathrm{da}} = -\frac{\nabla\phi}{\mathrm{a}\mathrm{H}}(7)$$

$$\nabla^{2} \,\phi = \frac{3}{2} \frac{\mathrm{H}_{0}^{2}\Omega_{0} \,\phi \delta_{\mathrm{dm}}}{\mathrm{a}}(8)$$

$$H^{2} = H_{0}^{2}(\frac{\Omega_{0}}{a^{3}} + \Omega_{\Lambda,0}) \,\Omega_{0} + \Omega_{\Lambda0} = 1$$
(9)

Here we specifically assumed a flat cosmological model with the cosmological constant characterized by the density parameter, $\Omega_{\Lambda 0}$ at red shift z = 0.

There are numerical factors in eqs.(7-8) that obscure the fact that the equations of characteristics are nothing but the equations of motion of particles under the force of gravity. These equations are almost the equations of the N-body problem in the comoving coordinates. However, there are differences. Characteristics cover the whole phase-space which we cannot do in simulations that use a finite number of particles. Instead, we approximate the phase-space by placing particles at some positions and giving them initial momenta. How exactly we place the particles depends on the problem to be solved. For example, if a large simulation volume is expected to be resolved everywhere with the same accuracy, then particles should be nearly homogeneously distributed initially and have the same mass. If instead a small region should be resolved with a higher resolution than its environment, than we place lots of small particles in the region and cover the rest of the volume with few large particles. Because we intend to produce an approximate solution for the continuous distribution of matter in space as described by the Boltzmann-Poisson equations, we may not even think that we solve the N-body problem an ensemble of point masses moving under the force of gravity. For example, at the initial moment the volume of a simulation may be covered by many small non-overlapping cubes (not points). Then each cube is treated as a massive particle with some size, mass, and momentum. So, instead of N point masses we have N small cubes. This is definitely a better approximation for the reality. Indeed, these types of approximations are used in many simulations. For example, in Particle-Mesh(PM) simulations dark matter particles are small cubes with constant density and size. In Adaptive Mesh Refinement (AMR) codes particles are also cubes with the size of the cube decreasing in regions with better force resolution. The last clarification is related to the baryons. In order to treat the baryons properly, we need to include equations of hydrodynamics and add gas density to the Poisson equation. We clearly do not do it in N-body simulations. Still, we cannot ignore baryons. They constitute a significant fraction of mass in the Universe. If we neglect baryons, there will be numerous defects. For example, they growth rate of fluctuations even on large scales will be wrong and virial masses will not be correct. In cosmological N-body simulations we assume that all the mass-dark matter and baryons is in particles and each particle

represents both dark matter and baryons with the ratio of the two being equal to the cosmological average ratio.

Simple N-body problem: pair-wise summation

We start discussion of numerical techniques with a very simple case: forces are estimated by summing up all contributions from all particles and with every particle moving with the same time-step. The computational cost is dominated by the force calculations that scale as N², where Nis the number of particles in the simulation. Because of the steep scaling, the computational cost of a simulation starts to be prohibitively too large for $N \ge 10^6$ However, simulations with a few hundred thousand particles are fast, and there are numerous interesting cases that can be addressed with N $)10^6$ particles. Examples include major-mergers of dark matter halos, collisions of two elliptical galaxies, and tidal stripping and destruction of a dwarf spheroidal satellite galaxy moving in the potential of the Milky Way galaxy. In these cases it is convenient to use proper, not commoving coordinates.

The problem that we try to solve numerically is the following. For given coordinates r_{init} and velocities v_{init} of N massive particles at moment $t = t_{init}$ find their velocitiesv and coordinates r at the next moment $t = t_{next}$ assuming that the particles interact only through the Newtonian force of gravity. If r_i and m_i are the coordinates and masses of the particles, then the equations of motion are:

$$\frac{d^{2}r_{i}}{dt^{2}} = -G \sum_{j \neq i, i \neq j} \frac{m_{j}(\vec{r}_{i} - \vec{r}_{j})}{\left|\vec{r}_{i} - \vec{r}_{j}\right|^{3}}$$
(10)

Where G is the gravitational constant. Two steps should betaken before we start solving equations (8) numerically First, we introduce force softening: we make the force weaker ("softer") at small distances to avoid very large accelerations, when two particles collide or come very close to each other. This makes numerical integration schemes stable. Another reason for softening the force at small distances is that in cosmological environments, when one deals with galaxies, clusters of galaxies, or the large-scale structure,

effects of close collisions between individual particles are very small and can be neglected. In other words, the force acting on a particle is dominated by the cumulative contribution of all particles, not by a few close individual companions. There are different ways of introducing the force softening. For mesh-based codes, the softening is defined by the size of cell elements. For TREE codes the softening is introduced by assuming a particular kernel, and it is different for different implementations. The simplest and often used method is called the Plummer softening. It replaces the distance between particles $\Delta r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ in eq.(10)with the expression $(\Delta r_{ij} + \epsilon^2)^{\frac{1}{2}}$, where ϵ is the softening parameter.



Figure 4: The Revolution Plot of Acceleration against distance

Second, we need to introduce new variables to avoid dealing with too large or too small physical units of a real problem. This can be done in a number of ways. For mesh-based codes, the size of the largest resolution element and the Hubble velocity across the element give scales of distance and velocity. Here we use more traditional scaling. Suppose M and R are scales of mass and distances. These can be defined by a particular physical problem. For example, for simulations of an isolated galaxy M and R canbe the total mass and the initial radius. It really does not matter what M and R are. The scale of time t₀ is chosen t₀ = $(GM/R^3)^{-\frac{1}{2}}$. Using M, R, and t₀ we can change the physical variables r_i, v_i, m_i into dimensionless variables using the following relations

$$\vec{\mathbf{r}}_{i} = \tilde{\mathbf{r}} \,\vec{\mathbf{R}}, \mathbf{v}_{i} = \mathbf{v}_{i} \,\frac{\vec{\mathbf{R}}}{\mathbf{t}_{0}}, \mathbf{m}_{i} = \tilde{\mathbf{m}}_{i} \,\mathbf{M}, \mathbf{t} = \tilde{\mathbf{t}} \,\mathbf{t}_{0}$$
(11)

We now change the variables in eq. (10) and use the Plummer softening

$$\widetilde{g}_{i} = -\sum_{j=1}^{\infty} \frac{\widetilde{m}_{j} (\widetilde{r}_{i} - \widetilde{r}_{i})}{(\Delta r_{ij} + \widetilde{\epsilon}^{2})^{3}/2} , \frac{d\widetilde{v}_{i}}{d\widetilde{t}} = \widetilde{g}_{i}, \frac{d\widetilde{t}_{i}}{d\widetilde{t}} = \widetilde{v}_{i}$$
(12)

Where, \tilde{g}_i is the dimensionless gravitational acceleration. Note that these equations look exactly as eq (10), if we formally set G=1 and $\in = 0$.

The simplest, but not the best, method to derive the Green functions is to consider $\phi_{i,j,k}$ and $\rho_{i,j,k}$ as amplitudes of the Fourier components of the gravitational potential in the computational volume and then to differentiate the Fourier harmonics analytically. This gives

$$G_{0}(k) = -\frac{1}{k_{x}^{2} + k_{y}^{2} + k_{z}^{2}} = -\left(\frac{L}{2\pi}\right)^{2} \frac{1}{i^{2} + j^{2} + k^{2}}$$
(13)

where $(k_x, k_y, k_z) = (2\pi/L)(i, j, k)$ are components of the wave-vector in physical units. A better way of solving the Poisson equation is to start with the finite-difference approximation of the Laplacian ∇^2 . Here we use a the second order Taylor expansion for the spacial derivatives:

$$\nabla^{2}\phi = \frac{\partial^{2}\phi}{\partial x^{2}} + \frac{\partial^{2}\phi}{\partial y^{2}} + \frac{\partial^{2}\phi}{\partial z^{2}}$$

$$\approx \left[\phi_{\iota+I,j,\kappa} - 2\phi_{\iota,j,\kappa} + \phi_{\iota,j-I,\kappa} - 2\phi_{\iota,j,\kappa} + \phi_{\iota,j-I,\kappa} + \phi_{\iota,j,\kappa+I} - 2\phi_{\iota,j,\kappa} + \phi_{\iota,j,\kappa-I} + \phi_{\iota,j,\kappa+I} - 2\phi_{\iota,j,\kappa} + \phi_{\iota,j,\kappa-I} + \phi_{\iota,j,\kappa+I} + \phi_{\iota,j,\kappa+I}$$

This approximation leads to a large system of linear algebraic equations: $A\phi = 4\pi G\rho$, where ρ is the vector on the right hand side, ϕ is the solution, and A is the matrix of coefficients. The solution of this matrix equation can be found by applying the Fourier Transformation. This provides another approximation for the Green functions:

$$G_{1}(k) = \frac{\Delta x^{2}}{2} \times \left[\cos\left(\frac{2\pi i}{N_{grid}}\right) + \cos\left(\frac{2\pi j}{N_{grid}}\right) + \cos\left(\frac{2\pi k}{N_{grid}}\right) - 3 \right]^{-1}$$
(15)

For small (i, j, k) eq.(14) gives the same results as $\phi = 4\pi G\rho$. However, at (i, j, k) close to N_{grid} the finite-difference scheme G₁ provides less suppression

for high-frequency harmonics and thus gives a stronger and more accurate force at distances close to the grid spacing Δx . The computer memory puts constraints on the PM method because the method requires a large 3-dimensionalmesh of size N_{grid}^3 while the force resolution increases only as the first power of N_{grid} : $\Delta x = L/N_{grid}$, where L is length of the computational box. As we start to increase the resolution, we quickly run of the computer memory.



Figure 5: Snapshot -profiles of the evolution of k and Δx for Green Functions

Concluding Remarks

An alternative approach to implement the numerical solution of the N-body problem is to make use of the simple codes of Mathematica or MaTLab. For direct simulations this approach can be very effective, thanks to the fact that the bottle neck of computation is just the evaluation of the gravitational force, which has a very simple expression. The special purpose hardware can then be interfaced with a general purpose computer, which takes care of all the other numerical operations required to solve the equations of motions. It can be seen, from the snapshot-profiles, the virulent notice of gravitational field, gravitational acceleration etc,...In this paper, it has been attempted to carry out simple N-body simulation using simple Mathematica built in codes such as List Plot, List Animate, Bessel J and other simple coding commands.

Acknowledgements

I am highly grateful to Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her kind permission to do and her encouragement to carry out this paper.

I would like to thank Professor Dr Aye Aye Thant, Department of Physics, University of Yangon, for her valuable guidance, kind encouragement, valuable help, and support in this paper.

Special thanks are due to Professor, Dr Thant Zin Naing, Retired Pro-Rector (Admin), International Theravāda Buddhist Missionary University, for his valuable guidance and helpful advice to carry out this work.

References

Aarseth S. J., Turner E. L., Gott III J. R., (1979), ApJ, 228,664

Appel A. W., (1985), SIAM Journal on Scientific and Statistical Computing, vol. 6, no.1, January 1985, p. 85-103.,6, 85

Bagla J. S., (2002), Journal of Astrophysics and Astronomy, 23, 185

Peebles P. J. E., (1970), AJ, 75, 13

Planck Collaboration et al., (2013), ArXiv e-prints

GRAVITATIONAL COLLAPSE IN SELF-SIMILAR SPACETIMES

Htwe Nwe Oo¹ and Thant Zin Naing²

Abstract

Attempts are made to give an alternative description of self-similar spacetimes which is proving to be very substantial and useful in astrophysics and general relativity. The metric for collapsing dust cloud is utilized in this formalism. The nature of gravitational collapse in self-similar spacetimes has been studied in detail and relevant physical interpretations of the results obtained are given. Some interesting results of the calculation have been visualized.

Keywords: self-similarity, gravitational collapse, collapsing dust, homothetic killing vector.

Introduction

Gravitational collapse is an important issue in general relativity and it is widely believed that it may be responsible for high energy objects in our universe. Energy theorems in relativity have shown that under reasonable energy conditions a matter cloud with sufficient mass would undergo a gravitational collapse. General relativistic field equations involve a system of highly nonlinear partial differential equations and hence analyzing a gravitational collapse scenario in general even in spherically symmetric spacetime is virtually impossible. Self-similar spacetimes have therefore been given considerable attention in recent applications. Due to the symmetry property of self-similarity equations in self-similar spacetime become an ordinary differential equation and therefore the study of a phenomena becomes much easier to analyze. In this study we therefore use self-similar spherically symmetric spacetimes to examine the gravitational collapse and its features. In astrophysics and cosmology the self-similar models are of great interest to the relativists and cosmologist alike. It is worthy to start with the very definition of self-similar spacetimes. A self-similar spacetimes is characterized by the existence of a homothetic killing vector field (Joshi, 1993).

^{1.} Dr, Assistant Lecturer, Department of Physics, Yangon University of Education.

^{2.} Retired Pro-rector (Admin), International Theravā da Buddhist Missionary University, Yangon

Self-Similar Spacetimes and Path of Photon

A spherical symmetric spacetimes is self-similar if it admits a radial area coordinate r and an orthogonal time coordinate t such that for the metric components g_{tt} and g_{rr} we have

$$g_{tt}(kt,kr) = g_{tt}(t,r)$$
$$g_{rr}(kt,kr) = g_{rr}(t,r)$$

for all k > 0. Thus, along the integral curves of the killing vector field all points are similar.

A spherical symmetric spacetimes (SSS) in co-moving coordinates is given by general form

$$ds^{2} = -A(t, r)dt^{2} + B(t, r)dr^{2} + r^{2}C(t, r)d\Omega^{2}$$

where $d\Omega^2 = d\theta^2 + \sin^2\theta d\phi^2$. If SSS is self-similar, self-similarity condition must hold, it must have a homothetic killing vectors, which means $t \rightarrow kt, r \rightarrow kr$ and the metric becomes,

$$ds^{2} = -A(kt,kr)dt^{2} + B(kt,kr)dr^{2} + r^{2}C(kt,kr)d\Omega^{2}$$

and parameters A,B,C are such that

$$A(t, r) = A(kt, kr)$$
$$B(t, r) = B(kt, kr)$$
$$C(t, r) = C(kt, kr)$$

The collapsing dust cloud is described by the self-similar metric,

$$ds^{2} = -dT^{2} + R^{2}dr^{2} + R^{2}(d\theta^{2} + \sin^{2}\theta d\phi^{2})$$
(1)

where

$$R^{\frac{3}{2}} = \frac{3}{2}\sqrt{F}(t_0(r) - t)$$
$$R^{\frac{3}{2}} = \frac{3}{2}\sqrt{F}\left(a - \frac{t}{r}\right)r^{\frac{3}{2}}$$

$$R = \left(\frac{3}{2}\right)^{\frac{2}{3}} F\left(a - \frac{t}{r}\right)^{\frac{2}{3}} r$$

To check the metric, one can proceed as follows:

$$A(t, r) = -1$$

$$A(kt, kr) = -1$$

$$A(kt, kr) = -1$$

$$A(t, r) = A(kt, kr)$$

$$B(t, r) = {R'}^2 = \left(\frac{3}{2}\right)^{\frac{2}{3}} F\left(a - \frac{t}{r}\right)^{-\frac{1}{3}} \left(\left(\frac{2t}{3r}\right) + \left(a - \frac{t}{r}\right)\right)$$

$$B(kt, kr) = \left(\frac{3}{2}\right)^{\frac{2}{3}} F\left(a - \frac{kt}{kr}\right)^{-\frac{1}{3}} \left(\left(\frac{2kt}{3kr}\right) + \left(a - \frac{kt}{kr}\right)\right) = {R'}^2$$

$$B(t, r) = B(kt, kr)$$

$$C(t, r) = \frac{R^2}{r^2} = \left(\frac{3}{2}\right)^{\frac{4}{3}} F^2 \left(a - \frac{t}{r}\right)^{\frac{4}{3}}$$

$$C(kt, kr) = \left(\frac{3}{2}\right)^{\frac{4}{3}} F^2 \left(a - \frac{kt}{kr}\right)^{\frac{4}{3}} = \frac{R^2}{r^2}$$

$$C(t, r) = C(kt, kr)$$

The above shows that the given metric is self-similar. The radial null geodesics in this metric is defined by $ds^2 = 0$ and $k^{\theta} = k^{\phi} = 0$ (Tolman, 1934). The geodesic equations for k^T and k^r from Lagrangian equation are

$$L = -k^{T^{2}} + R'^{2}k^{r^{2}} + R^{2}k^{\theta^{2}} + R^{2}sin^{2}\theta k^{\phi^{2}}$$
(2)
$$\frac{\partial L}{\partial T} = \frac{d}{d\lambda} \left[\frac{\partial L}{\partial k^{T}} \right]$$
$$k^{r^{2}} \frac{\partial R'^{2}}{\partial T} = \frac{d}{d\lambda} \left[\frac{\partial \left(-k^{T^{2}} \right)}{\partial k^{T}} \right]$$
$$\frac{dk^{T}}{d\lambda} + R'\dot{R}'k^{r^{2}} = 0$$
(3)

Similarly

$$\frac{\partial L}{\partial r} = \frac{d}{d\lambda} \left[\frac{\partial L}{\partial k^r} \right]$$

$$k^{r^2} \frac{\partial R'^2}{\partial r} = \frac{d}{d\lambda} \left[\frac{\partial \left(R'^2 k^{r^2} \right)}{\partial k^r} \right]$$

$$2R'R''k^{r^2} = 4R' \frac{dR'}{d\lambda} k^r + 2R'^2 \frac{dk^r}{d\lambda}$$

$$\frac{dk^r}{d\lambda} - \frac{R''}{R'} k^{r^2} + \frac{2}{R'} k^r + \left(\dot{R}' k^T + R'' k^r \right) = 0$$

$$\frac{dk^r}{d\lambda} - \frac{\dot{R}'}{R'} k^T k^r + \frac{R''}{R'} k^{r^2} = 0 \qquad (4)$$

Let k^a be tangent to radial null geodesics (i.e, $k^a k_a = 0 = k^a_{;b} k^b$) for the metric in equation(1) and $g_{ab} k^a k^b = 0$, for null condition. We have for radial null geodesics from equations (3) and (4),

$$g_{TT}k^{T^{2}} + g_{rr}k^{r^{2}} = 0$$

$$g_{TT}k^{T^{2}} = -g_{rr}k^{r^{2}}$$

$$\frac{k^{T^{2}}}{k^{r^{2}}} = \frac{-g_{rr}}{g_{TT}}$$

$$\frac{k^{T}}{k^{r}} = \sqrt{\frac{-g_{rr}}{g_{TT}}} = R'$$

$$k^{r} = \frac{1}{R'}k^{T}$$

$$\frac{k^{T}}{k^{r}} = R' \rightarrow \frac{dT}{dr} = R'$$

$$\frac{dk^{T}}{d\lambda} = -R'\dot{R}'k^{r'}$$

Where λ is affine parameter. The Kretschmann scalar of the metric is obtained as

$$K = \frac{16(21a^2r^2 - 10art + 5t^2)}{27(-3ar + t)^2(-ar + t)^4}$$

If we assume that r = r and t = ar, we get

$$K = \frac{16(21a^2r^2 - 10a^2r^2 + 5a^2r^2)}{27(-3ar + ar)^2(-ar + ar)^4}$$

Which gives us, $K = \infty$

Therefore, the points of unboundedness i.e., $K = \infty$ occur at (ar, r). Selfsimilarly implies that all variables of physical interest may be expressed in terms of the similarity parameter $X = \frac{t}{r}$.

$$X = \frac{t}{r}, \quad t = Xr$$
$$dt = Xdr + rdX$$
$$\frac{dt}{dr} = R'$$
$$\frac{Xdr}{dr} + \frac{rdX}{dr} = R'$$
$$X + \frac{rdX}{dr} = R'$$
$$\frac{rdX}{dr} = R' - X$$
$$\frac{dX}{dr} = \frac{R' - X}{r}$$
$$\int \frac{1}{r} dr = \int \frac{1}{R' - X} dX$$
$$ln r = -ln[-R' + X]$$

The above is the possible path of photon in gravitationally collapsing objects.



Figure: The profile of the Kretschmann **Figure:** The profile of the path scalar of the metric with an orthogonal of photon in gravitationally time coordinate t and a radial area collapsing objects coordinate r

Gravitational Collapse in Self-Similar Spacetimes

We would like to examine the determination of curvature strength of the naked singularity in order to decide on its seriousness and physical relevance and the mathematical calculations of Christoffel Symbols, Riemann Tensors, Ricci Tensors and Kretschmann Scalar of the metric.

The collapsing dust cloud is described by the self-similar metric,



profile Figure: of The homothetic coordinate R(t, r) in selfsimilar spacetimes.

the **Figure:** The profile of the homothetic coordinate R'(t, r) in self-similar spacetimes.

R

Here, **b** is constant and after differentiation we get

$$R' = \frac{b (3ar - t)}{3r(a - \frac{t}{r})^{\frac{2}{3}}}$$
(6)

From metric,
$$g_{11} = -1, g_{22} = {R'}^2$$

 $g_{33} = R^2, g_{44} = R^2 sin^2 \Theta$

To find some calculations, we have to use the following equations,

Christoffel Symbol are denoted by	$\nu, \Gamma^{\lambda}_{\mu\nu} = \frac{1}{2} g^{\lambda k} \big(g_{k\nu,\mu} + g_{\mu k,\nu} - g_{\mu\nu,k} \big)$
Riemann Tensor	$R_{abcd} = g_{d \in} R_{abc}^{\epsilon}$
Kritchmann Scalar	$K = R^{abcd} R_{abcd}$
Ricci Tensor $R_{\mu\nu}$	$= \Gamma^{\lambda}_{\mu\nu,\lambda} - \Gamma^{\lambda}_{\mu\lambda,\nu} + \Gamma^{\lambda}_{\mu\nu}\Gamma^{\sigma}_{\lambda\sigma} - \Gamma^{\sigma}_{\mu\lambda}\Gamma^{\lambda}_{\nu\sigma}$

Gravitatinal collapse of Bose-Einstein condensate dark matter halos

As a first step in the study of the time dynamics of the gravitationally bounded Bose-Einstein condensates, we have to chose a variational tril wave function. Instead of fixing it in an arbitrary way (by assuming, for example, that the initial density profile of the condensate has a Gaussian form), we require that $|\psi|^2$ satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla . \left(\rho \vec{\upsilon} \right) = 0 \tag{7}$$

For the density of the Bose-Einstein condensate we assume a general form

$$\rho(r,t) = \rho_0(t) + \rho_1(t)\rho_2(r), \tag{8}$$

where $\rho_0(t), \rho_1(t)$ and $\rho_2(r)$ are arbitrary functions of t and r to be determine. From a physical point of view, the trail density profile $\rho(t)$ is the sum of two terms, the first representing a "cosmological" type homogeneous term ρ_{hom} (t), while the second term ρ_{inhom} (t, r) represent the effect of the time-independent inhomogeneities in the dark matter halo. The inhomogeneous term is assumed to be separable in the variables t and r, so that $\rho_{inhmo}(t, r) = \rho_1(t)\rho_2(r)$.

Substitution in equations $\vec{v} = H(t)\vec{r}$ and $\rho(r,t) = \rho_0(t) + \rho_1(t)\rho_2(r)$, into the continuity equation Eq.(7) gives

$$\dot{\rho_0}(t) + 3\rho_0(t)\frac{\dot{R}(t)}{R(t)} + \rho_2(r) \times \left[\dot{\rho_1}(t) + 3\rho_1(t)\frac{\dot{R}(t)}{R(t)} + \frac{\dot{R}(t)}{R(t)}\rho_1(t)r\frac{\dot{\rho_2}(r)}{\rho_2(r)}\right] = 0$$
(9)

We determine the function $\rho_2(r)$ by imposing the condition $r\rho'_2(r)/\rho_2(r) = \text{constant} = \alpha > 0$, which leads first to

$$\rho_2(r) = \mathcal{C}_1 r^{\alpha},\tag{10}$$

where C_1 is an arbitrary constant of integration. Next we require that the term in the square bracket of Eq.(9) vanishes. Therefore, Eq.(9) gives the following two independent differential equations for the determination of the functions $\rho_0(t)$ and $\rho_1(t)$,

$$\dot{\rho_0}(t) + 3\rho_0(t)\frac{\dot{R}(t)}{R(t)} = 0, \tag{11}$$

And

$$\dot{\rho_1}(t) + (3 + \alpha)\rho_1(t)\frac{\dot{R}(t)}{R(t)} = 0, \qquad (12)$$

respectively. Hence, the general solution of Eq.(9) can be obtain as

$$\rho(r,t) = \frac{1}{R^{3}(t)} \Big[a_{0} + b_{0} \frac{r^{\alpha}}{R^{\alpha}(t)} \Big],$$
(13)

where a_0 and b_0 are arbitrary constants of integration. Since at the vacuum boundary of the condensate, where r = R(t), the density must satisfy the condition $\rho [R(t), t] = 0$, At ≥ 0 , we obtain for the two integration constants the condition $a_0 + b_0 = 0$.

Concluding Remarks

In this thesis some fundamental notions and basics of self-similar spacetime are given and attempts are made to derive the path of photon using simple tractable methods. The Kretschmann scalar is also calculated for spherical symmetric spacetimes metric. Self-similar solutions are derived and visualizations of some results are done with the help of mathematica. Autonomous phase plane, self-similar and scaling exact solutions with scalar field are given and some animation plots are visualized using mathematica.

Acknowledgement

I would like to thank Dr Khin Khin Win, Professor and Head, Department of Physics, University of Yangon, for her kind permission and encouragements to carry out this work.

I would like to thank Dr Aye Aye Myint, Rector, Yangon University of Education, for her kind permission and encouragements to carry out this work.

I would like to express my gratitude to Professor Dr Khin Swe Oo, Head of Department of Physics, Yangon University of Education, for her kind permission and encouragements to carry out this work.

Special thanks are due to Professor, Dr Thant Zin Naing, Retired Pro-rector (Admin), International Theravā da Buddhist Missionary University, for his valuable guidance and helpful advice to carry out this work.

References

Amendola L (1999) Phys Rev D 60 043501

Baenblatt G I (1996) Scaling "Self-similarity and Intermediate Astrophysics" (Cambridge: Cambridge University Press)

Joshi P S (1993) "Global Aspects in General Relativity" (Oxford: Clarendon Press)

Appendix

It is necessary to compute the Christoffel symbols for equation (1), from which we can get the curvature tensor. If we use labels (1,2,3,4) for (T, r, θ , ϕ) in the usual way, non zero Christoffel symbols are given by using Tensorpak. m package,

$$\begin{split} & \varGamma_{12}^{2} = \frac{2t}{3(3a^{2}r^{2} - 4art + t^{2})} \ , \varGamma_{13}^{3} = \frac{2}{-3ar + 3t} \ , \varGamma_{14}^{4} = \frac{2}{3ar + 3t} \ , \\ & \varGamma_{21}^{2} = \frac{2t}{3(3a^{2}r^{2} - 4art + t^{2})} \ , \varGamma_{22}^{4} = \frac{2b^{2}(3ar - t)t}{27r^{2}(ar - t) - (a - \frac{t^{2}}{r^{3}})} \ , \varGamma_{22}^{2} \\ & = \frac{2t^{2}}{-9a^{2}r^{3} + 12ar^{2} - 3rt^{2}} \ , \\ & \varGamma_{23}^{3} = \frac{3ar - t}{3ar^{2} - 3rt} \ , \varGamma_{24}^{4} = \frac{3ar - t}{3ar^{2} - 3rt} \ , \varGamma_{31}^{3} = \frac{2}{-3ar + 3t} \ , \varGamma_{32}^{3} \\ & = \frac{3ar - t}{3ar^{2} - 3rt} \ , \\ & \varGamma_{33}^{4} = -\frac{2}{3}b^{2}r\left(a - \frac{t}{r}\right)^{\frac{1}{3}} \ , \varGamma_{33}^{2} = \frac{3a(-ar + t)}{3ar - t} \ , \varGamma_{34}^{4} = \cot\theta \ , \varGamma_{41}^{4} \\ & = \frac{2}{-3ar^{2} + 3t} \ , \\ & \varGamma_{42}^{4} = \frac{3ar - t}{3ar^{2} - 3rt} \ , \varGamma_{43}^{4} = \cot\theta \ , \varGamma_{44}^{4} = -\frac{2}{3}b^{2}r\left(a - \frac{t}{r}\right)^{\frac{1}{3}}sin^{2}\theta \ , \varGamma_{44}^{2} \\ & = -\frac{3r(ar - t)sin^{2}\theta}{3ar - t} \ , \\ & \varGamma_{44}^{3} = -\cos\theta \sin\theta \ , \end{split}$$

From these we get the following nonvanishing components of the Riemanntensor

$$R_{1212} = \frac{2(3ar+t)}{9(3ar-t)(-ar+t)^2} , R_{1221} = -\frac{2(3ar+t)}{9(3ar-t)(-ar+t)^2} , R_{1313}$$
$$= -\frac{2}{9(-ar+t)^2} ,$$

$$\begin{split} R_{1331} &= \frac{2}{9(-ar+t)^2} \ , R_{1414} = -\frac{2}{9(-ar+t)^2} \ , R_{1441} = \frac{2}{9(-ar+t)^2} \ , R_{2112} \\ &= -\frac{2(3ar+t)}{9(3ar-t)(-ar+t)^2} \ , \\ R_{2121} &= \frac{2(3ar+t)}{9(3ar-t)(-ar+t)^2} \ , R_{2323} = \frac{4t}{9(-3ar-t)(-ar+t)^2} \ , R_{2332} \\ &= -\frac{4t}{9(-3ar-t)(-ar+t)^2} \ , \\ R_{2424} &= \frac{4t}{9(-3ar+t)(-ar+t)^2} \ , R_{2442} = -\frac{4t}{9(-3ar+t)(-ar+t)^2} \ , R_{3113} \\ &= \frac{2}{(3ar-3t)^2} \ , \\ R_{3131} &= -\frac{2}{(-3ar-3t)^2} \ , R_{3223} = -\frac{4t}{9(-3ar+t)(-ar+t)^2} \ , R_{3232} \\ &= \frac{4t}{9(-3ar+t)(-ar+t)^2} \ , \\ R_{3434} &= \frac{4}{9(-ar+t)^2} \ , R_{3443} = -\frac{4}{9(-ar+t)^2} \ , \\ R_{4224} &= -\frac{4t}{9(-3ar+t)(-ar+t)^2} \ , \\ R_{4244} &= -\frac{4}{9(-ar+t)^2} \ , \\ R_{4343} &= \frac{4}{9(-ar+t)^2}, \\ \\ R_{4343} &= \frac{4}{9(-ar+t)^2}, \\ \end{split}$$

We get non-zero values of Ricci Tensor

$$\begin{split} R_{11} &= -\frac{2}{3(3\ a^2r^2 - 4art + t^2)} \ , \\ R_{22} &= \frac{2b^2(-3ar + t)}{27r^2(ar - t)\left(a - \frac{t^2_3}{r}\right)} \ , \\ R_{33} &= -\frac{2b^2r(a - \frac{t}{r})^{\frac{1}{3}}}{9ar - 3t} \ , \\ \\ &= -\frac{2b^2r(a - \frac{t}{r})^{\frac{1}{3}}sin^2\theta}{9ar - 3t} \ , \\ \\ \\ Scalar Curvature is, \quad \\ R &= -\frac{4}{3(3a^2r^2 - 4art + t^2)} \ , \end{split}$$

and Krichman Scalar is, $K = \frac{16(21a^2r^2 - 10 art + 5t^2)}{27(-3ar+t)^2(ar+t)^2}$.

AXION DARK MATTER, CP VIOLATION PROBLEM IN QCD

Han Win Than¹ and Kyaw Zall Linn²

Abstract

Attempts are made to give a brief description of axion dark matter and its possible root from CP problem in strong interaction. First of all, the theoretical background of symmetry and symmetry breaking in particle physics have been reviewed in detail . Then, the role of Goldstone's theorem, Goldstone's bosons in Gauge theories are investigated. It has been shown that spontaneous symmetry breaking of gauge symmetry can be described by Higgs mechanism. The most popular solution to the CP problem in strong interaction : the addition of an additional $U(1)_{PQ}$ symmetric field and its quanta- axion is presented. A rough estimate of the axion mass is also conducted using currently available constraints on QCD and quantum cosmology.

Keywords: symmetry braking, Goldstone's theorem, Higgs mechanism, axion dark matter $U(1)_{PQ}$ symmetric field

Introduction

The axion is a hypothetical elementary particle postulated by the Peccei–Quinn theory in 1977 to resolve the strong CP problem in quantum chromodynamics (QCD). If axions exist and have low mass within a specific range, they are of interest as a possible component of cold dark matter. As shown by Gerard 't Hooft, strong interactions of the standard model, QCD, possess a non-trivial vacuum structure that in principle permits violation of the combined symmetries of charge conjugation and parity, collectively known as CP. Together with effects generated by weak interactions, the effective periodic strong CP-violating term, Θ , appears as a Standard Model input - its value is not predicted by the theory, but must be measured. However, large CP-violating interactions originating from QCD would induce a large electric dipole moment (EDM) for the neutron. Experimental constraints on the currently unobserved EDM implies CP violation from QCD must be extremely tiny and thus Θ must itself be extremely small. Since a priori Θ could have any value between 0 and 2π , this presents a "naturalness" problem for the standard model. Why should this parameter find itself so close to 0? (Or, why should QCD find itself CP-preserving?) This question constitutes what is known as the strong CP problem.

^{1.} Dr, Assistant Lecturer, Department of Physics, University of Yangon, Myanmar.

² Demonstrator, Department of Physics, University of Yangon, Myanmar.

In 1977, Roberto Peccei and Helen Quinn postulated a more elegant solution to the strong CP problem, the Peccei–Quinn mechanism. The idea is to effectively promote Θ to a field. This is accomplished by adding a new global symmetry (called a Peccei–Quinn symmetry) that becomes spontaneously broken. This results in a new particle, as shown by Frank Wilczek and Steven Weinberg, that fills the role of Θ , naturally relaxing the CP-violation parameter to zero. This hypothesized new particle is called the axion. The original Weinberg–Wilczek axion was ruled out. Current literature discusses the mechanism as the "invisible axion", which has two forms: KSVZ (Kim–Shifman–Vainshtein–Zakharov) and DFSZ (Dine–Fischler– Srednicki–Zhitnitsky).

It had been thought that the invisible axion solves the strong CP problem without being amenable to verification by experiment. Axion models choose coupling that does not appear in any of the prior experiments. The very weakly coupled axion is also very light because axion couplings and mass are proportional. The situation changed when it was shown that a very light axion is overproduced in the early universe and therefore excluded. The critical mass is of order 10^{-11} times the electron mass, where axions may account for the dark matter. The axion is thus a dark-matter candidate, as well as a solution to the strong CP problem. Furthermore, in 1983, Pierre Sikivie wrote down the modification of Maxwell's equations from a light stable axion and showed that axions can be detected on Earth by converting them to photons, using a strong magnetic field, the principle of the ADMX. Solar axions may be converted to x-rays, as in CAST. Many experiments are searching laser light for signs of axions.

Maxwell's equations with axion modifications

If magnetic monopoles exist then there is a symmetry in Maxwell's equations where the electric and magnetic fields can be rotated into each other with the new fields still satisfying Maxwell's equations. Luca Visinelli showed that the duality symmetry can be carried over to the axion-electromagnetic theory as well. Assuming the existence of magnetic charges and axions, Maxwell's equations read

Name	Equations
Gauss's Law	$\nabla . \left(E - c \kappa \theta B \right) = \frac{\rho_e}{\varepsilon_0}$
Gauss's Law for magnetism	$\nabla \left(B + \frac{\kappa}{c} \theta E\right) = \mu_0 \rho_m$
Faraday's Law	$\nabla \times (E - c\kappa\theta B) = -\partial_t \left(B + \frac{\kappa}{c} \theta E \right) - \mu_0 J_m$
Ampere-Maxwell Law	$\nabla \times \left(B + \frac{\kappa}{c} \theta E\right) = \frac{1}{c^2} \partial_t (E - c\kappa \theta B) + \mu_0 J_e$
Axion Law	$(\Box + m_a^2)\theta = -\kappa E.B$

Incorporating *the* axion has the effect of rotating the electric and magnetic fields into each other.

$$\begin{pmatrix} E^{\Box} \\ B^{\Box} \end{pmatrix} = \frac{1}{\cos\xi} \begin{pmatrix} \cos\xi & c\sin\xi \\ -\frac{1}{c}\sin\xi & cos\xi \end{pmatrix} \begin{pmatrix} E \\ B \end{pmatrix}$$

where the mixing angle \Box depends on the coupling constant \Box and the axion field strength $\boldsymbol{\theta}$

$tan\xi = -\kappa\theta$

By plugging the new values for electromagnetic field and into Maxwell's equations we obtain the axion-modified Maxwell equations above. Incorporating the axion into the electromagnetic theory also gives a new differential equation – **the axion law** – which is simply the Klein-Gordon Equation (the quantum field theory equation for massive spin-zero particles) with an source term.

A term analogous to the one that would be added to Maxwell's equations to account for axions also appears in recent (2008) theoretical models for topological insulators. giving an effective axion description of the electrodynamics of these materials. This term leads to several interesting predicted properties including a quantized magnetoelectric effect. Evidence

for this effect has recently been given in THz spectroscopy experiments performed at The Johns Hopkins University.

Gauge Transformation

Let G be a lie group, g is lie algebra and T^a the generators of the lie algebra where the index 'a' takes values from 1 to dim G.

$$[T^{a}, T^{b}] = if^{abc}T^{c}$$
$$Tr(T^{a} T^{b}) = \frac{1}{2} \delta^{ab}$$

The lie group is called abelian, if all structure constants f^{abc} vanish, it can be called non-abelian.

An example for abelian case in particle physics is given by QED with abelian group U(1) and, non-abelian case is given by QCD corresponding group SU(3). This non-abelian gauge group was first suggested by Yang and Mills in 1954 and the name called "Tang-Mills theory" which is another name of "Gauge theory".

The Search for QCD Axion

Dark matter remains the most compelling evidence of physics beyond the Standard Model (SM). Since we have only observed it through its gravitational effects, there is a wide range of possible dark matter candidates. A very interesting possibility is that dark matter is made of light bosonic fields which only interact extremely weakly with the SM. The QCD axion is a particularly well-motivated example of such weakly-coupled light fields.

Further, the axion makes the CP-violating QCD θ angle dynamical, with a minimum at θ = 0. Thus, the axion can naturally explain the severe constraints on CP violation in the strong sector, $\theta \le 10^{-10}$, from null measurements of the neutron/Hg electric dipole moments.

The mass of the QCD axion is set by its decay constant f_a . Its couplings to other SM fields are model-dependent, but are expected to be given by higher-dimension operators suppressed by f_a . Astrophysical observations impose a lower bound on the decay constant, $f_a \ge 10^9 \text{GeV}$ for generic couplings. On the other hand, axion decay constants of $f_a > 10^{12} \text{GeV}$ predict a dark matter abundance in excess of observations for generic initial

conditions. These two considerations determine the axion window, $10^9 \text{GeV} < f_a < 10^{12} \text{GeV}$.

 $\begin{aligned} & \mathsf{Table}\Big[\mathsf{Plot3D}\Big[\mathsf{BesselJ}\Big[\theta, \left(\mathfrak{m}^{2} \phi + \lambda \phi^{3}\right)\Big], \{\mathfrak{m}, \mathbf{1}, \mathbf{10}\}, \{\lambda, .5, 5\}, \mathsf{PlotRange} \rightarrow \{.01, .2\}, \\ & \mathsf{PlotLabel} \rightarrow \mathsf{Row}[\{"\phi=", \mathsf{PaddedForm}[\mathbf{1} \star \phi, 3]\}], \mathsf{Axes} \rightarrow \mathsf{True}, \mathsf{AxesLabel} \rightarrow \Big\{"\mathfrak{m}", "\lambda", "\frac{\partial \mathsf{V}}{\partial \phi}"\Big\}, \\ & \mathsf{ColorFunction} \rightarrow \mathsf{Function}[\{x, y, z\}, \mathsf{Hue}[\mathsf{Mod}[z, \mathbf{1}]]\}, \mathsf{ColorFunctionScaling} \rightarrow \mathsf{True}, \\ & \mathsf{DisplayFunction} \rightarrow \mathsf{Identity}\Big], \{\phi, \mathbf{1}, 9\}\Big] \end{aligned}$







Figure: Evolution of potential energy with respect to scalar function ϕ .

Conclusions

Axion-like bosons could have a signature in astrophysical settings. In particular, several recent works have proposed axion-like particles as a solution to the apparent transparency of the Universe to TeV photons. It has also been demonstrated in a few recent works that, in the large magnetic fields threading the atmospheres of compact astrophysical objects (e.g., magnetars), photons will convert much more efficiently. This would in turn give rise to distinct absorption-like features in the spectra detectable by current telescopes. A new promising means is looking for quasi-particle refraction in systems with strong magnetic gradients. In particular, the refraction will lead to beam splitting in the radio light curves of highly magnetized pulsars and allow much greater sensitivities than currently achievable. Axions may be produced within neutron stars, by nucleon-nucleon bremsstrahlung. From the simulated work shows that the evolution of potential energy with respect to scalar function is highly turbulent and rapidly changing nature.

Acknowledgement

I would like to thank Dr Khin Khin Win, Professor and Head, Department of Physics, University of Yangon, for her kind permission and encouragements to carry out this work.

I would like to thank Dr Aye Aye Thant, Professor, Department of Physics, University of Yangon, for her kind permission and encouragements to carry out this work.

Special thanks are due to Professor, Dr Thant Zin Naing, Retired Pro-rector (Admin), International Theravā da Buddhist Missionary University, for his valuable guidance and helpful advice to carry out this work.

References

- Abbott, L.; Sikivie, P. (1983). "A cosmological bound on the invisible axion". *Physics Letters* B. 120 (1-3): 133–136. Bibcode:1983PhLB..120..133A. doi:10.1016/0370-2693(83)90638-X.
- C. A. Baker et al., \An Improved experimental limit on the electric dipole moment of the neutron," Phys. Rev. Lett. 97 (2006) 131801, arXiv:hep-ex/0602020 [hep-ex].
- Duffy, Leanne D.; van Bibber, Karl (2009). "Axions as dark matter particles". New Journal of Physics. 11 (10): 105008. arXiv:0904.3346
- Georg; Beltrán, Berta. Axions: Theory, Cosmology, and Experimental Searches. Lecture Notes in Physics. 741. pp. 3–17. arXiv:hep-ph/0607268
- Peccei, R. D. (24 July 2006). "The Strong CP Problem and Axions". In Kuster, Markus; Raffelt,

SIMPLE SIMULATIONS OF MAGNETOHYDRODYNAMICS IN STAR FORMATIONS

San San Maw¹, Thant Zin Naing²

Abstract

Attempts have been made to implement simple simulations of MHD in star formations. Some simple and tractable numerical method is utilized to make the simulation more realistic and physically acceptable. Detailed coding are given in the Appendix.

Keywords: MHD, HFMWDs, simulation, white dwarfs

Introduction

The magnetohydrodynamics is the study of the magnetic properties and behavior of electrically conducting fluids. Examples of such magnetofluids include plasmas, liquid metals, salt water, and electrolytes. The word "magnetohydrodynamics" is derived from magneto-meaning magnetic field, hydro-meaning water, and dynamics meaning movement. The field of MHD was initiated by Hannes Alfven, for which he received the nobel Prize in Physics in 1970.

The fundamental concept behind MHD is that magnetic fields can induce currents in a moving conductive fluid, which in turn polarizes the fluid and reciprocally changes the magnetic field itself. The set of equations that describe MHD are a combination of the Navier-Strokes equations of fluid dynamics and Maxwell's equations of electromagnetism. These differential equations must be solved simultaneously, either analytically or numerically.

The Equations of Ideal MHD

The equations of ideal MHD describe the movement of a compressible conducting fluid subject to magnetic fields. In ideal MHD all dissipative processes are neglected, meaning that the fluid possesses no viscosity and its conductivity is assumed to be infinite. The ideal MHD equations (Strang, 1968).

^{1.} Dr, Assistance Lecturer, Department of Physics, West Yangon University.

^{2.} Retired Pro-rector (Admin), International Theravā da Buddhist Missionary University, Yangon.

$$\frac{\partial \rho}{\partial t} = \nabla .(\rho v) = 0 \tag{1}$$

$$\frac{\partial \rho v}{\partial t} + \nabla (v \rho v - bb) + \nabla P_{tot} = -\rho \nabla \phi$$
⁽²⁾

$$\frac{\partial E}{\partial t} + \nabla [(E + P_{tot})v - b(v.b)] = -\rho v. \ \nabla \phi$$
(3)

$$\frac{\partial b}{\partial t} - \nabla \times (v \times b) = 0 \tag{4}$$

expressing the conservation of mass, momentum, energy and magnetic flux, respectively. Here ρ is the mass density, v the velocity and $E = \rho e + \frac{\rho}{2}v^2 + \frac{b^2}{2}$ the total energy density being, the sum of internal, kinetic and magnetic energy densities. The magnetic field is given by $B = \sqrt{4\pi b}$ and $P_{tot} = p + \frac{b^2}{2}$ is the total pressure, being the sum of the gas pressure and the magnetic pressure. For the equation of state (EoS) one assumes an ideal gas law

$$p = \rho e(\gamma - 1), \tag{5}$$

where γ is the ratio of specific heats. General EoSs can be included, which is especially important for the simulation of CCSN where the EoS has to describe stellar matter in the very broad range of conditions prevailing during this event. The right hand side of the momentum and energy conservation equations detail the effect of gravitational forces onto the conserved variables.

The MHD equation (1) to equation (4) conserve the divergence of the magnetic field so that an initial condition

$$\nabla . \ b = 0 \tag{6}$$

remains true, consistent with the physical fact that magnetic monopoles have never been observed.

Numerical Solution of the MHD Equations

The MHD equation form a set of non-linear hyperbolic equations, which can in general only be solved by numerical means. Before we start describing the individual solution operators, we first introduce our notation. We discretise time into discrete steps Δt^n and space into finite volumes or cells $V_{i,j,k}$ where *n* labels the different time levels and the triple (i, j, k)denotes a particular cell. The vector $u = (\rho, \rho v_x, \rho v_y, E)^T$ denotes the conserved fluid variables. The solution vector $u^n_{i,j,k}$ contains the spatially averaged values of the conserved variables at time *t* in cell $V_{i,j,k}$

$$u_{i,j,k} = \frac{1}{V_{i,j,k}} \int_{V_{i,j,k}} u(x,t) dx dy dz,$$
(7)

where the cell volume $V_{i,j,k} = \Delta x \Delta y \Delta z$ is given by the assumed constant cell dimensions $\Delta x = x_{i+1/2} - x_{i-1/2}, \Delta = y_{i+1/2} - y_{i-1/2}, \Delta z = z_{i+1/2} - z_{i-1/2}$. Half-integer indices denote the intercell boundary. Further we define the cell face averaged magnetic field components at time *t* by

$$(b_x)_{i+1/2,j,k} = \frac{1}{S_{i+1/2,j,k}} \int_{S_{i+1/2,j,k}} b_x(x,t) dy dz$$
(8)

$$(b_{y})_{i,j+1/2,k} = \frac{1}{S_{i,j+1/2,k}} \int_{S_{i,j+1/2,k}} b_{y}(x,t) dx dz$$
(9)

$$(b_z)_{i,j,k+1/2} = \frac{1}{S_{i,j,k+1/2}} \int_{S_{i,j,k+1/2}} b_z(x,t) dx dy$$
(10)

where $S_{i+1/2,j,k} = \Delta y \Delta z$ denotes the cell face of cell $V_{i,j,k}$ located at $x_{i+1/2}$ and spanned by the zone increments Δy and Δz .

In an operator-split scheme the solution algorithm to the ideal MHD equations can be summarized as

$$u^{n+2} = L_{forward} \ L_{backward} \ u^n, \tag{11}$$

where

$$L_{forward} = L_x(\Delta t) B_x^{yz}(\Delta t) L_y(\Delta t) B_y^{xz}(\Delta t) L_z(\Delta t) B_z^{xy}(\Delta t)$$
(12)

$$L_{backward} = L_z(\Delta t)B_z^{xy}(\Delta t)L_y(\Delta t)B_y^{zx}(\Delta t)L_{zx}(\Delta t)B_x^{yz}(\Delta t)$$
(13)

are the forward and backward operator for one time step. The operators $L_{x,y,z}$ evolve the fluid and account for the source terms, while the *B* operators evolve the magnetic field. If the individual operators are second order accurate, then the application of the forward followed by the backward operator is second order accurate in time (Landau & Lifschitz, 1991). The numerical solution algorithm to the MHD equations is explicit. Therefore we impose the following time step

$$\Delta t^{n} = k.\min_{i,j,k} \left(\frac{\Delta x}{C_{i,j,k}^{n,x}}, \frac{\Delta y}{C_{i,j,k}^{n,y}}, \frac{\Delta z}{C_{i,j,k}^{n,z}} \right),$$
(14)

where

$$C_{i,j,k}^{n,d} = \max(v_{d,i,j,k}^{n,d} + c_{Fi,j,k}^{n})$$
(15)

is the maximum speed at which information can travel in the whole computational domain in direction d = x, y, z being the sum of the velocity component in d and the speed of the fast magnetosonic waves c_F . We typically set the CFL number k to 0.75.

Solving the Fluid MHD Equations

The evolution of the fluid variables u in the x-direction, we neglect the source terms from gravity. During this process the magnetic field is held

constant and interpolated to cell centers. Then mass, momentum and energy conservation in x-direction can be written as

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = 0, \tag{16}$$

where

$$F = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + P_{tot} + b_x^2 \\ \rho v_x v_y - b_x b_y \\ \rho v_x v_z - b_x b_z \\ (E + P_{tot}) v_x - b_x b. v \end{bmatrix}$$
(17)

is the flux vector.

Integrating equation (16) over a cell $V_{i,i,k}$ gives

$$\frac{\partial u_{i,j,k}}{\partial t} + \frac{1}{\Delta x} (F_{i+1/2,j,k} - F_{i-1/2,j,k}) = 0,$$
(18)

where the definition of the cell averaged values of equation (7) has been substituted and Gauss' theorem has been used. The numerical flux $F_{i+1/2,j,k}$ represents an average flux of the conserved quantities through the surface $S_{i+1/2,j,k}$

$$F_{i+1/2,j,k} = \frac{1}{S_{i+1/2,j,k}} \int_{S_{i+1/2,j,k}} F(x,t) dy dz$$
(19)

at given time t. Equation (18) is a semi-discrete conservative scheme for the conservation law of equation (16). In the following we focus on obtaining the numerical fluxes in a stable and accurate manner. Time integration of the ordinary differential equation (18) will be addressed later in this subsection.

Many schemes for the stable and accurate computation of the numerical fluxes have been devised in the literature. Godunov type methods

achieve this by solving either exact or approximate Riemann problems at cell interfaces (Godunov, 1959, Laney, 1998 & Toro, 1997). Through solving the Riemann problem, these methods ensure an upwind discretisation of the conservation law and hence achieve causal consistency. Due to the difficulty of solving the Riemann problem in the ideal MHD case, the algorithm of (Pen, Arras, & Wong, 2003) uses the relaxation scheme of (Jin & Xin, 1995). For detailed information on these type of methods we refer to (Jin & Xin, 1995, LeVeque & Pelanti, 2001). The idea of the relaxation scheme is to replace a system like equation (18) by a larger system

$$\frac{\partial u}{\partial t} + \frac{\partial w}{\partial x} = 0, \tag{20}$$

$$\frac{\partial w}{\partial t} + D^2 \frac{\partial u}{\partial x} = \frac{1}{\varepsilon} (F(u) - w), \qquad (21)$$

called the relaxation system. Here, the relaxation rate ε is a small positive parameter and D^2 is a positive definite matrix. For small relaxation rates, system of equation (20) rapidly relaxes to the local equilibrium defined by w = F(u). A necessary condition for solutions of the relaxation system of equation (20) to converge in the small ε limit to solutions of the original system of equation (20) is that the characteristic speeds of the hyperbolic part of equation (20) are at least as large or larger than the characteristic speeds in system of equation (16). This is the so-called subcharacteristic condition.

As (Jin & Xin,1995) we choose D = d. *I* to be a diagonal matrix. In order to fulfill the subcharacteristic condition the diagonal element *d* or the so-called freezing speed is chosen to be

$$d = |v_x| + c_{F_1} \tag{22}$$

where c_F is the speed of the fast magnetosonic waves, i.e. the fastest wave propagation speed supported by the equations of ideal MHD.

The key point in the relaxation system is that in the local equilibrium limit it has a very simple characteristic structure

$$\frac{\partial}{\partial t}(w+Du) + D\frac{\partial}{\partial x}(w+Du) = 0,$$
(23)

$$\frac{\partial}{\partial t}(w - Du) - D\frac{\partial}{\partial x}(w - Du) = 0, \qquad (24)$$

where $w \pm Du$ are then the characteristic variables. They travel with the "frozen" characteristic speeds $\pm D$ respectively.

System of equation (23), (24) can be easily recast into an equation for u and w. However, we are practically only interested in that for u

$$\frac{\partial u}{\partial t} + \frac{\partial F^+}{\partial x} + \frac{\partial F^-}{\partial x} = 0, \qquad (25)$$

where $F^+ = (w+Du)/2$ denotes the right travelling waves and $F^- = (w-Du)/2$ the left travelling waves in the *x*-direction. In the following we shall drop the indices of the other directions. Since this defines an upwind direction for each wave component, a first order upwind scheme results from choosing $F_{i+1/2}^+ = F_i^+$ and $F_{i+1/2}^- = F_{i+1}^-$. In this case, the total flux at the cell interfaces is readily evaluated to become

$$F_{i+1/2} = F_{i+1/2}^{+} + F_{i+1/2}^{-} = \frac{1}{2} (F_i + F_{i+1}) - \frac{1}{2} D(u_{i+1} - u_i) , \qquad (26)$$

where $F_i = w_i = F(u_i)$. For D we use the freezing speed

$$d = \max(d_i, d_{i+1}) \tag{27}$$

in order to satisfy the subcharacteristic condition.

Conclusion Remarks

In this paper, simple simulations for magnetohydrodynamics (MHD) have been presented using simple iteration and simple mathematica coding to study the numerical nature of MHD equations and it is simply observed that some of the numerical simulations give interesting 2D and 3D graphics which show the physical nature of the equations.

Acknowledgements

I would like to thank Dr Khin Khin Win, Professor and Head, Department of Physics, University of Yangon, for her kind permission and encouragements to carry out this work.

I would like to thank Dr Tin Maung Tun, Rector, West Yangon University, for his kind permission and encouragements to carry out this work.

I would like to express my gratitude to Professor Dr Moe Ohnmar, Head of Department of Physics, West Yangon University, for her kind permission and encouragements to carry out this work.

Special thanks are due to Professor, Dr Thant Zin Naing, Retired Pro-rector (Admin), International Theravā da Buddhist Missionary University, for his valuable guidance and helpful advice to carry out this work.

References

- Godunov, S. K., (1959). A difference method for numerical calculation of discontinuous solutions of the equations of hydrodynamics. Mat. Sb. (N.S.), 47 (89):271-306.
- Jin, S. and Xin, Z., (1995). The relaxation schemes for systems of conservation laws in arbitrary space dimensions. Comm. Pure and Appl. Math., 48:235-276.
- Landau, L. D., Lifschitz, E. M., (1991). Lehrbuch der theoretischen Physik, 10 Bde., Bd.8, Elektrodynamik der Kontinua. Deutsch, Harri.
- Laney, C. B., (1998). Computational Gasdynamics. Cambridge University Press.
- LeVeque, R. J., Pelanti, M., (2001). A class of approximate riemann solvers and their relation to relaxation schemes. J. Comput. Phys., 172(2):572-591.
- Pen, U. L, Arras, P., and Wong, S., (2003). A free, fast, simple, and efficient total variation diminishing magnetohydrodynamic code. ApJS, 149:447-455.
- Strang, G., (1968). On the construction and comparison of difference schemes. SIAM J.Num. Anal., 5:506.
- Toro, E. F., (1997). Riemann Solvers and Numerical Methods for Fluid Dynamics. A Practical Introduction. Springer-Verlag.



Appendix

Figure 1: The profile of total pressure of the magnetic field in term of p and b.



Figure 2: The profile of total energy of the magnetic field in term of ρ and v.



Figure 3: The profile of solution vector $u^{n}_{i,j,k}$ contains the spatially averaged values.

SYNTHESIS AND CHARACTERIZATION OF DYE-SENSITIZED SOLAR CELL BASED ON SILVER OXIDE NANOWIRES

Zin Min Myat¹, Zin Min Tun², Than Than Win³ and Yin Maung Maung¹

Abstract

In this paper, silver oxide (Ag₂O) nanowires grown onto ITO glass substrate from aqueous solution of silver nitrate (AgNO₃) and sodium hydroxide (NaOH) were used in dye-sensitized solar cells. Ag₂O nanowires were fabricated by using chemical bath deposition method at 300 °C and 400 °C for 1 h. Ag₂O nanowires were fabricated by using chemical bath deposition method (CBD). Phase formation and crystal structure of silver oxide were characterized by XRD analysis. The surface morphology of silver oxide nanowires were examined by SEM. The prepared nanowires structures were dye-sensitized with dragon fruit and assembled into a dye-sensitizer. Absorption and transmission properties of extracted dyes and silver oxide nanowires were carried out with UV-Vis spectroscopy. The DSSCs were converted the energy in light absorbed by dyes or pigments into other form of energy. Conversion efficiency (η_{con}) and fill factor (FF) were measured and determined by using I-V characteristics. Silver oxide (Ag₂O) nanowires photo-electrodes with dragon fruit dye sensitizers for DSSCs exhibited the optimum values of conversion efficiency 0.67 % at 300 °C and 0.63 % at 400 °C at two temperatures and it might be dye to good performance of anthocyanin molecules. Photovoltaic properties of silver oxide (Ag₂O) nanowires cells were measured and it was expected to utilize the dye sensitized solar cells applications.

Keywords: Ag₂O nanowires, CBD method, XRD, SEM, UV-Vis, I-V characteristics

Introduction

Dye sensitized solar cells (DSSCs) can be defined as photoelectrochemical solar cells. The cell is composed of sandwich electrodes, which are photoelectrode, counter electrode, and a redox electrolyte system. Both electrodes are mainly made from a transparent conductive oxide (TCO) coated glass. Fluorine doped tin oxide (ITO) on glass substrate are well

^{1.} Dr. Assistant Lecturer, Department of Physics, University of Yangon

^{2.} Department of Physics, West Yangon University

³ Department of Physics, Mandalay University of Distance Education

known materials as TCO applications due to having few surface electrical resistivity (Ωm^{-2}) and good optical transmission on the whole solar spectrum.

A typical DSSC consists of a transparent conductive oxide (TCO), semiconductor oxide, dye sensitizer, electrolyte and counter electrode. The working electrode is a nanoporous semiconductor oxide that is placed on conducting glass and is separated from the counter electrode by only a thin layer of electrolyte solution. The extension of the photoelectrode dye enables the collection of lower-energy photons. The dye is chemisorbed onto the semiconductor oxide surface. An ideal sensitizer should absorb a wide range of wavelengths and possess high thermal stability due to its strong binding to the semiconductor oxide. The photoanode of DSSCs is typically constructed using a thick film (~10 μ m) of TiO₂ or, less often, ZnO or Ag₂O nanoparticles [Matudnmura M et al 1980].

Dye sensitized solar cell (DSSC) is a device for the conversion of visible light into electricity, based on the sensitization of wide band gap semiconductor. The performance of the cell mainly depends on a dye used as sensitizer. Dye-sensitized solar cells (DSSCs) based on semiconductor electrodes have been investigated since1960. DSSCs are unique compared with almost all other kinds of solar cells in that electron transport, light absorption and hole transport are each handled by different materials in the cells. The sensitizing dye in a DSSC is anchored to a wide-band gap semiconductor such as TiO₂, Ag_2O or ZnO [Regan B O et al 1991].

Materials and Methods

Preparation of Silver Oxide (Ag₂O) seed layer films

The precursor solution of silver oxide nanoparticles were coated onto the indium doped tin oxide (ITO) /glass substrates by spin coating method. Firstly, the ITO /glass substrates were cleaned in a mixture solution of hydrochloric acid (HCl) and nitric acid (HNO₃) for 5 min. And then the substrates were also cleaned in a solution of acetone. These substrates were rinsed with distilled water and dried at room temperature. The prepared silver oxide nanoparticles were dissolved with 2-methoxyethanol ($C_3H_8O_2$) as solvent to form viscous paste at 120 °C for 3 h. This viscous paste was then coated onto indium doped tin oxide (ITO) /glass substrates at 3000 rpm for
30 s by spin coating technique. Silver oxide colloidal solution was deposited onto chemically cleaned ITO conductive glass substrates. The seed layer coated films were annealed at 300 °C and 400 °C for 1h for diffusion films. The crystal structure and morphology of silver oxide (Ag₂O) films were confirmed by XRD and SEM analysis. Optical transmission spectra of the silver oxide films were recorded using a UV- vis spectrometer. The block diagram of preparation of silver oxide (Ag₂O) seed layer films was shown in Figure 1.

Preparation of Silver Oxide (Ag₂O) Nanowires Photoelectrode

Silver oxide (Ag₂O) nanowires were fabricated by chemical bath deposition method. Firstly, in order to grow Ag₂O nanowires, the seed layer films were used in this experiment. The prepared Ag₂O solution was synthesized by mixing of 50 ml silver nitrate and 20 ml of hexamethylenetetramine (C₆H₁₂N₄) solution with deionized water (DIW) by using chemical bath deposition method (CBD). For Ag₂O nanowire preparation, the seed layer films were subsequently dipped in a mixture solution and annealed at 80 °C for 10 h. During this period, the reaction heterogeneous growth of nanowires was limited by homogeneous nucleation of Ag₂O nanoparticles. Finally, the substrates were taken out from the growth solution and rinsed with deionized water and annealed at 300 °C and 400 °C for 1 h. The morphological characterization of Ag₂O nanowires were examined by Scanning Electron Microscopy (SEM).

Preparation of Natural Dye Sensitizers from Dragon Fruit

Dragon fruit was used dye extract in this work. Firstly, the oxide layer of dragon fruit skins was peeled off and washed with water and cut to get small pieces. The dragon fruit skins were cured in boil water at 100 °C for 30 min to be softer and enhanced colour. Fresh dragon fruit skins weight (50 g) were mixed into 50 ml of ethanol and equal weight of other skins were also mixed into 50 ml of distilled water at room temperature. The mixtures were annealed at 120 °C for 1 h until the mixture show homogeneous in colour. After cooling, the pH level of dragon fruit skins was measured with a pH meter and found to be 5 for ethanol and 6 for distilled water. The optical properties of natural dye-sensitizer were examined by UV-vis spectroscopy. The block diagram of extract dye from dragon fruit skin was shown in Figure 2.



Figure 1: Block diagram of Ag₂O nanostructure of seed layer films



Figure 2: The block diagram of extract dye from dragon fruit skin

Results and Discussion

XRD analysis of Silver Oxide Seed Layer Films

X- ray diffraction is a powerful technique for investigating the structure of crystalline materials. The upper side of XRD profile was represented the observed profile while the lower side indicated the standard JCPDF (Joint Committee on Power Diffraction Standards) library file. The dominant peaks were compared the data from the library (or) standard file. They were well matched with standard library profile. Figure 3 (a-b) showed the XRD spectrum of Silver Oxide (Ag₂O) seed layer films. The dominant peaks were well matched with the library (or) standard file. The most dominant peak was also occur at (111) peak. X-ray diffraction (XRD) demonstrated the cubic structure of the Ag₂O films. The crystallite size of silver oxide silver oxide seed layer films were calculated 23.16 nm at 300 °C and 20.44 nm at 400 °C.



Figure 3: (a) XRD spectrum of Ag₂O seed layer film at 300 °C



Figure 3: (b) XRD spectrum of Ag_2O seed layer film at 400 °C

SEM Analysis of Ag₂O Nanowire

Ag₂O nanowires onto indium doped tin oxide (ITO/glass) were carried out to examine by SEM analysis. Figure 4 (a-b) indicated the SEM micrograph of Ag₂O nanowires. From SEM image, it was observed that the diffusion wire was smooth, irregular shaped cylindrical grains. In order to study the morphology and nano structural properties of fabricated Ag₂O nanowires arrays grown at 300 °C and 400 °C for the same growing time. These figures showed the SEM micrographs with the respective diameter and the lengths of Ag₂O nanowire photoelectrode. The Ag₂O nanowires were disorderly, and had a wide size distribution. The growth temperature is the key parameter to dominate the diameter Ag₂O nanowires. It could be seen that the Ag₂O nanowires grown oriented on the substrates. It can be seen from these figures, different structural and morphological changes were observed. The diameter and the length distributions between the Ag₂O nanowires for different growth temperature exhibited a significant difference which shows growth dense nanowires with diameters between (365 nm- 450 1nm) at 300 °C and (175 nm- 236 nm) at 400 °C respectively. According these results, the morphologies of the nanowires were varied strongly and sharp with different growing temperature. As a result, it was obvious that Ag₂O nanowire was significantly formed onto Ag₂O seed layer films at different deposition temperature.



Figure 4: (a) SEM image of asprepared silver oxide nanowires at 300 °C

Figure 4: (b) SEM image of asprepared silver oxide nanowires at 400 °C

UV-vis Analysis of dye solutions from dragon fruit skins

The absorption spectrum and the energy band gap of dragon fruit dyes were performed using UV-vis spectrometer (SMIMADZU). Figure 5 (a-b) shows the absorption spectra of distilled water and ethanol and the dye's ability to absorb photons from visible light spectrum. It was found that the maximum absorption of wavelength obtained by distilled water is about 533 nm and slightly red shifted compared to ethanol with the peak wavelength of 535 nm. Dragon fruits dye which is extracted using ethanol is resulted in deep coloured solutions. The wavelength range of spectrum laid between 400 nm to 700 nm. The dragon fruit showed good absorption level between 500 nm and 600 nm wavelength. Basically, the absorption was due to anthocyanin obtained in the dragon fruit. The measured and calculated values of UV-vis spectrum were described in Table 2.

 Table 2: Optical band gap energy and absorption coefficient of dragon fruit skin dye

Dyes	Extract solvent	Structural class	Peak absorbance (nm)	Absorption range (nm)	Energy band gap (eV)	Absorption coefficient, α (m ⁻¹)
Dragon	Ethanol	Betalain	535		2.32	2.16
fruit skin	Distilled water	pigment	533	400-600	2.33	2.03



Figure 5: (a) Absorption spectra of dragon fruit skin with distilled water



UV-vis Analysis of Silver Oxide Nanowires Films

The absorbance spectrum of silver oxide nanowires films on ITO glass substrates by using UV-vis Spectrometer. The wavelength range of spectrum lied between 190 nm and 1100 nm. The observed absorption peaks of silver oxide nanowires films were 314 nm at 300 °C and 416 nm at 400 °C. It was observed that the UV-vis absorption spectrum of silver oxide nanowires at 300 °C and 400 °C were shown in Figure 6 (a-b). The measured and calculated values of energy band-gap in UV-vis spectra of silver oxide nanowires were described in Table 3. The alternative method to observe the band gap is Beer-Lambert law. The $(\alpha h \upsilon)^2$ and h υ characteristic curve of Ag₂O nanowires films at 300 °C and 400 °C were shown in Figure 7 (a-b). On the characteristic curve, the extrapolating the straight line onto horizontal axis $((\alpha h \upsilon)^2 = 0)$, give the value of band gap and the obtained nanowires films had a direct band gap 1.79 eV for the absorbance spectrum at 300 °C and 2.06 eV for the absorbance spectrum at 400 °C.

Table 3: Optical band –gap energy of Ag₂O nanowires films at 300 °C and 400 °C

Temperature	Optical b	and gap (eV)	Standard band gap (eV)
(\mathbf{C})	Direct method	Beer-Lambert law	
300	1.95	1.79	13-24
400	2.16	2.06	1.5 2.4



Figure 6: (a) Absorption spectra of silver oxide nanowires film at 300 °C

Figure 6: (b) Absorption spectra of silver oxide nanowires film at 400 °C



Figure 7: (a) Photon energy for silver oxide nanowires film at $300 \text{ }^{\circ}\text{C}$



Figure 7:(b) Photon energy for silver oxide nanowires film at 400 °C

Photovoltaic Performance Analysis of Silver Oxide Nanowires

The photovoltaic performance analysis of fabricated DSSCs was carried out under the illumination of 5083 lux. The performance of Ag₂O nanowires at 300 °C and at 400 °C were defined by several parameters such as short-circuit current Isc and open-circuit voltage Voc obtained under illumination conditions. The current-voltage characteristics at different temperatures with natural dyes were represented in Figure 8 (a-b). These figures showed the solar cells behavior of natural dye sensitized solar cells. The maximum power point P_{max} was obtained by tangential point on I-V characteristic curve. By drawing the maximum power point onto X-axis, the maximum voltage (V_m) was obtained. By drawing the maximum power point onto Y-axis, the maximum current (I_m) was obtained. Based on the natural dye sensitizers, silver oxide nanowires coated counter electrodes were observed to be 0.67 % at 300 °C and 0.89 % at 400 °C. The detail analysis of short circuit current (Isc), short circuit current density (Jsc), open circuit voltage (Voc), fillfactor (FF) and conversion efficiency (η_{con}) of dye sensitized solar cells were shown in Table 4.

Specimen	lux	$I_{sc}(\mu A)$	V _{oc} (mV)	FF	η (%)
Ag ₂ O (300°C)	5086	330.36	115.89	0.78	0.67
Ag ₂ O (400°C)	5086	348.36	119.80	0.89	0.63

Table 4: Solar cell parameters of the cell with dragon fruit dye



Figure 8: (a) I-V characteristics curve of silver oxide nanowires DSSCs at $300 \ ^{\circ}\text{C}$



Figure 8: (a) I-V characteristics curve of silver oxide nanowires DSSCs at $400 \ ^{\circ}\text{C}$

Conclusion

Silver oxide nanowires were deposited onto ITO glass substrates by chemical bath deposition technique. Silver oxide nanoparticles with different sizes were synthesized using co-precipitation method. XRD analysis showed that nanoparticles in the fabricated films at 300 °C and 400 °C were crystallized in the cubic structure and their average crystallite sizes were observed to be 23.16 nm and 20.44 nm. According to SEM images, it can be said that the average diameter of silver oxide nanowires at 400°C (175 nm - 236 nm) is smaller than that of at 300 °C (365 nm- 450nm). The results showed that the silver oxide nanowires were successfully fabricated by chemical bath deposition technique. Natural dye was extracted from dragon fruit skins as organic dye materials. The optical absorption analysis indicated that dragon fruit dye has a wide transparency widow in the entire visible and near IR region. The result showed that the dye extracted from absorption wavelengths at 500 nm to 600 nm. It was revealed that anthocyanin dye from dragon fruit quite worked well as natural dye sensitizers for silver oxide

nanowires DSSCs. It was revealed that anthocyanin dye from dragon fruit quite worked well as natural dye sensitizers for silver oxide nanowires DSSCs. From the experimental photovoltaic parameters results, it was found that the efficiencies of Ag₂O nanowires photoelectrodes were 0.67 % at 300 °C and 0.63 % at 400 °C. The results have been pointed out the photovoltaic properties by measuring the I-V characteristics curve and calculating the fill factors and conversion efficiencies. It was proved that the extract dye from dragon fruit quite worked well as a natural dye sensitizers for DSSCs and they are promising to use in light energy harvesting application because of their environmental friendliness and low cost production.

Acknowledgements

I would like to thank Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her kind permission.

I would like to thank Professor Dr Aye Aye Thant, Department of Physics, University of Yangon, for her valuable advice in the preparation of this paper.

References

- Azulai D, Belenkova T, et al, Transparent Metal Nanowires Thin Films Prepared in Mesostructured Templates. Nano let, (2009) **9** 4246-4249.
- Andre R, Natalio F, et al, Adv. Funct. Matet. (2011) 21: 501-509.
- Boyle DS, Bayer A, et al, Characterization of ZnO thin films grown by chemical bath deposition. Thin Solid Films, (2000) 150:361.
- Chang H, Lo Y-J. Pomegranate leaves and mulberry fruits as natural sensitizers for dye sensitized solar cells. Solar Energy, (2010) 84:1833-1837.
- Greene LE, Yuhas BD, Law M, et al, Solution-grown zinc oxide nanowires. Inorg Chem, (2006) 45: 7535-7543.
- Hochabaum AI, Yang P, Semiconductor nanowires for energy conversion. Chem Rev, (2010) 110:527-546.
- Kalaiarasan E, Palvannan Tj, Taiwan Inst. Chem. Eng. (2014) 45: 625-634.
- Liu Y, Zhu G, Bao C, Yuan A, Shen X, Chin. J. Chem. (2014) 32: 151-156.
- Nakade, S. et al. Dependence of TiO_2 nanoparticle preparation methods and annealing temperature on the efficiency of dye-sensitized solar cells. J. Phys. Chem. (2002) B 106, 10004-10010.

Perkampus H. UV-vis Spectroscopy and Its Applications, Springer, (1992).

CHARACTERIZATION AND DIELECTRIC PROPERTIES OF ZINC TITANATE (ZnTiO₃) CERAMICS

Nway Han Myat Thin^{*}

Abstract

In this study, zinc titanate (ZnTiO₃) was prepared by solid state reaction method using zinc oxide (ZnO) and titanium oxide (TiO₂) in a molar ratio of 1:1. Three calcination temperatures (800° C, 900° C, 1000° C) at 2 h were selected to investigate the reaction of formation of zinc titanate (ZnTiO₃). Structural properties of ZnTiO₃ ceramics were characterized by X-ray Diffraction (XRD) technique. Scanning Electron Microscopy (SEM) technique was used to examine the surface morphology of ceramics. Frequency dependence of the dielectric properties of ZnTiO₃ was measured by LCR meter.

Keywords: ZnTiO₃ Ceramics, XRD, SEM, Dielectric Properties

Introduction

Ceramic materials are inorganic, non-inorganic materials made from compounds of a metal and non-metal. Ceramic materials may be crystalline or partly crystalline. They are formed by the acton of heat and subsequent cooling. Clay was one of the earliest materials used to produced ceramics, but many different ceramic materials are now used in domestic, industrial and building products. Ceramics can also be formed to serve as electrically conductive materials, objects allowing electricity to pass through their mass or insulators, materials preventing the flow of electricity. Electroceramics have numerous applications due to their specific structures and physical properties such as microelectronics or as individual circuit components, particulary as capacitors of sensor. These materials and their solid solutions are of a great interest for several applications to their easy synthesis by various methods (solid state reaction, sol-gel, hydrothermal or mechanochemical synthesis) and their properties (piezoelectricity, pyroelectricity, ferroelectricity). Due to their dielectric performances, they are mostly used in the electronic industry as capacitors, detectors, sensors, resonators, actuators, and memories.

^{*} Dr, Assistant Lecturer, Department of Physics, University of Yangon

In the present work ZnTiO3 compound was prepared by solid state reaction method followed by calcimined at different temperatures 800C, 900C and 1000C for two hours each. The structure, microstructure and dielectric properties of sintered ZnTiO₃ have been investigated. ZnTiO₃ compound is an attractive dielectric ceramics owing to its interesting dielectric properties in high frequency range.

Experimental

The ZnTiO₃ compound was prepared by conventional solid state reaction method. The 99.99% pure ZnO and TiO₂ powders were weighed in a molar ratio 1:1 using digital balance as the stating materials. The stating materials were then grounded in an agate mortar for 24 h with the aid of ethanol to make homogeneous and fine powder. Finally the fine powder was calcined at different temperatures 800°C, 900°C and 1000°C for 2h each in air chamber. The calcined powders at various temperatures were examined by X-ray diffractometry (XRD, Rigaku) using Cu K α radiation to indentify the possible phases formed after heat treatment. The surface morphology was examined by scanning electron microscopy (SEM JEOL - JCM -6000 Plu). After examining the structural properties, the ZnTiO₃ compound powders at different temperatures were cold press into cylindrical pellet of size 2.4cm diameter and 0.5cm thickness using hydraulic press with a pressure of 5 ton. Saturated solution of polyvinyl alcohol (PVA) was used as a binder for pellets. These pellets were sintered at 500°C for 2h each. The binder was burnt our during the sintering of the sample. The flat surfaces of pellets were be measured capacitance and resistance as a function of frequency (1kHz to 100kHz) using GW INSTEK LCR-8110G LCR Meter. The flow chart for preparation of ZnTiO₃ powders and ceramics were shown in figure (1).



Figure 1: Block diagram of preparation of ZnTiO₃ powders and ceramics

Results and Discussion

The experimental results and discussion from XRD and SEM measurement of $ZnTiO_3$ powders prepared at different temperatures 800°C, 900°C and 1000°C for 2 *h* each. The electrical properties of $ZnTiO_3$ ceramics were studied from the calculation of dielectric constant and resistivity.

Characterization of X-ray Diffraction

The X-ray diffractometry is mainly used for the identification and qualification of compounds by their diffraction patterns. The XRD patterns performed on the powder synthesized at various temperatures 800° C, 900° C and 1000° C show the presence of ZnTiO₃ (cubic). The X-ray diffraction patterns of zinc titanate powder at different temperatures (800° C, 900° C and 1000° C for 2h) were shown in figure 2(a-c). The XRD patterns of the powder showed (311), (220),(400), (422), (511) and (440) planes were produced. The diffraction angles, interplaner spacing, FWHM and crystallize size of (311) plane were listed in table (1).The crystallite sizes for all powder were calculated by Scherrer Formula,

$$D = \frac{0.899\lambda}{B\cos\theta}$$

where D is the crystalline size of the sample (nm), λ is the X-Ray wavelength (0.154056 nm), θ is the Bragg angle and B is observed FWHM (radian). As shown in XRD patterns, the diffraction line of (3 1 1) plane is found to the strongest in intensity (I=100%) and this plane (peak) is dominated on other peaks. XRD patterns revealed cubic phase of calcined zinc titanate powders. The obtained crystallite sizes can be taken as the nanosized crystalline materials due to the size lies between 1 nm –100 nm. The crystallite size of ZnTiO₃ powder is in nanometer range and apparently decreases with the increasing temperature.

plane				
Temperature (°C)	Diffraction angle (deg)	Interplaner spacing (Å)	FWHM (deg)	Crystallite size (nm)
800°C	35.341	2.538	0.191	45.61
900°C	35.476	2.528	0.193	45.16
1000°C	35.344	2.537	0.226	38.55

Table 1: Data obtained by XRD analyses of ZnTiO₃ powders for (311)



Figure 2: (a) XRD Pattern of ZnTiO₃powders prepared at 800°C



Figure 2: (b) XRD Pattern of ZnTiO₃ powders prepared at 900°C



Figure 2: (c) XRD Pattern of ZnTiO₃powders prepared at 1000°C

SEM Morphology of Zinc Titanate Powders

Morphology of zinc titanate powders was examined by scanning electron microscope. SEM image of the calcined ZnTiO₃ powders with various temperatures (800° C, 900° C and 1000° C for 2 h) each are shown in Figure 3 (a-c).These images show nearly spherical with a very narrow distribution centered at around 0.3-0.4 µm. The variation of grain size with different annealing temperatures was shown in table (2).The sphere like particles seemed to distribute homogeneously and the particle size decreases with the increase in the calcination temperature.

 Table 2: Average grain size of ZnTiO₃ powders with different temperatures from SEM image

Sr	Temperature (°C)	Time (<i>h</i>)	Grain Size (µm)
1	800	2	0.44
2	900	2	0.40
3	1000	2	0.33



Figure 3: (a) SEM photograph of ZnTiO₃ powders prepared at 800°C



Figure 3: (b) SEM photograph of ZnTiO₃ powders prepared at 900°C



Figure 3: (c) SEM photograph of ZnTiO₃ powders prepared at 1000°C

Dielectric Constant and Dissipation Factor of ZnTiO₃ Ceramics

Applied frequency dependence of resistance and capacitance value for $ZnTiO_3$ ceramics at various temperatures were measured by LCR meter. The higher dielectric constant makes these materials useful as capacitor and energy- storage devices materials. Variation of capacitance with respect to applied frequency for $ZnTiO_3$ ceramics at different temperatures (800°C, 900°C and 1000°C) were shown in figure (4). Decreasing of capacitance value was observed with respect to increasing of applied frequency. At the higher frequency region, saturated capacitance value was observed. The capacitance with the dielectric material is related to the dielectric constant (\mathcal{E}_r) is showed in equation.

$$\mathcal{E}_r = \frac{Cd}{\mathcal{E}_0 A}$$

Where C is capacitance of a capacitor, d is thickness of sample, \mathcal{E}_0 is dielectric constant of vacuum (8.854187818×10⁻¹²Fm⁻¹), A is area and \mathcal{E}_r is dielectric constant of sample. The frequency variation of dielectric constant of ZnTiO₃ ceramics at different annealing temperatures are shown in figure (5). It was observed that dielectric constant decreases with increasing frequency in all temperatures. High dielectric value was observed at lower frequency (1 kHz). It is seen that all the parameter decrease with increasing frequency. The higher dielectric constant makes these materials useful as capacitor and energy storage devices materials.

The dissipation factor $(\tan \delta)$ or DF is a measure of loss-rate of energy of a mode of oscillation (mechical, electrical, or electromechanical) in a dissipative system. DF will vary depending on the dielectric material and the frequency of the electrical signals. The frequency variation of dissipation factor of ZnTiO₃ ceramics at different annealing temperatures are shown in figure (6).

Electrical Resistivity of ZnTiO₃ Ceramics

Electrical resistivity is a fundamental property that quantifies how strongly a given material opposes the flow of electric current. The calculation of the resistivity was performed according to the following equation,

$$\rho = \frac{\pi d^2}{4} \frac{R}{L}$$

Where ρ *is* the resistivity, d is the diameter of the sample, R is the resistance and L is the sample thickness. The frequency variation of electrical resistivity of ZnTiO3 ceramics at different annealing temperatures are shown in figure (7). The variation of capacitance, dielectric constant, tan δ and resistivity values of of ZnTiO3 ceramics at different annealing temperatures are shown in Table (3).



Figure 4: Frequency variation of capacitance of ZnTiO₃ ceramic with different temperatures



Figure 5: Frequency variation of dielectric constant of ZnTiO₃ ceramic with different temperatures



Figure 6: Frequency variation of dissipation factor of ZnTiO₃ ceramic with different temperatures



Figure 7: Frequency variation of resistivity of ZnTiO₃ ceramic with different temperatures

Table 3: The variation of capacitance, dielectric constant, dissipationfactor and resistivity of ZnTiO3 ceramics with differenttemperatures

Temperature	f(], U, ,)	$\mathbf{C}(\mathbf{n}\mathbf{F})$	Dielectric	tons	Resistivity
(°C)	I(KHZ)	C(pr)	constant (E_r)	tano	(p)
800°C	1.00E+00	48.9	52	0.13	0.23
	1.20E+01	36.1	38	0.16	0.219
	2.30E+01	11.1	12	0.27	0.2
	3.40E+01	6.21	6.59	0.38	0.19
	4.50E+01	4.41	4.68	0.43	0.175
	5.60E+01	3.64	3.86	0.47	0.16
	6.70E+01	2.93	3.11	0.55	0.14
	7.80E+01	2.51	2.66	0.63	0.126
	8.90E+01	2.23	2.36	0.7	0.114
	1.00E+02	2.04	2.16	0.76	0.1
900°C	1.00E+00	63.2	67	0.11	0.142
	1.20E+01	59.8	63.5	0.12	0.137
	2.30E+01	26.1	27.6	0.2	0.132

Temperature	f(kHz)	C(pF)	Dielectric	tanδ	Resistivity
	3.40E+01	13.7	14.5	0.28	0.124
	4.50E+01	9.56	10.15	0.31	0.12
	5.60E+01	7.63	8.1	0.33	0.114
	6.70E+01	5.84	5.9	0.4	0.105
	7.80E+01	4.76	5.1	0.45	0.097
	8.90E+01	4.05	4.3	0.5	0.091
	1.00E+02	3.55	3.8	0.56	0.085
1000°C	1.00E+00	70.7	75	0.08	0.094
	1.20E+01	67.1	71	0.09	0.089
	2.30E+01	55.2	59	0.14	0.087
	3.40E+01	28.2	30	0.19	0.085
	4.50E+01	19.0	20	0.22	0.083
	5.60E+01	14.4	15.3	0.24	0.079
	6.70E+01	10.6	11.3	0.29	0.076
	7.80E+01	8.29	8.8	0.33	0.073
	8.90E+01	6.80	7.2	0.37	0.069
	1.00E+02	5.77	6.13	0.41	0.066

Conclusion

The crystallite size, micro structure and dielectric properties of ZnTiO₃ have been investigated. The solid state reaction method yields nano crystalline single phase ZnTiO₃ ceramics. The XRD pattern shows the formation of single phase cubic spinal structure for all the samples. The crystallite size of the samples decreases with the increase in temperature was observed in both XRD and SEM images. The decreasing trend of the dielectric constant and resistivity of ZnTiO₃ ceramics with increasing frequency are observed for all temperatures. These factors are normally taken into account when designing a capacitor for electronic application. Therefore ZnTiO₃ ceramic fabrication process and dielectric properties were quite suitable for ceramic capacitor.

Acknowledgements

I would like to thank Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon, for her kind permission.

I would like to thank Professor Dr Aye Aye Thant, Department of Physics, University of Yangon, for her valuable advice in the preparation of this paper.

References

- A. Chaouchi et al., (2010) Processing and Application of Ceramics 4, (2) 75-80
- A. Moulson, A. Herbert, Electroceramics: Materials, Properties, Applications, 2nd Ed. Wiley. New York, 2003
- C. Buchal and M. Siegert: Integr. Ferroelectric Vol. 35 (2001), P-1
- C. Carter, M. Norton. Ceramic Materials: Science and Engineering, Springer, New York, 2007
- C. Suryanarayana, M.C. Norton, X-ray Diffraction: A Practical Approach, Plenum Press, New York, 1998
- K. N. Harish (2013) Archive of Applied Science Research 5 (2) 48

K.Prasad et al., (1993) J. Master Sci 16 (6) 679

M. Yashima, R. Ali, Solid State Ionic 180 (2009) 120-126

P.K.Jain et al., (2010) Optoelectronics and Advanced Materials 4 (3) 299-304

S.A. Redfern, (1996) J. Phys. Condens Matte, Vol. 8, PP-8267

V. L. Mathe et al., (2002) J. Master Sci 25(4) 347

STRUCTURAL, MORPHOLOGICAL AND OPTICAL STUDIES OF ZINC OXIDE (ZnO) THIN FILMS PREPARED BY CHEMICAL BATH DEPOSITION TECHNIQUE

Thin Thin Kyu¹, Saw Shine Ko², Yin MaungMaung³, Than Than Win⁴

Abstract

In this study, Zinc Oxide (ZnO) thin films have been deposited by chemical bath deposition techniques on Indian Tin Oxide (ITO) glass substrate at 300°C and 400°C. Phase formation and crystal structure of Zinc Oxide thin films were studied by X-ray diffraction (XRD). Results of the Scanning Electron Microscopy (SEM)) were indicated the morphology of the sample surfaces. The optical band gap of Zinc Oxide thin films were studied by absorbent data using UV-Vis Spectrometry.

Keywords : Chemical bath deposition, ZnO, XRD, SEM, UV-Vis

Introduction

Amongst various other semiconducting materials, zinc oxide (ZnO) is widely studied because of its abundance in earth, environmental friendly nature, low cost, wide band gap, large exciton binding energy (60meV) at room temperature, high transmittance in the visible region and excellent thermal and chemical stabilities. Recently ZnO has been recognized as one of the intriguing candidates a wide range of technological applications that include transparent electrodes, piezoelectric, surface acoustic wave filters, photonic crystals, light emitting diodes, photodetectors, optical modulator waveguides, gas sensors, ultaviolet sensor, dye sensitized solar cells, solar cell and photo-catalysts. Many methods have been used to deposit ZnO for various applications. They include ac magnetron sputtering, dc magnetron sputtering, ion implantation, molecular beam epitaxy, metal organic chemical vapor deposition, sol-gel method, spray pyrolysis and chemical bath deposition method. The chemical bath deposition method has an advantage over other methods since it is very simple, it does not require sophisticated equipment, it uses low temperature and has low cost of deposition.

^{1.} Dr, Assistant Lecturer, Department of Physics, University of Yangon

^{2.} Dr, Assistant Lecturer, Department of Physics, University of Yangon

³ Dr, Associate Professor, Department of Physics, University of Yangon

^{4.} Dr, Associate Professor, Department of Physics, Mandalay University of Distance Education

Chemical Bath Deposition involves deposition of semiconductor thin films on substrates that are kept in the aqueous solutions. This method seems to be more suitable for synthesizing ZnO nanosheet electrodes with a high specific surface area. It has been reported that when ZnO nanosheets were applied in dye-sensitized solar cells, measured electron transport time in these systems was found to be much faster than in comparable mesoporous ZnO films. Together with the high internal surface area and good electrical conductivity, CBD ZnO films offer excellent visible light transmittance. DSSCs has shown that the light harvesting efficiency of film electrodes is influenced by its crystallinity, particle size, surface area, dye affinity, and film porosity. In this paper, thin films of ZnO have been deposited on ITO glass substrate using chemical bath deposition technique. The crystal structure and surface morphology of the film have been studied. The band gap energy and the effect of annealing temperature on band gap energy have also been investigated.

Experimental Procedure

The ZnO deposited onto the ITO substrates were prepared by the chemical bath deposition method at reaction solution temperature at $63.5 \sim 80^{\circ}$ C. The reaction bath is composed of Zinc chloride (ZnCl₂) and Sodium hydroxide (NaOH). An alkali solution of zinc hydroxide was first prepared. Initially, 6.8g of Zinc chloride was dissolved in 50ml of deionized water. After that, it is gradually stirred with magnetic stirrer with 300 rpm and this process at temperature raise to 80°C. And then 4 g of sodium hydroxide were mixed with 50 ml of deionized water. 25ml of sodium hydroxide solution treated drop by drop without touching to the wall of the container by using burets. The aqueous solution was turned into a milky white collide without any precipitation. The reaction solution was allowed to proceed for nearly two hours after complete addition of sodium hydroxide. After the complete reaction, the Indium Tin Oxide coated glass substrate was immersed vertically at the center of reaction solution in such a way that it should not touch the walls of the beaker. At the end of the deposition period, the observable films were washed with distilled water and drip-dried in air. Post

annealing temperature annealing of the films expelled the water molecules resulting Zinc oxide. In this study the annealing temperature were used at $300 \,^{\circ}$ C and $400 \,^{\circ}$ C respectively.



Figure1: Flow chart of preparation of ZnO thin film on ITO glass substrate with different annealing temperatures

Result and Discussion

Structural properties of ZnO thin film by XRD

To examine the crystal structure and phase formation of ZnO/ ITO thin films, they were performed using monochromatic CuKa radiation (λ = 1.54056 Å) operated at tube voltage 40kV and 40 mA (tube current). The X-ray diffraction patterns for zinc oxide thin films were shown in Fig. The upper side of XRD profile was represented the observed profile while the lower side showed the standard ICDD (International centre for Diffraction Data). The comparison between the observed and standard diffraction peal position and relative peak intensities conforms the hexagonal phase for the zinc oxide thin films. Fig 1(a) and (b) show the XRD pattern of the ZnO thin film annealed at 300°C and 400°C for 2h.The patterns of ZnO thin films deposited on ITO substrate revealed three dominant peak at 2 θ values of 32.24°, 35.90° and 36.80° corresponding to (100), (002) and (101) plane respectively at 300°C and 32.23°, 35.01° and 37.17° corresponding to (100), (002) and (101) plane respectively at 400°C. The well resolved XRD peaks of the diffraction pattern indicate that the ZnO thin film was well crystallized after the post-reaction annealing treatment. The strong and narrow diffraction peaks indicate that the material has a good crystallite size. The full width at half maximum (FWHM) and crystallites size was calculated using Debye Scherer's formula were given in Table 1, Table 2. The measured lattice parameters (a & c) and lattice distortion c/a for ZnO thin film at different annealing temperature was showed in Table 3.

Morphology and phase analysis of ZnO thin film

The microstructural properties of Zinc oxide thin films deposited onto ITO glass substrate were observed by SEM analysis. The SEM photograph shows nanosheet like structure. The width and thickness of the nanosheets were measured by using well known bar code system. Bar code size was formed to be 2μ m with magnification of 5000.SEM images of Zinc oxide thin films on the ITO glass substrate revealed sheet shape distribution some portion of the surface of the substrate. Fig 3(a) showed the SEM image of ZnO film at temperature 300°C and Fig 3(b) provided the sheet shape

structure on their film. The average size of nanosheets would be measured by the bar code system and its width were 105.44 nm, 107.11nm and thickness were 2 nm, 3nm at annealing temperature 300°C and 400°C respectively.

Optical Properties of ZnO thin film

The preparation of ZnO thin film, ZnO thin films were characterized by UV absorbance spectra. The optical properties of ZnO film are determined from absorbance measurement in the range of 190nm to 800nm for annealing temperature 300°C and range 190nm to 800nm for annealing temperature 400°C respectively. The maximum absorbance edge was found at 314nm for ZnO thin films for 300°C and 376nm for 400°C annealing temperature. The absorption spectrum of ZnO thin films was shown in figure 4(a) and (b). From the dependence of the absorption band edge on wavelength, the energy gap of the material can be determined. When the energy of the incident photon is greater than that of the band gap (hu>E_g) the absorption coefficient ' α ' is given by

$$\alpha = 2.3026 \text{ A/t} \dots (1)$$

where, t is thickness of the sample

A is the absorbance.

$$\alpha h\mu = A(h\mu - Eg)^{1/2}$$
------(2)

where, A is constant and hu is the photon energy.

From the curve αhv^2 versus hv, the band gap was identified by extrapolating the linear region of the curve to the energy axis. The energy band gap value of ZnO thin films were measured in figure 5(a) and (b). In these results, the band gap was examined to be 3.960eV and 3.302eV for annealing temperature 300°C and 400°C.

Table1:	The structural	parameter	of ZnO	thin	film	for	identified	peaks
	at 300 °C							

No.	Peak	FWHM (deg)	2-Theta(deg)	Crystallite size (nm)
1	(1 0 0)	0.092	32.239	93.61
2	(0 0 2)	0.332	35.900	26.28
3	(101)	0.390	36.800	22.43

Table 2: The structural parameter of ZnO thin film for identified peaks at 400 $^\circ \mathrm{C}$

No.	Peak	FWHM (deg)	2-Theta(deg)	Crystallite size (nm)
1	(1 00)	0.113	32.239	75.53
2	(0 0 2)	0.320	35.005	26.87
3	(101)	0.577	37.170	14.99

 Table 3: Lattice parameters (a & c) and lattice distortion c/a for ZnO thin film at different annealing temperature

Annealing temperature	a(Å)	c(Å)	c/a
At 300°C	3.2068	5.1804	1.6154
At 400°C	3.2047	5.1294	1.6005
Standard	3.2500	5.2000	1.6000



Figure. 2: (a) XRD diffractorgram of ZnO thin film annealed at 300°C



Figure 2: (b) XRD diffractorgram of ZnO thin film annealed at 400°C



Figure 3: (a) The SEM photograph of the ZnO thin film annealed at 300°C



Figure 3:(b) The SEM photograph of the ZnO thin film annealed at 400°C



Figure 4: (a) Absorption spectrum of the ZnO thin film annealed at 300°C



Figure 4: (b) Absorption spectrum of the ZnO thin film annealed at 400°C



Figure 5: (a) Plot of $(\alpha h\mu)^2$ versus photon energy of ZnO thin film annealed at 300° C



Figure 5: (b) Plot of $(\alpha h \mu)^2$ versus photon energy of ZnO thin film annealed at $400^{\circ}C$

Conclusion

The deposition of ZnO thin films prepared by the successive immersion of ITO glass substrate in solutions of NaOH and Zinc chloride reaction solution at 63.5°C ~80°C have been studied by Chemical Bath Deposition Technique. A sample of CBD technique was developed to synthesize interesting ZnO nanostructures. Hexagonal (wuritze structure) phase can be easily obtained by CBD method. At temperature of 300°C, the crystallite size was found to be 22.43nm at prominent peak (101) and 400°C provided 14.99 nm respectively. Therefore, we may deduce the crystallite size was decreased with increasing annealing temperature. Microstructural of the films changes on varying film precipitation conditions, particularly the annealing temperature. The surface morphology of deposited ZnO thin films on ITO substrate was showed nanosheets structure. The average width of nanosheets would be measured by the bar code system and its width and thickness were 105.44 nm, 107.11nm and 2 nm, 3nm annealing temperature at 300°C and 400°C. Optical band gap of the ZnO thin films, measured by employing a UV -Vis spectrophotometer, lies at 3.960eV and 3.302eV at 300°Cand 400°C annealing temperatures respectively. By the conclusion, the ZnO film is credible and promising use for thin film solar cell by nonexpensive and unsophisticated method.

Acknowledgement

I am highly grateful thanks Professor Dr Khin Khin Win, Head of Department of Physics, University of Yangon for her permission to do and her encouragement throughout this paper.

I also would like to thank Professor Dr Aye Aye Thant, Department of Physics, University of Yangon for her allowing me to do the paper.
References

- Annuar, K. et al (2010) "Effect of Bath Temperature on the Chemical Bath Deposition PbSe Thin Films", University Journal of Science, Engineering and Technology.6(2)126-132
- Avinash Dive S., Deepak., et al,(2015), "Growth structural optical and electrical properties of ZnO thin films Deposited by chemical bath deposition technique",<u>8</u>,189.
- Chen HG, Lian HD, Hung SP, Wang CF. J Cryst Growth 2013;362:231-4.
- Chu. D et al (2009) "Growth an Electrical Properties of ZnO Films Prepared by Chemical Bath Deposition Method", Phys. Status Solid A 206(4):718-723
- K.P. Vasudevan et al, (2017), "Structural, Morphological and optical properties of ZnO nanorods", Vol.03.No.01,pp 192-197
- Malevu T.D & Ocaya R.O., et al,(2015),"Effect of Annealing temperature on structural, Morphology and optical properties of ZnO nano-needles prepared by Zinc-Air cell system Method",<u>10</u>,1752.
- Lin JC, Lee CP, Ho KC. J Mater Chem 2012;22:1270-
- Rohidas B. Kale et al (2014), "Synthesis and characterization of ZnO nanostructures using modified chemical bath deposition method", Materials letters 137(2014) 401-404
- Shinde VR, Gujar TP, Lokhande CD. Sens Actuators B: Chem 2007; 123:701-6.

ANALYSIS OF TIME OF FLIGHT OF ⁸HE NUCLEI IN NUCLEAR EMULSION USING RANGE-ENERGY RELATION PROGRAM

Kyaw Thu^{*}

Abstract

A nuclear track emulsion (NTE) is exposed to 60MeV ⁸He nuclei. Measurements of decays of ⁸He nuclei stopped in nuclear track emulsion allow one to evaluate possibilities of alpha spectrometry. Thermal drift of ⁸He atoms is observed in nuclear emulsion. Knowledge of the energy and emission ranges of alpha particles allows one to derive the energy distributions of alpha decays $Q_{2\alpha}$. The presence of a tail of large values is established. Presented in this report is the time of flight estimate for ⁸He based upon data obtained from an emulsion stack exposed to 1.6GeV/c K⁻ mesons. The lifetime of ⁸He is about 0.1 s and the decays of ⁸He were obtained in a total estimated time of flight of ⁸He (\rightarrow ⁸Li+ β ⁻, (\rightarrow ⁸Be+ β ⁻) 2.6±0.21 psec. The forward to backward ratio indicates isotropic emission of ⁸Be (or ⁸Li) fragments. The emission of short recoils at the primary vertex shows a definite correlation with the ⁸Be (or ⁸Li) fragments.

Keywords: Range-energy relation program, KEK 373's emulsion plates, Computer-aided microscope system

Introduction

There have been quite a few experiments on the emission of ⁸He fragments from K⁻ interactions with emulsion nuclei at various incident beam energies. The experiments are helpful in understanding the nuclear structure and also the mechanism of fragmentation. For studying fragments with a charge greater than that of the a-particle,⁸He(also ⁸Li,⁹Li, ⁸B, ⁸Be) fragments have been chosen because of their characteristic decay into two α -particles, usually known as 'hammer tracks'. The hammer (HT) and hammer like(HLT) make the identification of ⁸He fragments very simple and unambiguous. In this paper we present the analysis on 60 HTs (HTLs) produced in the interaction of 1.6 GeV/c K⁻ with the emulsion nuclei. No effort, however, was made to distinguish between the ⁹Li, ⁸B, ⁸He and ⁸Li fragments in the HTs (HTLs).

^{*} Assistant Lecturer, Department of Physics, University of Yangon

More than 55 years ago, hammer and hammer like tracks of ⁸Be $\rightarrow 2\alpha$ were observed in nuclear track emulsion. They resulted from β decays of stopped ⁸Li and ⁸B fragments produced in turn by high energy particles as emulsion nuclei underwent splitting [C.F.Powell]. Another example is the first observation of the $2\alpha + p$ decay of the ⁹C nucleus via the 2+ state of the ⁸Be nucleus [M.S.Swami]. Due to the development of facilities for producing beams of radioactive nuclei, nuclear track emulsion turned out to be an effective tool for studying decays of light exotic nuclei with both neutron and proton excess. As a first step within this approach, the nuclear track emulsion was exposed to ⁸He nuclei with energy of ~ 60 MeV at the Kazuma Nakazawa Laboratory of Nuclear Reaction in July 2017. The features of ⁸He decays are depicted in Fig. 1 in accordance with [F. Ajzenberg Selove]. After the ⁸He nucleus is stopped and neutralized in the substance, the formed 8He atom remains unbound (noble gas) and, as a result of thermalization, can drift in the substance until it undergoes β decay. The half life of the ⁸He nucleus is $\tau_{\beta} = (119.0 \pm 1.5) \times 10^{-3}$ s[F. Ajzenberg Selove]. The lifetime of ⁸He is about 0.1 s and the decays of ⁸He were obtained in a total estimated time of flight of ⁸He as 2.6 ± 0.21 psec. This nucleus undergoes β decay to the 0.98MeV bound level of the⁸Li nucleus with a probability of 84% and energy $\Delta E = 9.7$ MeV. Then the ⁸Li nucleus with its half life $\tau_{\beta} = (838 \pm 6) \times 10-3$ s undergoes β decay to the 2+ level of the ⁸Be nucleus (3.03 MeV) with 100% probability and energy $\Delta E = 13$ MeV. Finally, the ⁸Be nucleus decays from its 2+ state with the width of 1.5 MeV to a pair of α particle. Figure 2 shows a mosaic macro photograph of the decay of the ⁸He nucleus stopped in nuclear track emulsion (one of 60 events observed in this investigation). The decay results in a pair of relativistic electrons (dotted tracks) and a pair of α particles (oppositely directed short tracks).



Figure1: Scheme of the main cascade decay channel for the ⁸He isotopes (Circles are photons (light) and neutrons (dark). Darker background indicates clusters)



Figure 2: Mosaic macrophotograph of the hammer (a) and hammerlike (b) decay of the ⁸He nucleus stopped in the nuclear track emulsion (horizontal track)

Experimental Procedure

This work was done using a stack consisting of 12 nuclear pellicles, each of size 25cm*24.5cm (thickness (~1mm) before development and (~0.5mm) after developmentinFig.3) exposed to the K⁻ beam of momentum 1.6 GeV/c at Kazuma Nakazawa Laboratory. Approximately 60 interactions

were picked up by an area scan using 50x magnifications with computer-aided microscope system in Fig 4. Each grey or black track which originated from a beam star was followed within the emulsion pellicle containing the primary star. The centre of each star was examined under a magnification of 100 x to detect the presence of a short hammer (hammer like) or recoil. All hammer and hammer like tracks were assumed to be due to ⁸Li, ⁸Be fragments. Only those ⁸Li, ⁸Be fragments which decayed at rest into two collinear α -particles (Space angle should be 180 ± 10 degrees) were picked up. In this respect the production rate given below is a lower limit.



Figure 3: Nuclear emulsion plate of KEK 373(After development)



Figure 4: Computer-aided microscope

Results and Discussion

Analysis of Hammer and Hammer like Decays

As the pellicle was scanned using a computer-aided microscope with a $50\times$ lens, the primary search for β decays of ⁸He nuclei was focused on hammer and hammer like events (Fig. 2). The absence of tracks of a decay electron in the observed event was interpreted as a consequence of the inadequately effective observation of all decay tracks in the emulsion pellicle. The most problematic background for selection by this criterion could arise from decays of ⁸Li nuclei. Figure 5 depicts the relation between the ranges L_α of α particles from the hammer decays and the energies E_{α} found from the splice interpolation of the range–energy calculation within the RER model. The average of the α particle ranges is $10.47 \pm 0.64 \mu$ m which corresponds to the average kinetic energy $\langle E(^{4}\text{He}) \rangle = 2.93 \pm 0.03$ MeV. The ranges L₂and L₃ of α particle in pairs exhibit a distinct correlation (Fig. 6). The distribution of the range differences L₂ – L₃ (Fig. 7) has ~1 μ m.

Knowing the energy and emission angles of α particle, we can obtain α decay energy distribution $Q_{2\alpha}$. The relativistically invariant variable Q is defined as a difference between the invariant mass of the final system M* and the mass of the primary nucleus M; i.e., $Q = M^* - M$. Here M* is defined as a sum of all products of the fragment four momenta $P_{i,k}$,

$$M^{*^2} = (\sum P_j)^2 = \sum (P_i P_k)$$

The $Q_{2\alpha}$ distribution (Fig. 12) mainly corresponds to the decays of ⁸Be nuclei from the excited 2+ state. Its average value $\langle Q_{2\alpha} \rangle$, however, turned out to be slightly greater than expected, which results from a small tail in the region of large $Q_{2\alpha}$ that obviously does not fit into the description by the Gaussian function. Applying the selection criteria L₂ and L₃< 12.5 µm and $\theta > 145^{\circ}$, we obtain $\langle Q_{2\alpha} \rangle = 3.01 \pm 0.1$ MeV which corresponds to the 2+ state. The reason why the tail arises in the $Q_{2\alpha}$ distribution is obscure and calls for further analysis. According to Fig. 6, the ranges L₂ and L₃correlate at values less than 12.5 µm as well. Therefore, an increase in ranges cannot be attributed to fluctuations of ranges due to recombination of He⁺² ions. Radioactive ⁸He gas can be used for measuring the ⁸He half-life at a new level of accuracy and for the laser spectroscopy of ⁸He. Of applied interest is the investigation of thin films by pumping ⁸He atoms with their particular penetrating power and depositing them onto detectors.



Figure 5: Determination of the α particle energy from the measured ranges



Figure 6: Distribution of ranges L_2 and L_3 in pairs of α particle.



Figure 7: Distribution of range differences L_2 - L_3 in pairs of α particle.



Figure 8: Energy $Q_{2\alpha}$ distribution of α particle pairs

Conclusions

This work demonstrates the capabilities of the recently reproduced nuclear track emulsion exposed to a beam of ⁸He nuclei. The test experiment allowed radioactive ⁸He nuclei to be independently identified by their decays as they stopped in the emulsion, the possibility of carrying out α spectrometry of these decays to be estimated, and the drift of thermalized ⁸He atoms in matter to be observed for the first time. The experiment proved the high purity of the beam of radioactive nuclei formed at the J-PARC facility with an energy ranging from 10 to 30 MeV/nucleon. The analysis of 60 decays of ⁸He nuclei can be a prototype for investigating decays of ^{8,9}Li, ^{8,12}B, ⁹C, and ¹²N nuclei in which the ⁸Be nucleus serves as a marker. The nuclear track emulsion can be used for the diagnostics of beams of radioactive isotopes. The statistics of the hammer and hammer like decays observed in this work is a small fraction of the flux of ⁸He nuclei, and the measured decays constitute of that fraction. This limitation was dictated by "reasonable" time and labor

expenditure. At the same time the nuclear track emulsion with implanted radioactive nuclei offers the basis for using computer-aided microscopes and range-energy relation program, making it possible to hope for unprecedented statistics of analyzed decays.

The present work indicates that there exists a correlation between the short recoils at the primary star and the emitted HTs (HLTs). Moreover, Presented in this report is the time of flight estimate for ⁸He based upon data obtained from an emulsion stack exposed to 1.6 GeV/c K⁻ mesons. And the decays of ⁸He were obtained in a total estimated time of flight of ⁸He as 2.6 ± 0.21 psec.

Acknowledgement

The author would like to thank Professor Dr Khin Khin Win, Head of Department of physics, University of Yangon for her kind permission to carry out this work. And then, I also would like to thank Professor Dr Aye Aye Thant, Department of physics, University of Yangon and Professor Kazuma Nakazawa, Head of Department of Physics, Gifu University, Japan.

References

- A. M. Rodin et al., Nucl. Instrum. Methods Phys. Res., Sect. B 204, 114–118 (2003).
- A. Knecht et al., Phys. Rev. C 86, 035506 (2012). 13. T. Stora et al., Europhys. Lett. 89, 32001 (2012).
- C. F. Powell, P. H. Fowler, and D. H. Perkins, Study of Elementary Particles by the Photographic Method (Per gamon, London, 1959), pp. 465–472.
- F. AjzenbergSelove, Nucl. Phys. A 490, 1–266 (1988); TUNL, Nuclear Data Evaluation Project. http://www.tunl.duke.edu/NuclData/
- Flerov Laboratory of Nuclear Reactions, U400M Accelerator Complex. http://flerovlab.jinr.ru/flnr/ u400m.html
- J. F. Ziegler, J. P. Biersack, and M. D. Ziegler, SRIM-the Stopping and Range of Ions in Matter (SRIM Co, 2008); Particle Interactions with Matter, SRIM-The Stopping and Range of Ions in Matter.
- K. L. Brown et al., (1980) CERN Yellow Report 8004.
- M. S. Swami, J. Schneps, and W. F. Fry, Phys. Rev. 103, 1134–1135 (1956).
- P. Mandal, D. K. Bhattacharya, M. Saha, P. K. Sen, and P. C. Bhattacharya, Phys, Calcutta University, Calcutta, India, 1976
- U. Rohrer, PSI Graphic Transport Framework based on a CERNSLACFERMILAB version by K.L. Brown et al. http://aea.web.psi.ch/Urs_Rohrer/ MyWeb/trans.htm

COMPARISON BETWEEN SINGLEPARTICLE ENERGY STATES OF ¹²_AC AND ¹²₆C

Cho Cho San¹, Khin Swe Myint²

Abstract

Nucleon single-particle energy states in ordinary nuclei and Λ single particle energy states in Λ -hypernuclei are compared to study the role of Λ particle in nuclear medium. So, we examined the single particle energy state in Λ hypernuclei ${}^{12}_{\Lambda}C$ and ordinary nuclei ${}^{12}_{6}C$. In our calculation, in order to get the single particle energy levels of ${}^{12}_{\Lambda}C$ and ${}^{12}_{6}C$, we used the phenomenological Woods-Saxon Λ -core nucleus potential and nucleonnucleus potential including spin-orbit term. Gaussian basis wave function is used in our consideration systems.

Key words: Λ single particle level, nucleon single particle level

Introduction

The study of the response of many-body system to a hyperon gives insight into the information of baryon-baryon interactions. The valuable information on the Λ -N interaction has an impact upon understanding of baryon-baryon interaction within the framework of SU (3) flavor symmetry. Since a bound Λ hyperon inside the nucleus can only decay via weak interaction, life time of hypernuclei is long enough to be observed and the binding data of hypernuclei provide a unique opportunity to know more about the Λ -nuclear interaction.(Hasegawa, T.,et al.,(1995))

Also the determination of the Λ spin-orbit interaction is very important to totally understand the nature of spin-orbit interaction of Λ and ordinary nucleus. It is known that the Λ -nucleus spin- orbit splitting is at least an order of magnitude smaller than that of the nucleon-nucleus interaction. Spin and orbit refer to the attributes of a single nucleon moving in the assumed potential. Such a term is found in atomic physics and it is due to the magnetic interaction of the magnetic dipole moment of the electron spin and the magnetic field experienced by the electron in its rest frame as moves through the Coulomb field of the nucleus. However, nuclear spin-orbit interaction

^{1.} Dr, Lecturer, Department of Physics, Mandalay University of Distance Education, Mandalay, Myanmar.

² Department of Physics, Mandalay University, Mandalay, Myanmar.

cannot be magnetic in origin as it is notstrong enough to explain the observed spin-orbit splitting. We have calculated Λ single particle energy ${}^{12}_{\Lambda}C$ and nucleon single particle energy levels of ${}^{12}_{6}C$ by using Λ -core nucleus and nucleon-nucleus phenomenological Woods-Saxon potentials including spin orbit term.

Glue-Like Role of Λ- Hypernuclei

The structure is modified when a hyperon, a Λ particle, is injected into the nucleus. There is no Pauli principle acting between the Λ and the nucleons in the nucleus. Therefore, the Λ particle can reside deep inside, and attract the surrounding nucleons towards the interior of the nucleus. Then, the Λ particle plays a 'glue like role' to produce a dynamical contraction of the core nucleus. Nuclei are compressed by the injection of a Λ particle such that the matter radius in some excited states is shrunk by as much as 30% due to the addition of a Λ particle.

A can occupy whatever single particle state, the ground state of the hypernucleus always corresponding to the hyperon in the 1s level. It is then clear that a Λ particle is a good probe of the inner part of nuclei. Actually, the Pauli principle is active on the u and d quarks of nucleons and Λ when they are very close to each other. With the exception of hypernuclei of the s-shell, the depth of the Λ -nucleus mean field is of about 30 MeV, it is less attractive than the one typical for a nucleon (50-55 MeV). This characteristic reflects the smaller range and the weakness of the Λ N interaction at intermediate distances with respect to the NN one. It is possible to reproduce the experimental single particle Λ levels using Woods-Saxon wells with the depth and appropriate radii. For s-shell hypernuclei the Λ single particle potential displays a repulsive soft core at short distance. A measure of this effect is given by the rms radii for a nucleon and a Λ in these hypernuclei: the hyperon rms radius is larger than the one for a nucleon. In order to study the Λ single-particle energy levels, we determine the Λ -nucleon spin-orbit splitting.

The Lambda Nucleon Spin-Orbit Splitting

The properties of baryon many-body systems, which contain not only nucleons but also hyperons with strangeness, link closely to the underlying hyperon-nucleon interaction. The determination of the Λ spin orbit interaction is very important to totally understand the nature of spin orbit interaction of Λ and ordinary nucleus. Several features of the Λ single-particle properties in the nucleus, being essentially different from those of the nucleon, have clearly emerged from these efforts. It is well accepted nowadays that the depth of the Λ -nucleus potential is around -30 MeV, which is 20MeV less attractive than the corresponding nucleon-nucleus one. The spin orbit splitting of single particle levels in Λ hypernuclei were found to be much smaller than their nucleonic counterparts, typically more than one order of magnitude. Such effect could originate from the weak tensor component of the Λ -N interaction. Moreover, the Λ , contrary to the nucleon, maintains its single particle character even for states well below the Fermi surface indicating a weaker interaction with other nucleons.

From the experimental motivation, the binding energy of ${}^{12}_{\Lambda}C$ which is observed from the emulsion experiment is -10.08 ± 0.18 MeV. Moreover the spectroscopic study of ${}^{12}_{\Lambda}C$ by the (π^+ , K⁺) reaction was reported by T. Haseagawa and his collaboration.

Hypernuclei structure calculations with core-excited states will be important in future analysis.

The Nucleon Nucleon Spin-orbit Splitting

Spin orbit splitting of nuclei is one of the main factors, which determine nuclear structure in nuclei both near and far from the closed shells. Spin and orbit refer to the attributes of a single nucleon moving in an averaged potential well. Spin-orbit splitting in atoms is due to the magnetic interaction of the magnetic dipole moment of the electron spin and the magnetic field experienced by the electron in its rest frame as it moves through the Coulomb field of the nucleus. However, the dynamical origin of the strong nuclear spin orbit force has not been fully resolved even up to date. The analogy with the spin orbit interaction in atomic physics gave the hint that it could be a relativistic effect. This idea has led to the construction of the relativistic scalar-vector mean field models for nuclear structure calculation. In these models the nucleus is described as a collection of independent Dirac-particles moving in self-consistently generated scalar and vector mean-fields. The footprints of relativity become visible through the large nuclear spin orbit coupling which emerges in that framework naturally from the interplay of two strong and counteracting (scalar and vector) mean-fields. The corresponding spin orbit term comes out proportional to the coherent sum of the very large scalar and vector mean-fields. In this sense, the relativistic mean-field model gives a simple and natural explanation of the basic features of the nuclear shell model potential.

The Λ-Core Nucleus Interaction

Single particle potential of hyperons is fundamental quantities in hypernuclei many-body systems, which are closely related to the properties of hyperon nucleon interaction. To investigate single particle energy levels of ${}^{12}_{\Lambda}$ C and ${}^{12}_{6}$ C, we employ the following potential, phenomenological Woods-Saxon A-core nucleus potential.

Phenomenological Woods-Saxon Λ-core Nucleus Potential

$$\mathbf{v}(\mathbf{r}) = -\mathbf{v}_{0}\mathbf{f}(\mathbf{r}) + \mathbf{v}_{s0}\left(\frac{\hbar}{m_{\pi}c}\right)^{2} \left(\vec{\ell}.\vec{s}\right) \frac{1}{r} \frac{\mathrm{d}\mathbf{f}(\mathbf{r})}{\mathrm{d}\mathbf{r}}$$
(1)

$$f(r) = \frac{1}{1 + e^{\left(\frac{r-R}{a}\right)}}$$

where, $v_0 =$ strength of the Woods-Saxon potential

 v_{so} = spin-orbit constant

$$\frac{\hbar}{m_{\pi}c}$$
 = Compton wavelength

a = diffuseness parameter

R = nuclear radius

The chosen parameters for nucleon are

$$v_0^N = 50 \text{ MeV}, v_{SO}^N = 14 \text{ MeV}, R = 1.25 \text{ A}^{\frac{1}{3}} \text{ fm}, a = 0.53 \text{ fm}$$
 (2)

The chosen parameters for lambda are

$$v_0^{\Lambda} = 30 \text{ MeV}, v_{SO}^{\Lambda} = 4 \text{ MeV}, R = 1.1(A - 1)^{\frac{1}{3}} \text{ fm}, a = 0.6 \text{ fm}$$
 (3)

The scalar product of $\vec{\ell}$ and \vec{s} is

$$\vec{\ell}.\vec{s} = \frac{1}{2} [j(j+1) - \ell(\ell+1) - s(s+1)]\hbar^2$$
(4)

Mathematical Formulation

Schrödinger equation for two-body bound system is $\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} + V(r)\right\}u(r) = Eu(r)$ (5)

The Gaussian form for wave function is

$$u(r) = r^{\ell+1} \sum_{j=1}^{N_b} c_j e^{-\left(\frac{r}{b_j}\right)^2}$$
(6)

$$\begin{cases} -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} - v_o f(r) + v_{so}\left(\frac{\hbar}{m_{\pi}c}\right)^2 (\vec{\ell}.\vec{s})\frac{1}{r}\frac{df(r)}{dr} \end{cases} \\ r^{\ell+1}\sum_{j=1}^{N_b} c_j e^{-\left(\frac{r}{b_j}\right)^2} = E r^{\ell+1}\sum_{j=1}^{N_b} c_j e^{-\left(\frac{r}{b_j}\right)^2} \end{cases}$$
(7)

By solving equation (7) we obtained the following norm matriterm, the kinetic energy term, the centrifugal term and the potential term.

The norm matrix term is

$$N_{ij}^{\ell} = \frac{(2\ell+1)!!\sqrt{\pi}}{2^{\ell+2} \left(\frac{1}{b_i^2} + \frac{1}{b_j^2}\right)^{\ell+\frac{3}{2}}}$$
(8)

The kinetic energy term is

$$\mathbf{T}_{ij}^{\ell} = -\frac{\hbar^{2}}{2\mu} \begin{bmatrix} \frac{4}{\mathbf{b}_{j}^{4}} \left(\frac{(2\ell+3)!!\sqrt{\pi}}{2^{\ell+3} \left(\frac{1}{\mathbf{b}_{i}^{2}} + \frac{1}{\mathbf{b}_{j}^{2}}\right)^{\ell+\frac{5}{2}}} \right) - \frac{4\ell+6}{\mathbf{b}_{j}^{2}} \left(\frac{(2\ell+1)!!\sqrt{\pi}}{2^{\ell+2} \left(\frac{1}{\mathbf{b}_{i}^{2}} + \frac{1}{\mathbf{b}_{j}^{2}}\right)^{\ell+\frac{3}{2}}} \right) + \\ \ell(\ell+1) \left(\frac{(2\ell-1)!!\sqrt{\pi}}{2^{\ell+1} \left(\frac{1}{\mathbf{b}_{i}^{2}} + \frac{1}{\mathbf{b}_{j}^{2}}\right)^{\ell+\frac{1}{2}}} \right) \end{bmatrix}$$
(9)

The centrifugal potential term is

$$F_{ij}^{\ell} = \frac{\hbar^2}{2\mu} \ell(\ell+1) \left(\frac{(2\ell-1)!!\sqrt{\pi}}{2^{\ell+1} \left(\frac{1}{b_i^2} + \frac{1}{b_j^2} \right)^{\ell+\frac{1}{2}}} \right)$$
(10)

The scalar product of $\Vec{\ell}$ and \Vec{s} is

$$\vec{\ell}.\vec{s} = \frac{1}{2} [j(j+1) - \ell(\ell+1) - s(s+1)] \hbar^2$$
(11)

For $j = \ell + \frac{1}{2}$ state, the potential term is

$$\mathbf{v}_{ij}^{\ell} = \int \mathbf{r}^{2\ell+2} \mathbf{e}^{-\left(\frac{1}{\mathbf{b}_{i}^{2}} + \frac{1}{\mathbf{b}_{j}^{2}}\right)\mathbf{r}^{2}} \left[\frac{-\mathbf{v}_{o}}{\frac{\mathbf{r}-\mathbf{R}}{1+\mathbf{e}^{-\mathbf{a}}}} + \mathbf{v}_{so}\left(\frac{\hbar}{\mathbf{m}_{\pi}\mathbf{c}}\right)^{2} \left(\frac{1}{2}\ell\right) \left(-\frac{1}{\mathbf{r}}\frac{\mathbf{e}^{-\mathbf{R}}}{\left(1+\mathbf{e}^{-\mathbf{a}}\right)^{2}}\frac{1}{\mathbf{a}}\right)\right] d\mathbf{r}$$
(12)

For $j = \ell - \frac{1}{2}$ state, the potential term is,

$$\mathbf{v}_{ij}^{\ell} = \int r^{2\ell+2} e^{-\left(\frac{1}{b_{i}^{2}} + \frac{1}{b_{j}^{2}}\right)r^{2}} \left[\frac{-\mathbf{v}_{o}}{\frac{r-R}{1+e^{-a}}} + \mathbf{v}_{so}\left(\frac{\hbar}{m_{\pi}c}\right)^{2} \left(\frac{-(\ell+1)}{2}\right) \left(-\frac{1}{r} \frac{e^{\frac{r-R}{a}}}{\left(1+e^{-a}\right)^{2}} \frac{1}{a}\right) \right] dr \quad (13)$$

The Hamiltonian is expressed by summing of kinetic energy term, centrifugal term and potential term as follows:

$$H_{ij}^{\ell} = T_{ij}^{\ell} + F_{ij}^{\ell} + V_{ij}^{\ell}$$
(14)

$$\sum_{j} H_{ij}^{\ell} c_{j} = E \sum_{j} N_{ij}^{\ell} c_{j}$$
⁽¹⁵⁾

By rewriting equation (15) in terms of matrix form as follows:

$$[H][c] = E[N][c]$$
⁽¹⁶⁾

The above equation (16) is numerically solved by using power inverse iteration method. Then we get the single particle energy levels ${}_{6}^{12}C$ and we compare them with the Λ -hypernuclei ${}_{\Lambda}^{12}C$.

Results and Discussion

We have calculated the single-particle energy levels for Λ -hypernuclei ${}^{12}_{\Lambda}C$ and ordinary nuclei ${}^{12}_{6}C$ by solving two-body time independent Schrodinger equation. In our calculation, we used the phenomenological Woods-Saxson central potential including spin orbit term in Λ -nucleus

interaction and nucleon nucleus interaction. Our calculated single-particle energy levels of Λ -hypernuclei and ordinary nuclei are as shown in table (1). The energy level diagram for Λ -hypernuclei and ordinary nuclei are displayed in figure (1). From Figure (1), it can be seen that the single particle energy level of ${}^{12}_{\Lambda}$ C in s-state is -10.11 MeV. The emulsion experiment is investigated that the single particle energy of ${}^{12}_{\Lambda}$ C in s-state is-10.08±0.18MeV. Our calculated results by using Woods-Saxson central potential including spinorbit interaction is in good agreement with the experimental data. The nucleon single particle energy level of ${}^{12}_{6}$ C is -27.5 MeV for s-state and-12.6 MeV and -7.69 MeV for $p_{3/2}$ and $p_{1/2}$ state respectively. There are three bound states for ${}^{12}_{6}$ C and only one bound state for ${}^{12}_{\Lambda}$ C. Therefore, the potential depth of Λ -

 $_{6}$ C and only one bound state for $_{\Lambda}$ C. Therefore, the potential deput of 7 nucleus interaction is shallower than that of nucleon-nucleus interaction.

Single particle energy state	$^{12}_{\Lambda}\mathrm{C}$	$^{12}_{6}{ m C}$
$1s_{1/2}$	-10.11 MeV	-27.5 MeV
1p _{3/2}		-12.6 MeV
1p _{1/2}		-7.69 MeV

Table 1: Single-particle energy levels of ${}^{12}_{\Lambda}C$, ${}^{12}_{6}C$



Figure 1: Single-particle energy level of ${}^{12}C, {}^{12}C$

Conclusion

We have investigated that the single particle energy levels of ${}^{12}_{6}C$ and ${}^{12}_{6}C$ by solving two-body time independent schrodinger equation. Gaussian basis wave function is used in our consideration system. The phenomenological Woods-Saxson potential including spin orbit term is used in A nucleus interaction and nucleon nucleus interaction. From our calculated results, it is concluded that the potential strength of A-nucleon interaction isabout one third that of nucleon-nucleon interaction.

Acknowledgements

I would like to thank Dr Aung Naing Soe, Pro-Rector, Mandalay University of Distance Education for his encouragement. I am grateful to the full support of Professor Dr Kay thi Nwe, Head of Department of Physics, Mandalay University of Distance Education. I am deeply indebted to Professor Dr Khin Swe Myint, Rector (Rtd), Emeritus Professor, Department of Physics, University of Mandalay for all her enthusiastic discussion, collaboration and encouragement.

References

Danysz, M. Pniewski, J., and Phil, J., Mag. 44 (1953) 348.

Hasegawa, T., et al., Phys. Rev. Lett.74 (1995) 224.

Henlay, E.M., (1991) "Subatomic Physics".

Millener, D. J., et al., Phys. Rev. C31(1985)499.

Motoba, T.et al., Nucl. Phys. A 534 (1991) 597.

Timura, H., et al., Nucl. Phys. A 639 (1998) 83c.

Vries, H., Jager, C.W and Vries, C. (1987), "Atomic Data and Nuclear Data Tables", 36.

Williams, W.S.C., (1991), "Nuclear and Particle Physics".

INVESTIGATION OF NICKEL CONTAINED FROM SULFIDE ORE DEPOSIT SAMPLES IN NAMTU MINE AREA BY MEASURING HALF-LIFE OF COBALT-58

Khin Su Su Han¹, Kay Thi Thin²

Abstract

The half-life of nickel in sulfide ore samples was determined by using neutron activation analysis. In NAA method, the samples were activated by Am-Be (α ,n) isotopic neutron source. Its strength is 550 mCi, average neutron energy is about 3 MeV and half-life is 432 years. After irradiation, the gamma radiation of the samples were collected and calculated by using GM (ST-360) counter. Since, the resulting half-life of the sample is 70 days, the possible reaction of nickel is confirmed as $\frac{58}{100}$ mCi = $\frac{58}{100}$

Ni (n, p) Co. The best choice is this nuclear reaction for ore sample. This reaction is confirmed by calculating the half-life of this reaction. $_{58}$ $_{58}$

Ni (n, p) Co is the best reaction because it has suitable energy and half-life.

Keywords: Rare Earth Metals, GM (ST-360) counter, Sulfide Ore Deposite Mine, NAA method

Introduction

Bawdwin Mine is the biggest Pb, Zn and Ag producer of Myanmar. The ore body is one of the largest and richest ever found. The geologic setting, ore type, metal zoning, alteration and geochemical characteristics all point out that the Bawdwin deposit is one of those of the well known massive sulfide deposits associated with felsic volcanism formed. The major Bawdwin ore body is that of the stratabound massive sulfide type, emplaced within the volcanoclastic rocks. The ore occurs as solid masses of sulfides, in places practically void of gangue minerals, as veins.

Here, the vertical metal zoning of Cu-Zn-Pb in the massive stratiform ore body and high Ni-Co-Cu in the underlying and cross-cutting loads of lower part of Mingtha and Chin are visualized.

^{1.} Lecturer, Department of Physics, Mandalay University of Distance Education, Mandalay, Myanmar.

^{2.} Pro-Rector, Meiktila University, Meiktila, Myanmar.

These sulphides, including galena (lead sulfide), sphalerite (zinc) and chalcopyrite (copper), accumulate at and just below the seafloor, where they form massive deposits that can range from several thousands to about 100 million tones. High concentrations of base metals (copper, zinc, lead) and especially precious metals (gold, silver) in some of these massive sulfide deposits have recently attracted the interest of the international mining industry. Many polymetallic sulfide deposits are also found at sites that are no longer volcanically active.

Massive sulphides formed in basaltic to and esitic environments of back-arc spreading centres (573 samples) are characterized by high average concentrations of zinc (17%), lead (0.4%) and barium (13%), but little iron. Polymetallic sulphides at back-arc rifts in continental crust (40 samples) also have low iron content but are commonly rich in zinc (20%) and lead (12%), and have high concentrations of silver (1.1%, or 2.304 g/s).

$$2FeS_{2} + 7O_{2} + 2H_{2}O \rightarrow 2Fe^{2+} + 4H^{+} + 4SO_{4}^{2-}$$

$$4Fe^{2+} + 4H^{+} + O_{2} \rightarrow 4Fe^{3+} + 2H_{2}O (2)$$

$$Fe^{3+} + 3H_{2}O \rightarrow Fe(OH)_{3} + 3H^{+} (3)$$

$$FeS_{2} + 14Fe^{3+} + 8H_{2}O \rightarrow 15Fe_{2}^{+} + 2SO_{4}^{2-} + 16H^{+}$$

These ore deposits have been formed during submarine volcanicexhalative processes while needed condition like pH - Eh is suitable for sea water, depth of topography and chemical composition of the water. Some of characteristics of type of ore deposits are:

- 1 Paragenesis of massive ore deposits, contain after 60 90% of sulfas, for example pyrite and pyrotite.
- 2 Type of these ore deposits, with increasing oxide ore deposits. likes iron ore deposits in central Iran and ore kiruna iron ore deposits in Sweden.
- 3 This type or deposits are divided into three groups:

a- Ore deposits with paragenesis of zinc-lead-copper

- b- Ore deposits with paragenesis of zinc- copper
- c- zinc- copper

Experimental Procedure

Sample Location (Sampling Site), Selection reaction and Preparation

Bawdwin Mines area (approximately about 12 square miles) lies at Namtu, Northern Shan State, Myanmar. Bawdwin mine is situated at longitude 97°23'24" E and latitude 23°05'24" N. The mining town of Bawdwin is situated in a narrow valley among a mountainous country rising up to 4600 feet above sea level and with V-shaped valleys. Bawdwin Mine is the biggest Pb, Zn and Ag producer of Myanmar. The ore body is one of the largest and richest ever found.

Bawdwin ore body with Pb, Zn, Ag is once one of the largest and richest ever found. It occurs in a NW-SE trending zone of about 8000feet long and 400-500 feet in width mostly along the eastern side of the Taungpeng-Hsenwi fault system. The ore body itself is about 3000 feet long and is well-defined. In the center of the ore shoot the ore was almost sulfides for a width of about 140 feet.

Each sample was weighed carefully by digital balance. A 40g of this ore granules from encapsulated in a polyethylene container was used in this work. This container was chosen due to its low background. Then all samples were put in a plastic bag in very close to the neutron source for one week irradiation time.

Threshold reactions of the types (n, p), (n, n'), (n, α) and (n, 2n) induced by the fast component of the fast neutron spectrum as well as the (n,γ) capture reactions produced by thermal and epithermal neutrons are well recognized.

Activation analysis with fast neutrons (fast neutron activation analysis , FNAA), using threshold reactions is not widely used, because of the lowflux density of fast neutrons in Am-Be neutron source, the small cross sections of many threshold reactions and the relatively high-threshold energy of neutrons.

Threshold reactions provide useful alternative reactions for the determination of certain elements by NAA if the (n,γ) reaction products are formed with unfavourable radioactive properties. As an example, determining

Ni using the ⁵⁸Ni (n,p) ⁵⁸ Co reaction ($T_{1/2}$ of ⁵⁸Co is 70.82 days) is favoured instead of using neutron capture reactions (⁶⁴Ni (n, γ) ⁶⁵Ni), which need pneumatic irradiation rabbit system due to the short half life time of ⁶⁵Ni.

Fe and Ni were determined in blue-green algae using the reactions 54 Fe (n, p) 54 Mn and 58 Ni (n, p) 58 Co. The iron isotopic abundances were determined in iron materials using threshold reactions. Fast determination of Fe by instrumental neutron activation analysis through the formation of 56 Mn from both 55 Mn (n, γ) 56 Mn and 56 Fe(n, p) 56 Mn using both reactor neutrons and epithermal neutron irradiation was described and evaluated. 58 Co production from natural nickel in nuclear reactor was described with particular consideration of interfering nuclear reaction.

The most abundant isotope of nickel is mass 58, and it is the most useful for the activation analysis with 14 MeV and 3 MeV neutrons. The best nuclear reaction for the identification of the isotope of interest should be chosen. Sometimes there is more than one reaction available for the same isotope. The possible induced nuclear reactions in Nickel ⁵⁸ Ni together with the reaction characteristics are shown in Table (1).

⁵⁸ Ni (n, p) ⁵⁸ Co is the best reaction because it has suitable energy and half-life. Moreover, the absorption reaction cross-section and target isotope ⁵⁸ abundance of the Ni (n, p) ⁵⁸ Co are relatively high Gamma emission probability (99%) from first peak energy (810.76keV) of this reaction is very high. It is also the endothermic reaction (Q-Value is negative) and threshold energy is lower than other reaction. Therefore, ⁵⁸ Ni (n, p) ⁵⁸ Co reaction is selected from four reactions. The decay scheme was shown in Figure (1). The best choice is this nuclear reaction for iron sample. (⁵⁸ Ni about 99%) This reaction is confirmed by calculating the half-life of this reaction.

Reaction	Gamma -energy (keV)	Half-life (days)	Gamma emission probability (%)	Threshold energy (MeV)	Isotopic abundance %
⁵⁸ Ni (n, p) ⁵⁸ Co	810.77	70.86	99.00	2.6	68.077
54 Fe (n, p) 54 Mn	834.85	312.12	99.97	2.8	5.845
$Mo_{92m}(n, p)$	934.44	2.576	99.07	6	14.48
⁹⁵ Mo (n, p) ⁹⁵ Nb	765.9	10.15	99.808	-	15.92

Table 1: Nuclear data for some threshold reaction

Half-Life Measurement of Irradiated Samples

The sample material is irradiated with neutrons from a neutron source. In this process, isotopes are converted into radioactive isotopes. While these isotopes decay, with half-life varying from seconds to years, they emit β -decay half-life and for detecting trace amounts of elements present in materials. These methods and data analysis techniques for making high precision measurements of nuclear beta decay half-lives. The change in the electron captures half-life of ⁵⁸Ni in pure Nickel. In addition, the beta-minus decay half-life of ⁵⁸Co.

Americium also alloys with Beryllium to form Am-Be which produces neutrons via the ⁹Be (α ,n) ¹²C reaction was used. ²⁴¹Am has a half-life of about 432 years. Although this isotopic decays by emitting alpha particles of about 5.4 MeV, these particles are following by gamma rays in the 40 to 60 keV region in the majority of the disintegrations. This gamma-ray emission make Americium appear less satisfactory than Plutonium for the preparation of neutron sources. For the Am-Be source in Physics lab, University of Mandalay, total neutron capture from the neutron source N=1.04×10⁶ neutrons/cm²s. Figure (2) shows the experimental set-up of the 550mCi 241 Am-Be neutron source irradiation facility.



Figure 1: The decay scheme of ⁵⁸Co



Figure 2: The experimental set-up of the 550mCi ²⁴¹Am-Be neutron source irradiation facility.

Experimental Set-up for Radiation Measurement

After irradiation, the gamma ray spectra of the radioactive ore samples were detected and analyzed by GM Counter. The experimental set-up for GM-ST360 counter is shown in Figure (3). Irradiate the sample for about 2 weeks by placing it in appropriate position in the ²⁴¹Am-Be Neutron (normally at the center of the coloum). Apply the operating voltage (1000V) for the GM Tube. Place the irradiated samples under the window of GM tube at a convenient distance (2cm) in order to get a good number of counts per second. Determine the background count rate (N) for each interval of 300 seconds (5minutes).



Figure 3: Experimental arrangement for GM-ST360 counter

To measure the half-life of Nickel-58

$$N(t) = N - \lambda N \Delta t, \tag{1}$$

where N(t) is the number of atoms that will be present at time t, N is the number of atoms present currently, λ is the decay constant, and Δt is the elapsed time. If the number of radioactive atoms remaining is plotted against time, curve can be obtained. The decay constant can be obtained from the slope of these curves (discussed more below).

A more common way of expressing the decay of radioactive atoms is the half-life. The half-life of a radioactive isotope is the time required for the disintegration of one-half of the atoms in the original sample.

activity, since activity =
$$\frac{N}{time}$$

(N= Each count of a GM tube represents one atom decaying and releasing one particle or ray of radiation.)

This is a separable differential equation that becomes

$$\int_{N_0}^{N} \frac{dN'}{N'} = -\lambda \int_{0}^{t} dt'$$
(2)

Thus, if we plot the natural log of the number of atoms (or activity) versus time, we will get a straight line with slope = dy/dx. This would allow us to find the decay constant. We will need the decay constant in the next step, which is to find the half-life of the radioactive isotope we are studying. Starting from Equation and applying a simple logarithmic identity,

Finally, we can solve for the half-time

$$t_{1/2} = \frac{\ln(2)}{\lambda} \tag{3}$$

Results and Discussions

The experimental work was performed at the Nuclear Research Laboratory, Department of Physics, and Mandalay University. In NAA experiment, ore samples were irradiated by using Am-Be (α , n) isotopic neutron source and then the induced gamma radiation were detected by using GM- ST360 Radiation Counter with windows and Macintosh software. Moreover, the absorption reaction cross-section and target isotope abundance of the Ni (n, p) Co are relatively high Gamma emission probability (99%) from first peak energy (810.76keV) of this reaction is very high. It is also the endothermic reaction (Q-Value is negative) and threshold energy is lower than other reaction. Therefore, Ni (n, p) Co reaction is selected from four

reactions. Note down the back ground count rate, before and after the experiment in order to subtract from the observed counts and record observations as shown in the Table (2). plot graph of log of the count rate (log N) versus time (second). The decay constant can be obtained from the slope of these curves (discussed more below). It was be a straight line as shown in figure (4). The slope of the straight line graph using the least square fit methods (use the formula)

$$m = (n \sum xy - \sum xy) / (\sum nx^2 - (\sum x)^2)$$
(4)

to determine the slope of the graph which gives the value of the decay constant.

Where n = number of observations

x = time interval

y = Log N

Table 2: Irradiation Measured data and Counting Conditions

Sr. No.	Time (min)	Counts	Net counts rate	Log N
1	5	1738	253.67	5.54
2	10	3257	231.77	5.45
3	15	4658	216.6	5.38
4	20	6082	210.17	5.24
5	25	7702	214.15	5.37
6	30	9248	214.33	5.37
7	35	10227	198.27	5.29
8	40	11039	182.05	5.20
9	45	11738	166.90	5.11
10	50	12334	152.75	5.03
11	55	13000	142.43	4.90
12	60	14360	145.4	4.90



Figure 4: Linear decay curve

Conclusion

Neutron activation of materials fallowed by using GM counter is an effective method for making measurements of nuclear beta decay half-lives and for detecting trace amounts of elements present in materials. In addition, the beta decay half-life of ⁵⁸Co is measured and compared with table of isotope library. Since, the resulting half-life of the sample is 70 days, the possible reaction of nickel is confirmed as Ni (n, p) ⁵⁸Co. The best choice is this nuclear reaction for ore sample. This reaction is confirmed by calculating the half-life of this reaction. Ni (n, p) ⁵⁸Co is the best reaction because it has suitable energy and half-life.

Acknowledgements

The authors are very much indebted to our teacher, Dr Aung Naing Soe, ProRector, Mandalay University of Distance Education, for allowing us to present this thesis.

The authors would like to express our sincere thanks to Professor Dr Kathi Nwe, Head of Department of Physics, Mandalay University of Distance Education, for her kind permission to carry out their research.

The authors are also thankful to our teachers of the ENP Laboratory, Department of Physics, University of Mandalay, for the encouragement during the period of this research.

Thank must also go to all our friends because of their reminiscent and sacrificial help to fulfill our desire within the fixed time.

References

- A. EI Abd, "Determination of Iron and Nickel in Geological Samples by Activation Analysis with Reactor Fast Neutrons", Reactor Physics Department, Egypt (2009).
- A.M. Hassan and J. Madani, "Neutron Activation Analysis of Saudi Hematite and Phosphate Samples Using the ²⁴¹Am-Be Neutron Irradiation Facility", Al-Azhar University, Egypt (1994).
- Dr Myint Lwin Thein and U Than Naing, "Stratigraphic and Tectonic Aspects of the Bawdwin Sulfide Ore Deposit", University of Yangon (1983).

"Massive Sulfide Ore Deposits", http:// en.wikipedia.org/wiki/ Volcanogenic.htlm (2012).

Z.Molnar, "Neutron Activation Analysis", http://www.reak.bme.hu/Education/Wignercourse/Wigne Minuals/Budapest/NEUTRON-ACTIVATION ANALYSIS.htm (2002).



REAL-TIME AUDIO TRANSMISSION SYSTEM BASED ON VISIBLE LIGHT COMMUNICATION

Ei Ei Minn¹, Kyaw Zwa Soe²

Abstract

A simple prototype of an optical wireless audio system by using laser diode as a source for the transmitter has been proposed. In this project, we designed and implemented a wireless optical transmitter and receiver system that established an audio communication at some distances with weak signal via visible light communication. The wavelength that used for this project is 635 nm which is visible wavelength range. Based on the experimental results, the visible light communication system can work successfully within in distance up to 30 meters. This project is successfully improved the transmission distance and signal coverage area effectively with low cost of hardware, high communication speed and almost no limit to bandwidth.

Keywords: Optical wireless communication, free space optical, laser, audio transmission

Introduction

The Optical wireless communication (OWC) also known as Free Space optical (FSO) system is a system that modulates visible or infrared (IR) beams through the atmosphere to propagate any data signals in a system that transfer a signal via visible light usually the wavelength is 380 nm to 740 nm through free space. In other words, it uses light to propagate the signal or to transmit the data in free space, FSO system uses light as the optical source such as a light emitting diode (LED) or laser diodes (LD) to transmit a data instead of enclosing the data stream in a glass fiber but it transmits the modulated light beam through the air. Hence, OWC is gaining reception in an increasing to the number of sectors of science and industry, owing to it is a very unique combination of the features such as extremely high bandwidth, rapid deployment time, license and tariff-free bandwidth allocation, low power consumption, weight and size.

The system using visible light technology has become a significant advantage over a radio frequency (RF). Therefore, optical wireless visible light knowledge seems to be perfect for managing wireless communication in

¹ Dr, Professor, Department of Physics, University of Computer Studies (Mandalay)

² Rector, University of Computer Studies (Mandalay)

the future. Furthermore, visible light transmission does not interfere with the existing RF system and does not controlled by the Federal communication commission (FCC) regulations. In addition, this project can build some privacy for sending and receiving data as visible light does not penetrate the wall, thus providing a level of privacy in the area.

Moreover, the newest publications have attracted considerable interest in using wireless optical communication links in aircraft and space vehicles. Using on-board wireless optical communication has great potential for size, weight, power, cost and EMI reduction. Therefore, this project will provide the initial drive to transmit voice and music by the light source and propagate through free space to be received with improving the distance up to 30 meters. Furthermore, this project also undertakes as a solution for problems about limited distance for transmitting the audio signal and reduces the noise.

Figure 1 shows the basic diagram of the optical wireless audio system or free space optical system (FSO) where the system is called line of sight (LOS) simplex communication system. The light from transmitter must be transmitted in straight lines without any divergence or scattering. It is divided into two main parts consisting of a transmitter circuit and a receiver circuit.



Figure1 : Basic Diagram of the Optical Wireless Audio System

System Operation

The system consists of a transmitter which is fed from the audio signal source and a receiver which picks up the modulated laser signal from transmitter.

There are two basic types of modulation that can be applied to this application, AM (amplitude modulation) and FM (frequency modulation). An AM system has the advantage of being extremely simple, but it has a major drawback in that any non-linearity in the system produces distortion on the audio output signal. In practice quite significant levels of distortion would almost certainly result, and it is better to use an FM system where nonlinearity in the laser diode, laser diode driver, and photo detector do not affect the audio output quality. The block diagram for audio transmission is shown in Figure 2.

The receiver must convert the variation in frequency back into an audio signal using some form of frequency to voltage converter. The photo detector is connected in a potential divider circuit which is in turn connected across a voltage source. The varying light level is thus converted to varying resistance through the detector element, and to a varying voltage by the potential divider circuit. The equipment uses a simple FM set up and the block diagram for the audio receiving is shown in Figure 3.



Figure 2 : Block Diagram for Audio Transmission System



Figure 3: Block Diagram for Audio Receiving System

Circuit Design

3.1 Transmitter Circuit

Figure 4 shows the circuit diagram of the transmitter circuit for audio signal. This circuit is slightly more simple of the two devices, and really consists of little more than a VCO (Voltage Controlled Oscillator). The output frequency of VCO is dependent on the control voltage, and this voltage is modulated by the audio input signal. An FM system is not distortion less though, to obtain a good quality audio output, the VCO and the frequency to voltage converter at the receiver must have good linearity.

The transmission circuit is more than just a VCO, and one of the additional stage is a buffer stage at the output which provides a reasonably high drive current to the laser diode. The circuit is designed around IC 3 which is a CMOS 4046 BE phase-locked loop, but in this circuit only the VCO section of the device is utilized. C_6 , R_6 and VR 1 are the timing components, and VRI is adjusted to match the center frequency of the transmitter VCO to that of the PLL decoder in the receiver circuit.

The output of the VCO is fed to the anode of semiconductor laser diode via resister R_7 and coupling capacitor C_7 . When the power is applied to the laser diode via resister R_8 , the generated laser beam output is about 635 nm and current flow into the laser diode is about 50mA. ICI is the input buffer stage and it will give enough high input impedance. The low pass filter is based on IC 2 which also operates as a unity voltage gain buffer stage. The filter gives the system a band width of about 15 kHz. This is marginally less than the full audio range, but is sufficient to provide a very respectable audio


Figure 4: The Complete Circuit Diagram of the Transmitter Circuit for Audio Signal

3.2 Function of Phase-Locked Loop

A phase locked loop provides the frequency to voltage conversion. The phase comparator, low pass filter and VCO make up the phase locked loop. The relative phase and frequency of the input signal and the VCO are checked by the phase comparator, which provides a series of output pulses. These pulses are integrated by the low pass filter to produce a reasonably smooth control voltage for the VCO. If the VCO is at a lower frequency than the input signal or even if it is just slightly lagging the input signal in phase, the output from the low pass filter goes to a high voltage and boosts the operating frequency of the VCO. Similarly, if the VCO is at a higher frequency than the input frequency, or leading it in phase, the output of the low pass filter goes to a low voltage. This reduces the VCO's operating frequency.

There is a negative feedback action here which results in the VCO locking on to the same frequency as the input signal, and also keeping in phase with it. This assumes that the input frequency is within the locking range of the circuit.

3.3 Receiver Circuit

The circuit diagram of the receiver circuit for audio signal appears in Figure 5. A phototransistor is used as the light detector, and this provides good sensitivity at the high carrier frequency and we use laser light as the carrier frequency. TR 2 is a gain phototransistor, and the collector to emitter resistance of TR 2 is connected with R9 to form a potential divider across the supply lines. The pulses of light cause the collector to emitter resistance of TR 2 to fall slightly, and this generates small negative pulses at the collector of TR 2. The output from the detector circuit is guite low at typically only a few mV RMS or less. A two stage gain amplifier is used to boost and clip the signal to give virtually square wave output to drive the frequency to voltage converter circuit. TR 3 is connected as a high gain common emitter amplifier, and it produces the first stage of amplification. IC 4 is connected as an inverting amplifier with a voltage gain of 20 dB, and this provides the second stage of amplification. The clipped signal at the output of IC 4 is compatible with the input of IC 5, which is another 4046 BE CMOS phase-locked loop. In this case it is used as the phase-locked loop detector. The link across pin 3 and 4 connects the output of the VCO to the input of the phase detectors (only the one of which is used here). R_{19} and C_{12} form the low pass filter between the phase comparator's output and the control input of the VCO while C_{12} and R_{17} are the VCO's timing components. R₁₈ is the load resistor for the built-insource follower buffer stage of IC 5, so demodulated audio can be taken from pin 10 of IC5.

IC 6 is used as the basis of the low pass filter at the output of the unit, and this is essentially the same as the filter at the input of the transmitter. The output from IC 6 is fed to the input of IC 7, which is an audio power amplifier. This provides an excessive output signal for most headphones, and resister R_{24} is therefore used to attenuate the output signal. The circuit will handle signal voltage of up to about 1V RMS or so with distortion of under 1%. The current consumption of the audio receiving circuit is about 12mA.



Figure 5: The Complete Circuit Diagram of the Receiver Circuit for Audio Signal

Result and Discussion

Figure 6 shows the complete prototype of optical wireless audio system. Both transmitter and receiver work by using battery (9V). Transmitter uses semiconductor laser as a data carrier. Transmitter uses frequency modulation to produce a series of audio signal encoding. Then, the receiver will receive the signal light, demodulate and enforce signals that can be sent by voice amplifier where the music can be heard. One can observed that the recent circuit setting can give a good or satisfactory results with a fairly high input level of around 250 mV to 1V RMS.

This project can operate up to 30m distance. If one can align the transmitted laser beam to reach the light sensor (phototransistor) of receiving circuit, so it can be used as a remote device for several purpose. The operating range is mainly depended on the laser output power.



(a) Transmitter Circuit



(b) Receiver Circuit



Conclusion

A method for transmitting and receiving of audio signal within a specified distance interval was presented. We recommend to improve the efficiency of optical wireless transmission by using laser diodes (LD) as the light source, because the LD can hit the laser over long distance with low noise. Therefore, this system is a good system and has high potential of commercialization that can be used in various applications such as wireless communication in the museum, airplane, intercom, TV sound system, closed circuit cameras and remote control devices.

If stereo operation is required, the most simple way of achieving this is to use a separate transmitter and receiver circuit for each channel. Furthermore, this project will proceed to transmit audio and video simultaneously with low noise in the future.

Acknowledgements

We would like to thank University of Computer Studies (Mandalay), Ministry of Education, Government of the Union of Myanmar which has financially supported this research to be accomplished.

References

- A. Beaver, M. Hannon, and A. Jalilzadeh, Infrared FM Audio Communication System, 2011.
- A. C. Boucouvalas, Indoor Ambient Light Noise and its Effect on Wireless Optical Links, *IEEE Proc. Optoelectronics, vol. 143. No.*6, Dec. 1996, 334-338.
- E. Chan, Wireless Optical Links for Airplane Applications, *IEEE, Photonics Society Summer* Topical Meeting Series, 2012, 76-77.
- H. Manor and S. Arnon, Performance of an optical wireless communication system as a function of wavelength. *Appl Opt.* 42,2003, 4285-4294.
- J.M. Kahn and J.R Barry, Wireless Infrared Communications, *Proceedings of the IEEE, vol,* 85, no, 2. February 1997, 265-298.
- Najmiah Radiah Mohamad, Chau Man Siang, Ahmad Sadhiqin MohdIsara, Adie MohdKhafe, AzahariSalleh, NurFatihahAzmi, Electromagnetic Levitator, *International Conference on Computer and Communication Engineering (ICCCE)*, 2012, 3
- R. Kawano, Y. Matsuya. T. Ishihara, J-1. Inoue, and Y. Kado, Voice Ubique Ultra Small High Quality Infrared Audio Receiver, Proc. IEEE Int. Conf. Consumer Electron. 2005, 285-286.
- W. Huang and H. Yang, Comparative study on three methods of wireless receiving of audio signal, 2nd inter, Conf. on. Artificial Intelligence, Management Science and Electronic Commerce (AIMSEC), 2011, 1994-1997.

COUPLED-CHANNELS ANALYSIS FOR HEAVY-ION FUSION REACTIONS OF $^{16}O + ^{A}X$ SYSTEMS

No No Htike¹, Nyein Wint Lwin²

Abstract

In this work, we have studied the fusion cross sections and fusion barrier distributions of heavy-ion collision at energy near and below the Coulomb barrier. The coupled-channels method has been applied to analyze the intrinsic characters of colliding systems. Firstly, we evaluate fusion cross sections for systems having different collective environments. Next, we calculate the fusion cross section and fusion barrier distribution for fixed projectile and different target (i.e., ${}^{16}O + {}^{A}X$ systems where the target has different intrinsic characters such as rotation and vibration). To this end, we compare the experimental fusion cross sections with those from calculations with and without coupling using the same potential parameters of the selected systems. The calculated results indicate the sensitivity of fusion cross sections on types of static and dynamic deformations. The results show that the coupled-channels calculations reproduce the fusion cross sections very well but barrier distribution deviate from the experimental results in the high energy region.

Keywords: nuclear structure, rotation, vibration

Introduction

This study focuses on the fusion cross section and fusion barrier distribution of heavy-ion collisions at energies around the Coulomb barrier are strongly influenced by couplings of the relative motion of the colliding nuclei to several nuclear intrinsic motions. In order to take into account those couplings, the coupled-channels approach has been a standard tool. In this approach, one often uses experimental information on nuclear intrinsic degrees of freedom, such as rotation and vibration. We will apply this approach particularly to the ¹⁶O + ^AX systems where the target nuclei have different intrinsic characters, and compare with the experimental results. The structure of colliding nuclei will be investigated from the effects of nuclear intrinsic motion on barrier distribution.

^{1.} Demonstrator, Department of Physics, University of Nursing, Mandalay.

^{2.} Associate Professor, Department of Physics, Mandalay University of Distance Education.

Coupled-Channels Formalism for Heavy-Ion Fusion Reactions

In order to take into account excitations of the colliding nuclei during the fusion, we assume the following Hamiltonian:

$$H(\mathbf{r},\xi) = -\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r}) + H_0(\xi) + V_{coup}(\mathbf{r},\xi),$$
(1)

where r is the coordinate for the relative motion between the projectile and target nuclei, and μ is the reduced mass. H₀(ξ) is the intrinsic Hamiltonian, ξ representing the internal degrees of freedom. V(r) is the potential for the relative motion and V_{coup} (**r**, ξ) is coupling Hamiltonians between the relative motion and intrinsic degrees of freedom, respectively. The coupled-channels equations are obtained by expanding the total wave function in terms of the eigen functions of H₀(ξ). This leads to

$$\left[-\frac{\hbar^2 d^2}{2\mu dr^2} + \frac{J(J+1)\hbar^2}{2\mu r^2} + V(r) - E + \epsilon_n \right] u_n^J(r) + \sum_{n'} V_{nn'}(r) u_{n'}(r) = 0, \qquad (2)$$

where, ϵ_n is the excitation energy for the n-th channel. In deriving these equations, we have employed the iso-centrifugal approximation and replaced the angular momentum for the relative motion by the total angular momentum, J. This approximation has been found to be valid for heavy-ion systems, and reduces considerably the dimensions of the coupled-channels problem. We impose the following boundary conditions in solving the coupled-channels equations:

$$u_{n}^{J}(r) \rightarrow H_{J}^{(-)}(k_{n}r)\delta_{n,0} - \sqrt{\frac{k_{0}}{k_{n}}} S_{n}^{J} H_{J}^{(+)}(k_{n}),$$

(3) Here, $k_n = \sqrt{2\mu(E - \epsilon_n)/\hbar^2}$ is the wave number for the n-th channel, where n = 0 represents the entrance channel. S_n^J is the nuclear S-matrix, and $H_J^{(-)}$ and $H_J^{(+)}$ are the incoming and the outgoing Coulomb wave functions, respectively. Using the S-matrix, the fusion cross sections are calculated as

$$\sigma_{\rm F}({\rm E}) = \frac{\pi}{k_0^2} \sum_{\rm J} (2{\rm J}+1) P_{\rm J}({\rm E}), \tag{4}$$

where,
$$P_J(E)$$
 is the penetrability and is related to the nuclear S-matrix by
 $P_J(E) = 1 - \left| \sum_n S_n^J \right|^2$.

Representation of Barrier Distribution

Extensive experimental as well as theoretical studies have revealed that the inadequacy of the potential model which can be attributed to the effects of the couplings of the relative motion between the colliding nuclei to several nuclear intrinsic motions. Among possible intrinsic excitations of a nucleus, the most relevant nuclear intrinsic motions to heavy-ion fusion reactions are low-lying vibrational excitations with several multi-polarities, or rotational motions of deformed nuclei.

The large enhancement of the fusion cross section, and the strong isotope dependence, are caused by the coupling of the relative motion between the projectile and target to their intrinsic degrees of freedom. The effects of channel coupling can be interpreted in terms of the distribution of fusion barriers and the underlying structure of the barrier distribution can be detected by taking the first derivative of penetrability. In order to point out the several important features of the fusion barrier distribution related with the channel coupling effects, it is important to use the barrier distribution representation. That is, the effects of channel coupling can be interpreted in terms of the distribution of fusion barriers and the underlying structure of the barrier distribution can be detected by taking the first derivative of penetrability is given by

$$D_{\text{fus}}(E) = \frac{d^2(E\sigma)}{dE^2}.$$
 (5)

From this expression, it is clear that the first derivative of the product of fusion cross section σ_f and the centre of mass energy E with respect to the energy, $d(E\sigma)/dE$, is proportional to the penetrability of the s-wave scattering. The fusion barrier distributions are obtained with the point difference formula with the energy step of $\Delta E = 2 \text{MeV}$ in order to be consistent with the experimental barrier distribution.

Results and discussion

This section describes the fusion cross sections and barrier distributions for ${}^{16}O + {}^{A}X$ systems (i.e., the same projectile and different targets) such as ${}^{16}O + {}^{58}Ni$, ${}^{62}Ni$, ${}^{92}Zr$ and ${}^{166}Er$ reactions are presented. The calculations were performed using the code CCFULL and the relevant parameters used in the calculation are listed in Table (1). The nuclear potential is assumed to have a Woods-Saxon shape and the depth parameter of the potential was chosen to reproduce the experimental fusion barrier heights.

The low lying excitation levels of target nuclei suggest that three of the target nuclei, ⁵⁸Ni, ⁶²Ni and ⁹²Zr have vibrational nature and ¹⁶⁶Er have rotational nature. Firstly, the fusion of 16 O and the two Ni isotopes: 16 O + 58 Ni, ⁶²Ni systems are considered and the calculated results are shown in Fig.(1) and (2), respectively. The single quadrupole and octupole phonon coupling to the (2^+) and (3^-) states taken into account for both ${}^{16}O + {}^{56}Ni$ and ${}^{62}Ni$ systems. The energies and deformation values of the low lying states are given in Table (2).



barrier distribution for taken from [7].

Fig.1.The results of coupled channels Fig.2.The results of coupled channels calculations and the corresponding calculations and the corresponding ¹⁶O+⁵⁸Ni barrier distribution $^{16}\text{O}+^{62}\text{Ni}$ for reaction. The experimental data are reaction. The experimental data are taken from [7].

The calculated fusion cross section and fusion barrier distribution are shown in upper and lower panels. The solid lines and dotted lines are calculated results with and without coupling. One can see that the calculated results of the fusion cross sections slightly overestimate the experimental data at low energy region. The extracted fusion barrier distributions well reproduce experimental data although it does not give height of the barrier. The features of the barrier distribution are the same in both results, but the peak positions are slightly shifted to low energy due to the coupling effects.

Next, the reaction of same projectile and heavier target such as ${}^{16}\text{O} + {}^{92}\text{Zr}$ system will be studied. For fusion with ${}^{16}\text{O}$ and vibrational target, ${}^{92}\text{Zr}$, we considered the coupling of one quadrupole phonon to (2^+) state and three octupole phonons to (3^-) states of the target nucleus, ${}^{92}\text{Zr}$. The results of fusion cross section (upper panel) and barrier distribution (lower panel) are shown in Fig.(3). In the figures, the solid lines show the calculated results with coupling and dotted lines are without coupling. We have performed the calculation with different number of phonons for target nucleus as in the previous section and it is found that the energy dependence of the subbarrier fusion cross section is almost insensitive to the addition of multiphonon excitation of the target but the barrier distribution is strongly sensitive on this effect.

Finally, the fusion reaction of ¹⁶O with heavy deformed nucleus, ¹⁶⁶Er, has been studied. In the calculation, the low lying quadrupole excitation (2^+) state of ¹⁶⁶Er and inert projectile, ¹⁶O, are taken into account and the results are displayed by solid lines in Fig.(4). Figure captions are same as above interpretation of fusion cross section and barrier distribution for ¹⁶O+¹⁶⁶Er system. It is found that the calculated results of fusion cross section and fusion barrier distribution gives good agreement with the experimental data. Thus, we can investigate the structure of heavy elements and get the information of the colliding nuclei from barrier distribution.



Fig.3: The results of coupled channels **Fig.4:** The results of coupled calculations and the corresponding channels calculations and the barrier distribution for ${}^{16}O + {}^{92}Zr$ corresponding barrier distribution for reaction. The experimental data are ${\rm ^{16}O}$ 166Er + reaction. The taken from [8]. experimental data are taken from [9].

Table 1: The potential parameters used in the coupled channels calculations. The barrier parameters obtained are also given. The values of barrier depth (V_B), barrier position (R_B) and curvature ($\hbar\omega$) for each system are taken from [7, 8, 9].

Desetions	V ₀	r ₀	a	VB	R _B	ħω	
Reactions	(MeV)	(fm)	(fm)	(MeV)	(fm)	(MeV)	
¹⁶ O+ ⁵⁸ Ni	95.50	1.130	0.610	31.62	9.51	3.92	
$^{16}\text{O}+^{62}\text{Ni}$	98.73	1.135	0.630	30.94	9.74	3.82	
$^{16}\text{O} + ^{92}\text{Zr}$	135.00	1.200	0.460	42.44	10.37	5.00	
$^{16}\text{O} + ^{166}\text{Er}$	110.50	1.130	0.750	64.70	11.39	4.23	

Table.2: The energies and deformation values of low-lying 2^+ , 3^- states for the different nuclei. The excitation energies and $\beta(E_2)$ and $\beta(E_3)$ values are taken from [10]

Nucleus	λ	E*(MeV)	$\beta_{\lambda}(or) \beta_{4}$
58NT:	2^{+}	1.454	0.183
INI	3-	4.474	0.198
62NI:	2^{+}	1.172	0.198
INI	3-	3.756	0.197
⁹² 7.	2^{+}	0.934	0.101
Ζſ	3-	2.340	0.280
166 _E ,	2+	0.080	0.238
Eľ			$0.006(\beta_4)$

Summary and Conclusion

In summary, we have used the coupled-channels method to evaluate the effects of coupling for the systems such as ${}^{16}O + {}^{58}Ni$, ${}^{16}O + {}^{62}Ni$, ${}^{16}O + {}^{92}Zr$ and ${}^{16}O + {}^{166}Er$ reactions. The coupled-channels approach has been applied to investigate heavy-ion fusion reactions at energy near and below the Coulomb barrier. We have discussed the role of collective excitations on barrier distribution using recent experimental data and compared the calculated results of fusion cross section and fusion barrier distribution for ${}^{16}O + {}^{A}X$ systems with the experimental data. It is found that the fusion cross section and fusion barrier distribution of coupling results well reproduce the experimental data and hence able to investigate the structure of the colliding nuclei. Thus the coupled-channels formalism is very applicable to clearly see the structure of heavy elements in nuclear fusion reactions.

Acknowledgement

I would like to thank Dr Lei Lei Win, Professor and Head of Physics Department, University of Mandalay, for her encouragement and permission.

References

- A.B. Balantekin, et al., Phys. Rev. C28 (1983) 1565.
- K.Hagino, et al., Prog. Theor. Phys. 128 (2012), 1061-1106.
- K. Hagino, "Ph.D. Thesis", Tohoku University (1998).
- K. Hagino, et al., Comp. Phys. Comm. 123 (1999) 143.
- J.O. Newton, et al., Phys. Rev. C64 (2001) 64606.
- J.O. Fernandez Niello, et al., Phys. Rev. C43 (1991) 2303.
- M. Beckerman, Rep. Prog. Phys. 51 (1988) 1047.
- N. Keeley, et al., Phys, A628 (1998) 1.
- O. Tanimura, Phys. Rev. C35, 1600 (1987); Z. Phys, A327, 413 (1987).

https://nucleus.iaea.org/Pages/nu-dat-2.aspx.

IMPROTANCE OF TRANSFER CHANNELS IN SUB-BARRIER FUSION REACTIONS

Su Mon Myat¹, Nyein Wint Lwin²

Abstract

The role of neutron transfer is investigated in the heavy-ion fusion reactions of ⁴⁰Ca+⁴⁸Ca and ⁴⁰Ca+¹²⁴Sn systems by using coupled-channel method. The calculated fusion cross sections and barrier distributions are compared with the experimental data. The calculations are performed with the inclusion of vibrational coupling for target nuclei in both systems. The calculated fusion cross sections with channel couplings give better agreement compare with no-coupling calculations. But extracted barrier distributions still deviate from the experimental data. The Q-values of two neutrons transfer reactions ⁴⁸Ca (⁴⁰Ca, ⁴²Ca) ⁴⁶Ca and ¹²⁴Sn (⁴⁰Ca, ⁴²Ca) ¹²²Sn show 2.621 MeV and 5.410 MeV, respectively. The inclusion of neutron transfer channel in the calculations reproduces the experimental fusion cross sections and barrier distributions.

Keywords: Heavy-ion fusion reactions, Coupled-channel method, Neutron transfer

Introduction

The process in which two colliding nuclei come close together to form a compound nucleus either by overcoming or by quantum tunneling through the potential barrier is known as nuclear fusion reaction. The simplest theoretical way to understand the fusion of the two nuclei is the one dimensional (1D) potential model, wherein the projectile is assumed to penetrate through potential barrier between two interacting nuclei and form a composite nucleus. However, at energies below the Coulomb barrier, the extensive experimental as well as theoretical studies have revealed that there is an anomalously large enhancement in the fusion cross section over the predictions of (1D) barrier penetration model. It indicates that the fusion of two nuclei is a complex rearrangement process which involves a large number of the degrees of freedom and a strong coupling between the projectile-target relative motion and the internal degrees of freedoms. As a result fusion reactions have become the most studied processes to explore the importance of structural as well as dynamical effects in the compound nuclear reactions.

^{1.} PhD Student, Department of Physics, Mandalay University.

^{2.} Dr, Associate Professor, Department of Physics, Mandalay University of Distance Education.

Moreover, the importance of neutron transfer in increasing the sub-barrier fusion probabilities was also established. The coupling to a transfer degree of freedom is in general weaker than couplings to collective excitations.

However, when the coupling is sufficiently large, e.g., for a transfer channel with a positive Q-value it expected that the transfer coupling leads to an extra enhancement of fusion cross sections below the Coulomb barrier. It has been known well that two-neutron transfer reactions provide a unique tool to study the pair correlation between nucleons. The effects of collective surface vibrations on fusion were also considered in a semi classical picture, again resulting in a distribution of fusion barriers. The experimental measurements of the fusion barrier distribution (BD) represent a new stage in the study of heavy-ion fusion. The fusion BD analysis is valuable tool to understand the fusion mechanism of two heavy nuclei and the role of their internal degrees of freedom leading to fusion. The fusion BD has been shown to be sensitive to the data related to the nuclear structure, such as the nuclear shapes, the multiple excitations, and the anharmonicity of nuclear surface vibrations etc. For this purpose, high precision measurements of the fusion cross-section data are required and have been reported for many systems.

The aim of the present work is to investigate the importance of neutron transfer channels on the calculations of the fusion cross section and the fusion barrier distribution for the systems ${}^{40}Ca{}^{+48}Ca$ and ${}^{40}Ca{}^{+124}Sn$.

Theoretical framework

Coupled-channels method

The effect of the nuclear structure can be taken into account in a more quantal way using the coupled-channels method. In this method, consider a collision between two nuclei in the presence of the coupling of the relative motion between the center of mass of the colliding nuclei, $\vec{\mathbf{r}} = (r, \hat{\mathbf{r}})$ to a nuclear intrinsic motion ξ . The total Schrödinger equation can be transformed to a set of coupled equations

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_0(r) - E\right]u_n(r) + \sum_m V_{n,m}(r)u_m(r) = 0$$
(1)

where,

$$V_{n,m}(r) = \varepsilon_n \,\delta_{n,m} + \int d\xi \,\varphi_n^*(\xi) \,V_{coup}(r,\xi)\,\varphi_m(\xi) \tag{2}$$

is the coupling matrix elements. These equations are called the coupledchannels equations and are solved by imposing the boundary conditions

$$u_n(r) \to e^{-ik_n r} \delta_{n,0} + R_n e^{ik_n r} \qquad r \to \infty, \tag{3}$$

$$\to T_n \ e^{-ik_n r} \qquad \qquad r \to -\infty, \tag{4}$$

where $k_n = \sqrt{2\mu (E - \varepsilon_n)/\hbar^2}$ is the wave number of the n-th channel and we have assumed that the intrinsic motion is in the ground state (n = 0) before the collision. T_n is interpreted as the transmission coefficient, the penetrability through the Coulomb barrier is given by

$$P(E) = \sum_{n} \frac{k_n}{k_0} \left| T_n \right|^2.$$
⁽⁵⁾

Then, the fusion cross section is given by

$$\sigma_{fus}(E) = \frac{\pi}{k^2} \sum_{J} (2J+1) P^J(E).$$
(6)

Pair-transfer coupling

For the two-particle transfer couplings, the macroscopic form factor for the transfer between the ground states is usually used

$$F_{trans}(r) = F_{tr} \frac{dV_N(r)}{dr}$$
⁽⁷⁾

where F_{tr} is the coupling strength parameter and $V_N(r)$ is the nuclear potential for the system.

Fusion barrier distribution

The first derivative of the product of fusion cross section σ and the centre of mass energy E with respect to the energy $d(E\sigma)/dE$, is proportional to the penetrability of the s-wave scattering

$$\frac{d(E\sigma)}{dE} = \frac{\pi r_B^2}{1 + \exp[-\frac{2\pi}{\hbar\Omega} (E - V_B)]} = \pi R_B^2 P_0(E).$$
(8)

This equation immediately leads to a relation between the first derivative of the penetrability and the fusion cross section

$$\frac{d^2(E\sigma)}{dE^2} = \pi r_B^2 \frac{2\pi}{\hbar\Omega} \frac{e^{2\pi(E-V_B)/\hbar\Omega}}{\left(1 + e^{2\pi(E-V_B)/\hbar\Omega}\right)^2} = \pi R_B^2 \frac{dP_0(E)}{dE}.$$
 (9)

This quantity, which is conventionally called fusion barrier distribution, is peaked at the height of the Coulomb barrier for the *s*-wave scattering.

Results and Discussion

⁴⁰Ca+⁴⁸Ca System

The coupled-channels calculation of fusion cross section as well as fusion barrier distribution for heavy-ion fusion reaction of ${}^{40}\text{Ca}{+}^{48}\text{Ca}$ system by including the 3⁻ (octupole) state of ${}^{40}\text{Ca}$, [P:(3⁻)] and the 2⁺ (quadrupole) and 3⁻ (octupole) states of ${}^{48}\text{Ca}$, [T:(2⁺) (3⁻)].

The results of coupled-channels calculations performed by using the CCFULL code are compared with the experimental data in Fig (1.a) and (1.b). The left panel is the fusion cross section and the right panel is the fusion barrier distribution. The dashed line represents the calculations of without including the coupling effects, i.e., the target and the projectile are assumed to be inert in which the calculations of the fusion cross section fail to reproduce the experimental data at and below the Coulomb barrier. The calculations including the coupling effects without neutron transfer channel [P:(3⁻); T:(2⁺) (3⁻)³] is shown by dotted line which underestimated the experimental data.

The solid line represents the coupling effects with neutron transfer channel [P:(3⁻); T:(2⁺) (3⁻)³ + 2n], where the calculated fusion cross section agrees with the experimental data. We can see in this figure, the calculations with neutron transfer channel coupling reproduce the experimental data for the fusion cross section as well as the fusion barrier distribution. The Woods-Saxon parameters are taken to be V₀ = 68.05 MeV, r₀ = 1.16 fm, and a₀ = 0.66 fm. The Q-value of the neutron pick-up channel of the 2n-transfer reaction ⁴⁸Ca (⁴⁰Ca, ⁴²Ca) ⁴⁶Ca is 2.621 MeV. The low-lying excitations energies and the deformation parameters are E₃ = 3.737 MeV, and β_3 = 0.411 for ⁴⁰Ca and, E₂ = 3.831 MeV, E₃ = 4.506 MeV, β_2 = 0.10, and β_3 = 0.18 for ⁴⁸Ca.

⁴⁰Ca+¹²⁴Sn System

The calculations of the fusion cross section and fusion barrier distribution are presented in Fig (2.a), and (2.b). For ⁴⁰Ca+¹²⁴Sn case, the coupling to the 3⁻ state of 40 Ca, [P:(3⁻)] and the 2⁺ and 3⁻ states of 124 Sn, [T:(2⁺) (3)] were included. The dashed line in Fig (2.a) and (2.b) represents the calculations without including the coupling, i.e., both projectile and target are inert. The coupling without neutron transfer and with neutron transfer channels are defined by dotted and solid lines. The results of fusion cross section which include the coupling with neutron transfer channel agree well with the experimental fusion cross section, and the corresponding fusion barrier distributions reproduce the experimental barrier distribution than those of without neutron transfer channel. The O-value of the 2n-transfer reaction ¹²⁴Sn (⁴⁰Ca, ⁴²Ca) ¹²²Sn is 5.410 MeV. The Woods-Saxon parameters are taken to be $V_0 = 98.05$ MeV, $r_0 = 1.2$ fm, and $a_0 = 0.66$ fm. The low-lying excitations energies and the deformation parameters are $E_3 = 3.737$ MeV, and $\beta_3 = 0.411$ for ⁴⁰Ca and E₂ = 1.132 MeV, E₃ = 2.603 MeV, $\beta_2 = 0.096$, and $\beta_3 = 0.106$ for ¹²⁴Sn.



Figure1: The results of the coupled-channels calculations for ⁴⁰Ca+⁴⁸Ca system for the fusion cross section (left panel) and the corresponding fusion barrier distribution (right panel), respectively. The experimental data are taken form.



Figure 2: The results of the coupled-channels calculations for ⁴⁰Ca+¹²⁴Sn system for the fusion cross section (left panel) and the corresponding fusion barrier distribution (right panel), respectively. The experimental data are taken from.

Conclusion

The importance of transfer channels are investigated for the systems ${}^{40}\text{Ca}+{}^{48}\text{Ca}$ and ${}^{40}\text{Ca}+{}^{124}\text{Sn}$. It can be concluded that coupling of the low lying states with neutron transfer channels in ${}^{48}\text{Ca}$ and ${}^{124}\text{Sn}$ target nuclei are very essential and leads to enhance the fusion cross section calculations and also leads to reasonable agreement with the experimental fusion barrier distributions. Furthermore, the enhancement of fusion cross sections can be observed at low energies below the Coulomb barrier due to the positive Q-value neutron transfer effect. Therefore, the two nucleon transfer enhancement of sub-barrier fusion reactions is very important for these two cases.

Acknowledgement

I thank to Professor Dr. Lei Lei Win, Head of Physics Department, University of Mandalay, for her encouragement and permission.

References

- A. M. Stefanini, et al., J. Phys. G 87 (1997) 1401.
- A. M. Stefanini, et al., Phys. Let. B 728 (2014) 639
- C. L. Jiang, et al., Phys. Rev .C 82 (2010) 41601
- G. Potel, et al., Rep. Prog. Phys. 76 (2013) 106301.
- K. Hagino, et al., Comp. Phys. Comm. 123 (1999) 143.
- L. F. Canto, et al., Phys. Rep. 424 (2006) 1.
- S. G. Steadman and M. J. Rhhoades-Brown, Ann. Rev. Necl. Part. Sci. 36 (1986) 649.
- V. V. Sargsyan, et al., Phys. Rev. C 88 (2013) 064601.
- Z. Kohley, et al., Phys. Rev.C 87 (2013) 064612.

INVESTIGATION OF ENVIRONMENTAL POLLUTION IMPACTS ON RADON LEVELS AND ELEMENTAL CONTENTS IN AGRICULTURAL SOIL SAMPLES FROM MYINGYAN TOWNSHIP

Khin Sandar Khaing¹, Kalyar Thwe²

Abstract

Environmental pollution impact is the most important issue of our time. Soil and water pollution, in particular, have historically impacted on food safety which represents an important threat to human health. In this research work, twelve agricultural soil samples collected from the four places of agricultural area of Photokephyu Village in Myingyan Township were analyzed scientifically for environmental pollution protection purpose. To estimation of the nuclear pollution, especially radon concentration, surface and mass exhalation rates, and effective dose were carried out by Solid State Nuclear Track Detection. The soil samples were determined by Energy Dispersive X-Ray Fluorescence Method for elemental concentrations quantitatively. The measurement results radon level found in this study were below the action level recommended by the ICRP. In EDXRF results, the toxic elements were not found in the samples. Results reveal that there is no significant public health risk from radon and elemental concentrations in the study region. The present investigation is useful from the health and environmental point of view.

Keywords: SSNTD, EDXRF, agricultural soil, environmental pollution, health risk

Introduction

Radiation is a natural part of the environment in which we live. All people receive exposure from naturally occurring radioactivity in soil, water, air and food. The largest fraction of the natural radiation exposure we receive comes from a radioactive gas, radon and its daughter. When radium decays, a radon and an alpha particle produced then the radon atom moved into an adjacent crystal by recoil effect from ejected α -particle. The rate at which radon escapes from soil into the surrounding air is known as radon exhalation rate of the soil. Solid state nuclear track detectors, known as passive method, are widely used for radon measurements. The CR-39 detector is very sensitive

¹ Dr, Lecturer, Department of Physics, East Yangon University

² Dr, Professor, Department of Physics, University of Mandalay

for the detection of α -particles, particularly, emitted by radon and their progeny. The metal elements are naturally introduced in the environment through rocks harshness, and also by a variety of human activities through industrials, cattle raising and agricultural. Fe, Zn, Cu and Mn are essential micronutrients to the growing of aquatic organisms. While metals such Cd, Pb, and Hg are not necessary to the growing of these organisms, they are toxic even in trace amounts. However, above the allowed limit of each element, and all metals have a high degree of toxicity in the environment. EDXRF is an analytical method for qualitative as well as quantitative determination of elements in a sample, independent of their chemical forms. This study was undertaken for the purpose of estimating the radon concentration, radon exhalation rates and annual effective dose measurements in agricultural soil samples from Photokephyu Village in Myingyan Township, by using CR-39 SSNTDs. This measurement results were compared with the limit of ICRP Recommendation values. To analyze the elements contained in these samples, the energy dispersive x-ray fluorescence (EDXRF) system (Shimadzu EDX-720 spectrometer) was used. To estimate the radiological hazard associated with them to the general population living for agriculture in the study areas of Myingyan Township.

Materials and Methods

Sample Collection and Processing

Twelve soil samples were collected from surface soil, depth 15 cm and depth 30 cm at four places of agricultural studied areas in Photokephyu Village (Myingyan Township). The collected soil samples were dried at room temperature for a week. After drying, the samples were crushed to a fine powder and sieved through a small mesh size to remove the larger grains size and render them more homogenous. The map and photograph of the studied area is shown in Figure1. The list of sample and description of sample location are shown in Table1.



Figure 1: The map and photograph of the studied area in Myingyan Township

Sample	Depth of Collected	Location of Collected Sample					
Name	Sample	in Studied Area					
S ₁₁	Surface layer of soil	east					
S ₁₂	15 cm						
S ₁₃	30 cm						
S ₂₁	Surface layer of soil	west					
S ₂₂	15 cm						
S ₂₃	30 cm						
S ₃₁	Surface layer of soil	south					
S ₃₂	15 cm						
S ₃₃	30 cm						
S ₄₁	Surface layer of soil	north					
S ₄₂	15 cm						
S ₄₃	30 cm						

Table 1: The List of Sample and Description of Collected Sample Location

Experimental Details of SSNTD Measurements

In the present investigation, "Sealed Can Technique" was used to study radon concentration, radon exhalation rates and annual effective dose. Dried and sieved sample (100 g) was placed at the bottom of a cylindrical sealed Can of height 5.5 cm and diameter 7.5 cm. The schematic diagram and photograph of the Can technique are shown in Figure 2.



Figure 2: The schematic diagram and photograph of the Can Technique

Initially, the mouth of the cylindrical Can was sealed without CR-39 plastic track detector for one month so as to acquire equilibrium between radium and radon members. The CR-39 detectors were square in shape, $1 \text{ cm} \times 1 \text{ cm}$ in size. The CR-39 is a small piece of plastic that is sensitive to tracks of highly ionizing particles such as alpha particles. Thereafter, the cover was replaced quickly by a cover fitted with CR-39 detector faced the sample. The detectors were exposed for a period of about 100 days. In sealed Can technique, the material of interest has enclosed in a 'cylindrical plastic Can' and sealed for a period of three weeks in order to get secular equilibrium between radium and radon.

After the 100 days period of exposure, the CR-39 detector samples were chemically treated by etching using 6.25 N solution of NaOH at temperature of 70°C, for 6 hours. The temperature was kept constant with an accuracy of $\pm 1^{\circ}$ C. At the end of etching process, the detectors were washed thoroughly with water and then air-dried. The number of alpha tracks of each detector was counted visually using optical microscope with a magnification of 400X. Then, the track density of detector samples were obtained by taking the average of twenty fifth views in the microscope. The area of one Field of View (FoV) is 0.00332 cm^2 . The photograph of optical microscope is shown in Figure 3.



Figure 3: The photograph of optical microscope

The alpha track density of each detector was calculated as the relation:

Alpha Track Density = $\frac{\text{Average number of alpha tracks counted in all fields of view}}{\text{Counted area (one field of view)}}$

The standard error in the average number of alpha track counts and alpha track densities were calculated as:

Standard Deviation (
$$\sigma$$
) = $\sqrt{\frac{\sum_{i=1}^{n} (x_i - \overline{x})^2}{N}}$, Standard Error = $\frac{\sigma}{\sqrt{N}}$

The radon concentration was found by using this formula:

$$C_{Rn} = \frac{\rho}{KT}$$

Where ρ is track density (track /cm²), K is the calibration factor (0.23 tracks cm⁻² d⁻¹ per Bq m⁻³), and T is the exposure time (100 days).

Exhalation rates in terms of surface and mass were calculated from the following equations.

$$E_{x} = \frac{CV\lambda}{A[T + \lambda^{-1}\{e^{-\lambda T} - 1\}]}$$
$$E_{M} = \frac{CV\lambda}{M[T + \lambda^{-1}\{e^{-\lambda T} - 1\}]}$$

Where, C is integrated radon exposure concentration (Bqm⁻³), V is volume of Can (0.00024 m³), T is exposure time (100 days), M is mass of the sample in Can (0.1kg), λ is the decay constant for radon (0.1825 day⁻¹) and A is area of the (0.0044 m²).

According to the UNSCEAR (2000) report, annual mean effective dose H is estimated using the following equation:

$$\mathbf{H} = \mathbf{C} \times \mathbf{E} \times \mathbf{F} \times \mathbf{T} \times \mathbf{D}$$

Where C stands for the radon concentration (Bq m⁻³), E is the equilibrium factor for indoor that is set as 0.36, O is the occupancy factor taken as 0.8, T is time in hours in a year (8760 hy⁻¹) and D is the dose conversion factor $(9 \times 10^{-6} \text{ m Sv}^{-1} (\text{Bq m}^{-3})^{-1} \text{ h}^{-1})$.

Experimental Details of EDXRF Technique

Each one sample was pressed with hydraulic press weighing 5 tons a pellet with a diameter in 2.5 cm. Each soil samples was analyzed using Shimadzu EDX-720 (Japan) spectrometer. The Shimadzu EDX-720 detects these x-rays and quantitatively determines which elements are present in the material. The Shimadzu EDX-720 is an Energy Dispersive XRF system, kwon as EDXRF. This indicates that the x-rays are detected using a semiconductor detector, which permits multi-element, simultaneous analysis.

EDX-720 spectrometer system consists of an x-ray generator and x-ray tube, a detector, a sample chamber, measuring electronics system and personal computer. Figure 4 illustrates the functional diagram and photograph of EDX-720 spectrometer system. The Shimadzu EDX-720 is equipped with high level Fundamental Parameter (FP) software for the determination of organic materials using scattered x-rays in addition to the characteristic lines. This

spectrometer can operate either under normal air pressure or in vacuum. The powder sample pellets were placed in the samples chamber which can measure sixteen samples at on time.



Figure 4: The functional diagram and photograph of EDX-720 spectrometer system

The EDX-720 spectrometer was x-rays tube excited system with Rh target at its optimum conditions of (50 kV, 25 μ A). A high resolution semiconductor detector, Si (Li) detector, was used in the system. The detector can be stored at room temperature but the working temperature of the detector must be kept at liquid nitrogen (-170°C). The detector has an area of 10 mm². The resolution FWHM of the Si (Li) detector system was (<155 eV). Each pellet was run for 99 seconds and the x-ray spectra were analyzed in IBM PC using EDX-720 software. The software utilizes the personal computer functions to transfer data to hard disk.

Results and Discussion

Determination of Radon levels in Soil Samples

The photograph of the alpha tracks on the detector samples (S_{43}) is shown in Figure 5. The measurement results of radon levels in soil samples from agricultural studied area are shown in Table 2. Figure 6 shows the radon concentration in agricultural soil samples from different locations. The variation of radon surface and mass exhalation rates and annual effective dose in different samples are shown in Figure 7. The radon concentrations ranging from 6.77 \pm 3.39 Bq m⁻³ to 84.31 \pm 15.66 Bq m⁻³ with an average value of 41.55 \pm 8.32 Bq m⁻³. The surface exhalation rate has been found to vary from 0.07 \pm 0.04 to 0.88 \pm 0.16Bq m⁻² day⁻¹ with an average value of 0.43 \pm 0.09 Bq m⁻² day⁻¹. The mass exhalation rate has been found to vary 0.003 \pm 0.002 to 0.039 \pm 0.007 Bq kg⁻¹ day⁻¹ with an average value of 0.019 \pm 0.004 Bq kg⁻¹ day⁻¹. The annual effective dose varies from 0.15 to 1.91 m Sv y⁻¹ with an average value of 0.94 m Sv y⁻¹.



Figure 5: The photograph of the alpha tracks on the detector samples (S_{43})

Sample No.	Alpha Track Density (tracks cm ⁻²)	Radon Concentration (Bq m ⁻³)	Radon surface exhalation rate (Bq m ⁻² day ⁻¹)	Radon mass exhalation rate (Bq kg ⁻¹ day ⁻¹)	Annual Effective Dose (m Sv yr ⁻¹)	
S ₁₁	759.04 ± 250.08	32.79 ± 10.80	0.34 ± 0.11	0.015 ± 0.005	0.74	
S ₁₂	915.66 ± 188.82	39.55 ± 8.16	0.41 ± 0.09	0.018 ± 0.004	0.89	
S ₁₃	1686.75 ± 252.42	72.86 ± 10.90	0.76 ± 0.11	0.034 ± 0.005	1.65	
S ₂₁	156.63 ± 78.44	6.77 ± 3.39	0.07 ± 0.04	0.003 ± 0.002	0.15	
S ₂₂	746.99 ± 175.09	32.27 ± 7.56	0.34 ± 0.08	0.015 ± 0.003	0.73	
S ₂₃	1024.10 ± 296.80	44.24 ± 12.82	0.46 ± 0.13	0.020 ± 0.006	1.00	
S ₃₁	686.75 ± 171.79	29.67 ± 7.42	0.31 ± 0.08	0.014 ± 0.003	0.67	
S ₃₂	831.33 ± 78.26	35.91 ± 3.38	0.38 ± 0.04	0.017 ± 0.002	0.82	
S ₃₃	1096.39 ± 211.82	47.36 ± 9.15	0.50 ± 0.10	0.022 ± 0.004	1.08	
S_{41}	650.60 ± 55.54	28.10 ± 2.40	0.29 ± 0.03	0.013 ± 0.001	0.64	
S ₄₂	1036.14 ± 189.16	44.76 ± 8.17	0.47 ± 0.09	0.021 ± 0.004	1.02	
S ₄₃	1951.81 ± 362.49	84.31 ± 15.66	0.88 ± 0.16	0.039 ± 0.007	1.91	
Average	961.85 ± 192.56	41.55 ± 8.32	0.43 ± 0.09	0.019 ± 0.004	0.94	
Maximum	1951.81 ± 362.49	84.31 ± 15.66	0.88 ± 0.16	0.039 ± 0.007	1.91	
Minimum	156.63 ± 78.44	6.77 ± 3.39	0.07 ± 0.04	0.003 ± 0.002	0.15	

Table 3: The measurement results of radon levels in soil samples fromagricultural studied area



Figure 6: The radon concentration in agricultural soil samples from different locations



Figure 7: The variation of radon surface and mass exhalation rates and annual effective dose in different samples

Discussion of SSNTD Measurements

All measured values of the radon concentrations are much lower than the recommended ICRP action level of 300 Bq m⁻³. The values of radon concentrations obtained from the study are found to be linearly dependent with exhalation rates. All measured annual effective dose values are below the limit of the recommended action level of 5 m Sv y⁻¹. According to these results one can say that, the soil in this area is advisable. Therefore, we can estimate that collected area was not found the pollution of radioactive radiation.

Determination of Elemental Concentration in Soil Samples

The quantitative results of the soil samples are given in Table 3. The comparison graphs of average elemental concentrations in 12 soil samples are given in Figure 8. The comparison graphs of iron, calcium, potassium and titanium concentrations in 12 soil samples are shown in Figure 9. In qualitative results, the major elements contained in soil samples are observed as silicon, iron, calcium, potassium and titanium. The silicon (Si) was found as major element and the iron (Fe) was second major element in all soil samples. The minor elements were found as zirconium (Zr), manganese (Mn), strontium (Sr), zinc (Zn), chromium (Cr), vanadium (V), yuttium (Y), copper (Cu) and rubidium (Rb) were found in all soil samples.

Commla	Elemental Concentration (W%)												
Sample	Si	Fe	Ca	K	Ti	Zr	Mn	Sr	Zn	Cr	Rb	V	Y
S ₁₁	43.89	29.79	11.98	9.86	2.67	0.57	0.51	0.28	0.13	0.07	0.07	0.11	0.07
S ₁₂	47.95	29.95	7.79	9.88	2.67	0.51	0.53	0.26	0.13	0.09	0.09	0.08	0.05
S ₁₃	48.58	28.73	8.36	9.76	2.65	0.67	0.54	0.26	0.13	0.11	0.06	0.11	0.07
S ₂₁	43.69	31.99	13.08	7.22	2.38	0.28	0.57	0.37	0.08	0.14	0.02	0.11	0.05
S ₂₂	43.75	34.07	10.46	7.46	2.53	0.35	0.61	0.44	0.10	0.07	0.01	0.07	0.05
S ₂₃	46.32	29.91	11.66	7.76	2.51	0.32	0.59	0.39	0.11	0.09	0.02	0.09	0.05
S ₃₁	45.52	35.46	5.37	9.30	2.80	0.30	0.66	0.20	0.17	0.11	0.44	ND	0.07
S ₃₂	42.24	38.32	5.39	8.87	2.74	0.29	0.69	0.21	0.18	0.11	0.03	ND	0.08
S ₃₃	46.49	33.75	6.29	9.15	2.68	0.37	0.61	0.25	0.16	ND	0.08	0.11	0.07
S ₄₁	46.15	35.15	5.50	8.81	2.70	0.25	0.61	0.19	0.18	0.09	0.06	0.10	0.06
S ₄₂	43.49	37.34	5.68	8.83	2.81	0.31	0.67	0.21	0.20	ND	0.09	0.13	0.07
S ₄₃	46.67	34.89	5.81	8.34	2.68	0.31	0.59	0.20	0.16	ND	0.63	0.13	0.06
Average	45.40	33.28	8.11	8.77	2.65	0.38	0.60	0.27	0.14	0.07	0.09	45.40	33.28

 Table 3: Quantitative Results of Agricultural Soil Samples for EDXRF

 Analysis

ND→ Not Detected



Figure 8: Comparison graph of average elemental concentrations in 12 soil samples



Figure 9: Comparison graphs of iron, calcium, potassium and titanium concentrations in 12 soil samples

Discussion of EDXRF Measurements

From the quantitative results, the occurrences of the large amount of heavy metal iron concentration were obtained in most soil samples. All of them, the largest amount of the iron concentration (38.32%) were obtained in the soil sample (s_{32}) from the 15cm depth of the study area. The collected soil sample between the different places and depths were obtained difference elemental concentration in EDXRF analysis. From the EDXRF analysis, the toxic elements in weight% level were not found.

Conclusion

The Can technique containing CR-39 plastic track detectors have been used for the measurement of radon concentrations, surface and mass radon exhalation rates, annual effective dose and for the measurement of elemental concentration in soil samples collected from various locations of selected agricultural area.

From the SSNTD's results presented in this study, the lowest values of all measurement results were found in the surface layer of soil sample from west of selected agricultural area in Photokephyu Village while the highest average values of all measurement results were found in the depth 30cm of soil sample from north of selected agricultural area in Photokephyu Village. All measurement results in soil samples are much lower than the recommended ICRP action level. This study shows that the value of radon level increases with the increase in depth. The result shows that this area is safe as for as the health hazards of radon are concerned. From the EDXRF analysis, the radioactive elements and other heavy elements were not determined within weight% level. There were not found toxic elements in weight% level. This studied area is advised to be used as agricultural areas.

Nowadays the environmental health problems tend to apply to an even greater extent to developing countries. Every effort should be made up to keep the concentrations of toxic elements, heavy elements and radioactive elements as low as possible in future for checking of the elemental pollution. The present study will be helpful to understand radiation level in the study area for further studies.

Acknowledgements

I would like to express great indebtedness to Rector Dr Kyaw Kyaw Khaung, Pro Rector Dr Nilar Kyi and Dr Nilar Aung, East Yangon University, for their encouragement to make present research paper. I wish to express my genuine thanks Professor Dr Khin Mya Mya Soe, Professor & Head, Department of Physics, East Yangon University, for her kind permission to carry out this research. I would like to express thankful to Professor Dr Thet Naing, Professor of Physics Department, East Yangon University, for his guidance with this research.

References

- Aamir Abdullah Mohammed., (2013), "Concentration Measurements of Radon, Uranium and Background of Gamma Rays in Air at the University of Baghdad – Al-Jadiriyah Site" University of Baghdad, Department of Physics.
- Abd-Elmoniem A.Elzain, (2016), "A Study of Radium Concentration and Radon Exhalation Rate in soil Samples from Kassala Town, Sudan Using SSNTDs," Department of Physics, University of Kassala ,Kassala , Sudan.
- Assad H. Ismail and Mohamad S. Jaafar, (2010), "Hazards Assessment of Radon Exhalation Rate and Radium Content in the Soil Samples in Iraqi Kurdistan Using Passive and Active Detecting Methods", International Journal of Environmental, Chemical, Ecological and Geophysical Engineering Vol:4, No-10.
- ICRP Publication 115, (2010), Lung Cancer Risk from Radon and Progeny and Statement on Radon.
- Lindgren E S, (1994), "X-ray Fluorescence Analysis: Energy Dispersive", Chalmers University of Technology and Goteborg University, Sweden.

STUDY ON STRUCTURAL AND MAGNETIC PROPERTIES OF YTTERBIUM DOPED ZINC FERRITE PREPARED BY SOLID STATE METHOD

Zar Zar Myint Aung¹, Aye Aye Thant²

Abstract

Rare earth, ytterbium doped Zinc ferrites: Zn $(Yb_xFe_{1-x})_2O_4$ with x=0.0000, 0.0125, 0.0250, 0.0375 and 0.0500 were prepared by the solid state method. Effect of Ytterbium doping on structural and magnetic properties of Zinc Ferrite is reported. The phase formation of the prepared samples was analyzed by X-ray diffraction. The appropriate variations in lattice parameters and cell volume confirmed the successful substitution of Fe³⁺ ions with Yb³⁺ ions at octahedral sites. The bulk density (D_b) and X-ray density (D_x) were also significantly varied by increased Yb³⁺ contents. XRD analysis reveal pure spinel phase in all the samples, without traces of secondary phases. The magnetic measurements were performed by using a soft magnetic Hysteresis Graphs Meter (DX-2012SD). It was found that saturation magnetic induction and coercivity followed decreasing trend with substation of Fe³⁺ ions by Yb³⁺ ions.

Keywords: XRD, structural, magnetic, ytterbium doped zinc ferrite

Introduction

Spinel ferrites have received special attention over the last years as important magnetic compounds of vital technological interest due to their useful applications. These materials are successfully used in different fields like in high frequency devices, microwave devices, catalysis, photocatalysis and magnetically guided drug delivery. The general formula for spinnel ferrites is AB_2O_4 , where A is divalent metal ion (eg. cobalt, nickel and zinc) B is usually iron usually substituted sometimes with other trivalence metals ions Rare earths.

The properties of these compounds are relied to the distribution of cations between tetrahedral (A) and octahedral (B) sites. Therefore, the structural and magnetic properties can be influenced by the synthesis methods, chemical-composition, particle size or doping and can be fine-tuned by changing the amount of doping Rare Earth elements.

¹ Dr, Demonstrator, Physics Department, Lashio University

^{2.} Dr, Professor, Physics Department, University of Yangon
Material and Method

Experimental procedure

Rare earth doped Zinc ferrites were prepared $Zn(Yb_xFe_{1-x})_2O_4$ with x=0.0000, 0.0125, 0.0250, 0.0375 and 0.0500 by the solid state method.. The raw materials such as ytterbium oxide, zinc oxide and ferrite oxide were used as the source materials. The required amount of the ZnO, Yb₂O₃ and Fe₂O₃were weighed with digital balance. The raw materials of ZnO, Yb₂O₃ and Fe₂O₃were taken in stoichiometric proportions.

These oxide materials were mixed with standard weight percentages according to their stoichiometric calculation by using the following equation.

$$ZnO + (x)Yb_2O_3 + (1-x)Fe_2O_3 \rightarrow Zn(YbFe)_2O_4 + 3O_2$$

All compositions have been mixed in an Agate mortar and ground for 5 hours. After mixing and grinding, the mixture has been pre sintered at 900°C for 5 hours in a furnace with heating rate of 20°C/min and cooled to room temperature with the same rate. After that, the powder and the mixture has been ground with an Agate motor for 1hour. Then, the powder has been pressed into pellets and toriods by uniaxial hydraulic press at a pressure of 5tons.

The sintering temperature should start from 1000 °C which is 100 °C higher than the pre-sintering temperature. This condition is required for densification of Ferrite in standard solid state methods. Therefore, the sintering temperature was chosen as 1000 °C with time duration for 5 hours to densify $ZnFe_2O_4$ and Yb doped $ZnFe_2O_4$ magnetic ferrite by standard solid state method.

The ytterbium doped zinc ferrite samples were characterized by using X-ray Diffraction. The magnetic characterization was carried out using a soft magnetic Hysteresis Graphs Meter (DX-2012SD).

Results and Discussion

Structural Analysis

The XRD spectrum of the sample final sintered at 1000 °C as shown in Figure 1. As seen in XRD spectra cubic spinel structure of zinc ferrite was found to be stable at final sintering temperature. The lattice constant and crystallite size of $Zn(Yb_xFe_{1-x})_2O_4$ calculated data are shown in Table 1. The lattice parameter obtained for pure zinc ferrite is in good agreement with the reported value.

The diffraction peaks corresponding to $(2\ 2\ 0)$, $(3\ 1\ 1)$, $(4\ 0\ 0)$, $(4\ 2\ 2)$, $(5\ 1\ 1)$ and $(4\ 4\ 0)$ reflection planes and the absence of any extra peak show that all the samples have attained single phase cubic structure. This implies that the Yb³⁺ ions have been completely dissolved into the spinel lattice of zinc ferrite.

In order to fulfill the structural properties, the theoretical (X-ray) density was calculated using equation, $D_x = \frac{8 M}{Na^3}$ where, $D_x = X$ -ray density, M= the molecular weight (gm) of the sample, N= Avogadro's number (per mol), and a= the lattice parameter in angstrom and bulk density by equation $D_b = \frac{m}{\pi r^2 h}$ Where, m = the mass of pellet, r = the radius of the pellets, h = the thickness of the pellets and D_b = the bulk density.

Table 2 shows the bulk density and apparent porosity of sintered temperature along with Yb compositions. The bulk density and X-ray density increased with increasing Yb content which indicated improvement in grain growth upon Yb substitution. The bulk density is found to be 62.92 % of X-ray density for the final sintering temperature of in average. Moreover, the bulk density increased with increasing Yb concentration, indicating improved densification by the substitution of Yb for Zn(Yb_xFe_{1-x})₂O₄in the ferrite. This indicated that the rate of densification decreased with the decreasing Yb content. Moreover, the Yb played an important role during sintering of the ferrites. The porosity for all the compositions was calculated by equations $P = 1 - \frac{D_b}{D_x}$ where, P = porosity, D_b = bulk density and D_{x =} X-ray density.

The smaller values of " D_b " than those of " D_x " confirmed the presence of pore in all the compositions. The formation of pores was decreased with the increase in Yb concentration. Therefore, it agrees well with the variation of density with Yb concentration. According to literature, the increased densification in this case was due to the presence of excess Zn in the system. The excess Zn arose due to the Yb substitution for Fe in the ferrite.



Figure 1: XRD patterns of Zn(Yb_xFe_{1-x})₂O₄ pellets sintered at 1000 °C

Table 1:Lattice constant and	crystallite size of 2	Zn(Yb _x Fe _{1-x}) ₂ O ₄ sintered at
1000 °C		

Sample of	Lattice Constant	Crystallite size
composition "x"	(Å)	(nm)
0.0000	8.47	44.29
0.0125	8.47	41.09
0.0250	8.47	37.80
0.0375	8.55	36.78
0.0500	8.55	31.68

No	Samples of composition "x"	Mol.wt. (g/mol)	X-ray density (g/cm ³)	Bulk density (g/cm ³)	Porosity
1	0.0000	241.07	5.27	3.62	0.31
2	0.0125	244.00	5.36	3.74	0.30
3	0.0250	246.93	5.41	3.75	0.29
4	0.0375	249.86	5.42	4.03	0.26
5	0.0500	252.79	5.48	4.16	0.24

Table 2: Values of X-ray density, bulk density and porosity of $Zn(Yb_xFe_{1-x})_2O_4$ sintered at 1000 $^\circ C$





The lattice constant of ytterbium-substituted zinc ferrite is observed to be larger than that of zinc ferrite. An increase in lattice constant with increase in Yb³⁺ ion content is expected because of the large ionic radius of Yb³⁺ (0.858 Å) compare to that of Fe³⁺(0.67 Å).

The ytterbium substitution zinc ferrite changes in the lattice constant and this may probably be the reason for the observed shift of XRD peaks with ytterbium substitution. The theoretical (X-ray) density of zinc ferrite is in agreement with that of the zinc ferrite because it increases with increase in ytterbium concentration.

Magnetic Properties of Zn(Yb_xFe_{1-x})₂O₄

The magnetic properties of $Zn(Yb_xFe_{1-x})_2O_4$ were measured by using Soft Magnet DC Meter (DX-2012SD) under the static (DC) state. Table 3 shows the initial permeability (μ_i), maximum permeability (μ_m), saturation magnetic induction (B_s) and remanence (B_r) of sintered ferrites along with their coercive force which were measured at room temperature.

Moreover, it was observed that H_c increased by increasing doping contents of Yb³⁺ ions. It might be due to the effect of denser microstructure with Yb³⁺ ions substitution in spinel lattice. It is interesting to note that the corecivity significantly increased at x = 0.0250 of Yb substitution compared to that of undoped ones. It has also been reported that if the squareness ratio is greater than 0.5 (B_r / B_s \geq 0.5), then the compounds are in single magnetic domain and if this ratio is less than 0.5 (B_r / B_s \leq 0.5), then the compounds are in multi-magnetic domains. In this work, it was observed that the squareness ratios for all samples are greater than 0.5 and therefore it confirmed the formation of single domain structure in ZnYbFe₂O₄ ferrites. Therefore, in these ZnYbFe₂O₄ ferrites, decrease in B_s and increase in H_c with respect to doping contents made them electromagnets.

Composition "x"	μ _i mH/m	μ _m mH/m	B _r (T)	B _s (T)	B _r /B _s	H _c (A/m)
0.0000	0.055	2.273	0.053	0.062	0.854	3.43
0.0125	0.040	1.682	0.037	0.044	0.840	3.48
0.0250	0.018	1.266	0.029	0.034	0.852	3.50
0.0375	0.018	1.266	0.029	0.034	0.852	3.50
0.0500	0.018	1.266	0.048	0.034	1.410	3.50

Table 3: Magnetic data for Zn(Yb_xFe_{1-x})O₄ sintered at 1000 °C



Figure 3: The variation of saturation magnetic induction of $Zn (Yb_xFe_{1-x})_2O_4$ with different Yb concentration (x)

Conclusion

In this experiment of ytterbium doped on the zinc ferrite $Zn(Yb_xFe_{1-x})_2$ O₄with x=0.0000, 0.0125, 0.0250, 0.0375 and 0.0500 were synthesized by using solid state method. XRD analysis confirmed the formation of single phase structure, without any secondary phase in all the compositions. The substitution of ytterbium in zinc ferrite has resulted in an increase in lattice constant. Moreover, it was observed that coercivity H_c increased by increasing doping contents of Yb³⁺ ions. It might be due to the effect of denser microstructure with Yb³⁺ ions substitution in spinel lattice. This is proved that the substitution of small amount of ytterbium rare earth (RE) ions in ferrite can also tune the magnetic properties.

The result obtained in this work suggested that $Zn(Yb_xFe_{1-x})_2O_4$ crystalline ferrites are suitable materials for microwave devices applications

Acknowledgement

This research was totally done at Department of Physics in University of Yangon, Myanmar (2017-2018).

References

- Anu Rana., Thakur, O. P. &Vinod Kumar., (2011). Effect of Gd³⁺substitution on dielectric properties if nano cobalt ferrite, *Material letters*, Vol.65, pp. 3191-3192.
- Busca, G., Finocchio, E., Lorenzelli, V., Trombetta, M. & Rossini, S. A. (1996). IR study of alkene allylic activation on magnesium ferrite and alumina catalysts, *Journal of Chem. Soc*, Vol.92, pp. 4687-4693.
- Ge-Liang Sun, Jian-Bao Li, Jing-Jing Sun & Xiao-Zhan Yang, (2004). The influences of Zn²⁺ and some rare-earth ions on the magnetic properties of nickel–zinc ferrites, *Journal of Magnetism and Magnetic Materials* 281: 2–3, pp.173-177.

Goldman, A., (1990). Modern Ferrite Technology. Van Nostrand, New York.

- Jang, Hong S.J. and Lee J.S., (January, 2009). Synthesis of Zinc Ferrite and its Photocatalytic Application under Visible Light, *Journal of the Korean Physical Society*, Vol.54, No.1, pp.204-208.
- Jitendra Pal Singh, Hemanut Kumar, Ayush Singhal, Neelmanee Sarin, Srivastava, R.C., and Keun Hwa Chae, (2016). Solubility limit, magnetic interaction and conduction mechanism in rare earth doped spinel ferrite, *An interdisplinary peer-reviewed international Journal*, <u>www.appslett.com</u> DOI:10.17571/ appslett.2016.02001.
- Kadam, G.B., Shelke, S.B. and Jadhav K.M., (2010). Structural and electrical properties of Sm³⁺ DOPED Co- Zn Ferrite, *Journal of Electronic and Electrical Engineering*, ISSN: 0976–8106 & E-ISSN: 0976–8114, Vol. 1, Issue 1, 2010, PP-15-25
- Khan, M. A., Islam, M. U., Ishaque, M., Rahman, I. Z., Genson, A. & Hampshire, S., (2009). Structural and physical properties of Ni–Tb–Fe–O system, *Material Characterization* Vol.60 (1), pp.73-78.
- LiviuSacarescu, Daniel Timpu, Nicoleta Lupu and Valeria Harabagiu, (March, 2015). Magnetic properties of nanosized Gd doped Ni-Mn-Cr ferrites prepared using the sol-gel autocombustion technique, *j.jmmm.(Journal of Magnetism and Magnetic Materials)* 378, pp92-97.
- Lijun Zhao, Hua Yang, Xueping Zhao, Lianxiang Yu, Yuming Cui &Shouhua Feng., (2006). Magnetic properties of CoFe2O4 ferrite doped with rare earth ion, *Materials Letters*, Vol.60: pp1-60

STRUCTURE AND MAGNETIC PROPERTIES OF NANOCRYSTALLINE NiZnFe₂O₄ PREPARED VIA CONVENTIONAL CERAMIC METHOD

Myat Shwe Wah¹, Min Maung Maung², Naing Win³ and Than Htun⁴

Abstract

Nanocrystalline Nickel-Zinc ferrite was synthesized by conventional ceramic method. The metal oxide of Ni, Zn and Fe were used as precursors for NiZnFe₂O₄. The structural characterizations were made for the samples with a chemical formula Ni_x Zn_{1-x} Fe₂O₄ (x = 0.1, 0.3, 0.5 and 0.7mol). The obtained nanocrystalline Ni-Zn ferrite was analysed and discussed through structural, morphological and magnetic characterization. Formation of pure NiZnFe₂O₄ phase was confirmed by X-ray diffraction analysis (XRD). The determined material's nanocrystalline structure was additionally supported by scanning electron microscopy (SEM). The magnetic hysteresis loop was recorded by means of a Magnet-Physik(EP-3).

Keywords: nanocrystalline, nickel-zinc ferrite (NiZnFe₂O₄),conventional ceramic method, XRD,SEM.

Introduction

Among the different mixed ferrites, Ni-Zn ferrites have a good utility as a conducted noise suppressor material in various electromagnetic interfaces compared to other ferrites. Because of their high resistivity, relatively high permeability and low eddy current loss. These soft magnetic materials, crystallizes in the spinel structure of the type $(Zn_{1-x}Fe_x)$ (Ni_xFe_{2-x}) O₄, where the metallic cations Fe₃₊/Zn₂₊ occupy the tetrahedral A sites, and the metallic cations Fe₃₊/Ni₂₊ occupy the octahedral B sites. It is known that magnetic properties of ferrites are sensitive to preparation technique and their microstructures.

The electrical and magnetic properties of such ferrites depend strongly on distribution of cations at the tetrahedral (A) and octahedral (B) sites in the lattice. It is well known that zinc ions can be used to alter the saturation

^{1.} Dr, Lecturer, Department of Physics, Mawlamyine University, Myanmar

² Associate Professor, Department of Physics, University of Dawai, Myanmar

³ Lieutenant Colonel, Department of Physics, Defence Services Academy

⁴ Professor and Head, Department of Physics, Mawlamyine University, Myanmar

magnetization. It is believed that the addition of zinc ions also affects the lattice parameter and it would therefore be expected to change the Curie temperature of the material. The substitution of divalent ions in pure ferrites leads to the modification of the structural, electrical and magnetic properties. There are the synthesis of Ni-Zn ferrites using different techniques like, refluxing process , ceramic , hydrothermal , combustion, co-precipitation, reverse micelle process, spark plasma sintering, micro emulsion and ball milling, etc.

Among these methods, the conventional solid-state reaction route is widely used for the production of ferrite because of its low cost and suitability for large scale production. In this work, the systematic doping of Ni content on the magnetic properties of Ni-Zn ferrite was synthesized by solid state double sintering method.

Experimental

Nickel-Zinc ferrites were prepared by solid state sintering method. The starting materials were nickel oxide(NiO), and, zinc oxide (ZnO) and ferrite oxide(Fe₂O₃) all of analytical grade. The structural characterizations were made for the samples with a chemical formula $Ni_x Zn_{1-x} Fe_2O_4$ (x = 0.1, 0.3, 0.5 and 0.7) mol. The metal oxides will be mixed and grind in A-gate mortar. The mixture will be pre-sintered at 800°C in the furnace. Afterwards the powder was pressed into pellets of thickness 3 mm and a diameter of 10 mm with press by applying a pressure of 2 $tons/in^2$. The pellet will be sintered at 1000°C in the furnace for one hour to obtain spinel phase. The final sintering was done at 1000°C. The structural characterizations of all samples were carried out by X-ray diffraction (XRD) and conforms the well defined single phase spinel structure. XRD data were taken at room temperature using $CuK\alpha$ radiation. Morphological, elemental composition characterizations of all prepared samples were performed by high resolution scanning electron microscopy. The Magnetic measurements were carried out by using Magnet-Physik (EP-3).



Figure 1: Flow chart for coventional synthesis of NiZnFe₂O₄ fine powder

Results and Discussion

XRD Analysis

The measured results of metal ions are consistent well with the stoichiometric values of samples, indicating that the compositions of asobtained samples are in agreement with those of anticipated stoichiometry. The X-ray diffraction patters of the samples are shown in Figure 2. The XRD pattern of metal ions presents a broad diffraction peak located at 22.04°. In Figure2, The main diffraction peaks appeared at $2\theta = 18.28^{\circ}$, 30.17° , 35.52° , 43.17° , 53.53° , 57.06° and 62.76° correspond to (111), (220), (311), (400), (422),(511) and (440) crystal planes of the spinel structure with the characteristic reflections of the Fd3m cubic group (JCPDS CARD 01-1108).All the Nickle substituted zinc ferrites of the various compositions show the crystalline cubic spinel structure. The sharp peaks represents that all ferrites are crystalline nature of single phase.



Figure 2: XRD spectrums of powder (NiZnFe₂O₄)

According to the Scherrer equation:

$$D = \frac{k\lambda}{\beta \cos\theta} \tag{1}$$

where D is the particle size (nm), b is the full width at half maximum diffraction peak, is the diffraction angle and k(0.15418 nm) is the wavelength of X-ray.

The average crystallite sizes of the NiZnFe₂O₄(NZF) nanoparticles estimated from the equation (1) were showed in Table 1. The average size of NZF nanoparticle decreases with the increase of x. The lattice parameter of individual composition was calculated by using the formula:

$$a = d[h^2 + k^2 + l^2]^2 \tag{2}$$

where, a = lattice constant; d = inter planar distance; and (h, k, l) are the Miller indices.

The calculated lattice constant "a" is seen to increase from 8.47Å to 8.38 Å with decrease in nickle content as reported in Table 1. The lattice parameter is found vary linearly with decreasing nickle concentration, there by indicating that the Ni-Zn ferrite system obeys Vegard's law . A similar behavior of lattice constant with dopant concentration was observed by

several investigators in various ferrite systems. The variation in lattice constant with nickle content can be explained on the basis of the ionic radii of Ni²⁺ (0.78 Å) ions is lower than that of Zn²⁺ (0.82 Å).

Sample	Crystallite size (nm)	Lattice parameter (A [°])
$Ni_{0.1} Zn_{0.9} Fe_2O_4$	37.8	8.4702
$Ni_{0.3}Zn_{0.7}Fe_2O_4$	33.9	8.4490
$Ni_{0.5}Zn_{0.5}Fe_{2}O_{4}$	32	8.4160
$Ni_{0.7}Zn_{0.3}Fe_{2}O_{4}$	29	8.3860

Table 1: The variation of lattice parameter for intense reflection peaks $NiZnFe_2O_4$

Figure 2 showed the XRD spectrums of the powder heat treated at 1000°C using high temperature solid state sintering method. Theamount of crystalized size decreased with variable of molecular ratios. X-ray density (dx) was determined using the following relation

$$D_x = \frac{ZM}{Na^3}$$

where Z is the number of molecules per unit cell (Z = 8), "M" is the molecular weight and "N" is the Avogadro's number. The values of the bulk density, X-ray density and the percentage of porosity for Ni-Zn ferrites are given in Table 2.

Table 2: Bulk density-ray density and porosity data for mixed Ni-Zn ferrites

Sr. No.	Ferrite composition	Bulk density Gm/cm ³	X-ray density Gm/cm ³	Porosity
2	X = 0.1	4.52	6.55	30.99
3	X = 0.3	4.89	6.60	25.90
4	X = 0.5	5.27	6.67	20.98
5	X = 0.7	5.65	6.75	16.29



Figure 3: Variation of bulk density and X-ray density with composition

It can be seen from the table that the bulk density increases and the porosity decreases progressively with addition of nickel to zinc ferrite. Zinc ferrite having the least porosity, this conforms the observation that the addition of nickel to zinc ferrite results the densification of the material. The variation of bulk density with nickel content for mixed Ni-Zn ferrite is shown in the Figure 3. It may be seen from the figure that bulk density increases linearly with the increase of nickel content.

Scanning Electron Microscopy (SEM)

The scanning electron microscope (SEM) images of all prepared samples are given in Figure 3(a, b, c & d). The morphology and the size distribution of the NiZnFe₂O₄ nanoparticles were determined using SEM. Typical SEM images of NiZnFe₂O₄ synthesized particles are shown in Figure 4. SEM micrograph depicts that the samples contain micrometrical aggregation of tiny particles. The existence of high dense agglomeration indicates that pore free crystallites are present on the surface. The SEM images show the agglomerated form of NiZnFe₂O₄ nanoparticles. As the nanoparticles possess high surface energies, they tend to agglomerate and grow into larger assemblies.



Figure 4: SEM images of Ni-Zn ferrite (x=0.1,0.3,0.5 and 0.7)

Magnetic Properties

Figure 5 shows the magnetic hysteresis loop of four NZF samples in applied magnetic field in the room temperatureby using Magnet-Physik (EP-3). The corresponding magnetic parameters such as the remanence (Br), intrinsic coercivity (H_{CJ}), normal coercivity (H_{CB}) and maximum energy product (BH)_{max} of ferrites were described in table 3. The Hc is the physical quantity used to measure the magnetic field intensity. In general, the Hc is influenced by many factors, including the anisotropic constant, the saturation magnetization, the comprehensive factors such as grain size, lattice stress and the defects of crystal surface and internal.



Figure 5: B-H graph of NiZnFe₂O₄ (a) x = 0.1, (b) 0.3, (c) 0.5 (d) 0.7 mol (e) comparison of all compositions

Samplas	Remanence Normal coericivity		Relative	
Samples	$(\mathbf{B_r})(\mathbf{T})$	(\mathbf{H}_{CB}) $(\mathbf{k}\mathbf{A}/\mathbf{m})$	permeability(µ _r)	
Ni _{0.1} Zn _{0.9} Fe ₂ O ₄	0.00137	1.29	8.45E-01	
Ni _{0.3} Zn _{0.7} Fe ₂ O ₄	0.00160	1.10	1.16E+00	
Ni _{0.5} Zn _{0.5} Fe ₂ O ₄	0.0104	5.54	1.49E+00	
Ni _{0.7} Zn _{0.3} Fe ₂ O ₄	0.0173	8.07	1.71E+00	

Table 3: The characteristic quantities magnetic field in ferrite samples.

The magnetic properties of ferrite materials showed that the values of the relative permeablility greater than one as a paramagnet type. Only one ratio showed that less than one as a diamagnetic type in $Ni_{0.1} Zn_{0.9} Fe_2O_4$. It will be focusing on optimizing the material properties and implementing the material in various electronics and magnetic application.

Conclusion

The mixed Ni-Zn ferrite samples are prepared and observed the following conclusions. The fact that the NiFe₂O₄ nanoparticles belonged to the cubic spinal structure was established by XRD. That the nanoparticles agglomerated to form spherical-shaped particles was also confirmed and made clear by the SEM analysis. The lattice parameter decrease with increase of nickel content, the bulk density increases linearly with nickle content, SEM pictures shows that the morphology of the particles is very similar. The values of bulk density, x-ray density increase gradually reaches the maximum value as Ni²⁺composition is increased.

Acknowledgements

I would like to express appreciation to Rector Dr Aung Myat Kyaw Sein, Pro-rector, Dr Mie Mie Sein and Pro-rector Dr San San Aye, Mawlamyine University for their encouragement and kind permission to undertake the present research. I also would like to thank to Professor

Dr Than Htun, Head of Department of Physics, Mawlamyine University for his encouragement and kind permission to carry out this research. I am deeply indebted to Professor Dr Yin Yin Myint, Department of Physics, Mawlamyine University for her kind permission to carry out this research work.

References

- C. J. Brinker and G. W. Scherer, (1990), "Sol-Gel Science", Academic Press, San Diego,.
- P. K. Roy and J.Bera, (2009), "Electromagnetic properties of samarium-substituted NiCuZn ferrite prepared by auto-combustion method", J. Magn. Magn. Mater., , Vol.321, pp. 247-251.

William E. Lee and W. Mark Rainforth, "Ceramic Microstructure", (CHAPMAN & HALL)

- Y. Ichiyanagi, M. Kubota, S. Moritake, Y. Kanazawa, T. Yamada, T. Uehashi, (2007), "Magnetic Properties of Mg-ferrite nanoparticles", J. Magn. Magn. Mater., Vol.310, pp 2378-2380.
- Z. Yue, W. Guo, J. Zhou, Z. Jui and L. Li, (2003), "Synthesis of nanocrystalline ferrites by sol-gel combustion Process: the influence of pH value of solution", J. Magn. Magn. Mater., Vol.270, pp. 216-223.

THEORETICAL INVESTIGATION ON Λ (1405) RESONANCE WITHIN $\overline{K}N$ FRAME WORK OF $\overline{K}N - \Sigma^+\pi^-$ COUPLED CHANNEL

Mar Mar Htay*

Abstract

We calculated various range parameters and different strength parameters of Λ (1405) with resonance state for $\Sigma^+\pi^- \rightarrow \Sigma^+\pi^-$. Firstly we solved Schrodinger equation by using separable potential for $\Sigma^+\pi^- \rightarrow \Sigma^+\pi^$ channel to obtain various differential cross sections with energies for various strength parameters and different range parameters. It is reduced the resonance state of $\Sigma^+\pi^-$. Secondly, we investigated the various strength and range parameters of seperable potential for Λ (1405) resonance within $\overline{K}N$ frame work of $\overline{K}N \rightarrow \Sigma^+\pi^-$ coupled channel. It is observed that the parameter sets of $\overline{K}N$ interaction can be constructed for $\Sigma^+\pi^-$ resonance and $\overline{K}p$ bound state. Therefore, we constructed the new model **A** and **B** for $\overline{K}N$ interaction.

Keyword: Resonance state, coupled channel and $\overline{K}N$ interaction.

Introduction

1.1 Reviews of Theoretical Investigation and Experimental Observation

The resonant state of Λ (1405) with J = 1/2, I = 0, S = -1, called Λ (1405), is located below the $\overline{K}N$ threshold, and decays to $\Sigma \pi$. The chiral dynamics theories suggested two poles in the coupled $\overline{K}N - \Sigma \pi$ scheme and they determined Λ (1405) with level width 120 MeV, to which counter arguments were given. More recently, J. Esmaili et al. analyzed old bubble-chamber data of stopped- K⁻ on ⁴He with a resonant capture process, and found the best-fit value to be $M = 1405.5^{+1.4}_{-1.0}$ MeV/c². Hassanvand et al. analyzed recent data of HADES on, $p+p \rightarrow p+K^+ + \Lambda(1405)$, and subsequently deduced $M = 1405^{+11}_{-9}$ MeV/c² and $\Gamma = 62 \pm 10$ MeV. Now, the new PDG values have been revised to be $M = 1405.1^{+1.3}_{-1.0}$ MeV/c² and $\Gamma = 50.5 \pm 2.0$ MeV, upon adopting the consequences of these analyses.

^{*} Dr, Lecturer, Department of Physics, Monywa University

Therefore, we investigated a model $\overline{K}N$ quasi-bound state by changing the strength and range of the $\overline{K}N$ interaction. The purpose of this work is to perform theoretical investigation on a Λ (1405) within $\overline{K}N$ frame work of $\overline{K}N - \Sigma^+\pi^-$ coupled channel.

Resonance State in Single Channel

2.1 Calculation of Resonance State for Single Channel

The Λ (1405) resonance is an I=0 quasi-bound state of $\overline{K}N$, which is embedded in continuum of $\Sigma \pi$ as a kind of Feshbach resonances. A model for low-energy meson-baryon interaction in the strange sector is presented. The interaction is described in terms of separable potentials with multiple partial waves considered.

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\mathbf{r}) + v(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$
(1)

Separable potential is $v(\mathbf{r},\mathbf{r}') = g(\mathbf{r})Y_{00}\frac{\overline{V}_0}{b^3}g(\mathbf{r}')Y_{00}$ (2)

The time independent Schrodinger equation can be written as

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\mathbf{r}) + \frac{\overline{v}_0}{b^3}g(\mathbf{r})Y_{00}\int g(\mathbf{r}')Y_{00}\psi(\mathbf{r}')d\mathbf{r}' = \frac{\hbar^2}{2\mu}k^2\psi(\mathbf{r})$$
(3)

$$-\frac{d^{2}}{dr^{2}}u(r) + G_{0}rg(r)\int_{0}^{\alpha}g(r')u(r')r'dr' = k^{2}u(r)$$
(4)

Where,
$$G_0 = \frac{2\mu}{\hbar^2} \overline{v}_0 \frac{1}{b^3}$$
 (5)

Where,
$$G \equiv G_0 \int_0^\alpha g(r') u(r') r' dr'$$
 (6)

We employ Yukawa type form factor as $g(r) = \frac{b}{r}e^{-\frac{r}{b}}$ (7)

The inhomogeneous equation is
$$-\frac{d^2}{dr^2}u_0(r)+G.rg(r)=k^2u_0(r)$$
 (8)

The solution of inhomogeneous equation is $u_0(r) = Ae^{-\frac{r}{b}}$ The solution of homogeneous equation is $u_1(r) = a \sin(kr + \delta)$

From equation (8), we get the equation as

$$\frac{G}{G_0} = -\frac{1}{2}b^2 a \sin \delta + a \frac{kb}{1+k^2b^2}b^2 \cos \delta + a \frac{1}{1+k^2b^2}b^2 \sin \delta \qquad (9)$$

By solving equation (10)

$$\sigma_{tot} = \frac{4\pi}{k^2} \frac{k^2 b^2}{k^2 b^2 + \frac{1}{4} \left\{ 1 - k^2 b^2 + \frac{1}{S} (1 + k^2 b^2)^2 \right\}^2}$$
(10)

Where, $S = \frac{1}{2}G_0 b^5 = \frac{1}{2}\frac{2\mu}{\hbar^2}\overline{v}_0 b^2$, $S = \text{strength parameter } B_0 = \frac{\hbar^2}{2\mu}\frac{1}{b^2}$,

 B_0 = dynamic pole parameter, b = potential range parameter.

We solved numerically equation (10) by using FORTRAN CODE to obtain resonance state. The results are shown in next section.

2.2 Bound and Resonance Pole

The single channel Schoredinger eqation is

$$-\frac{d^2}{dr^2}u_0(r) + G.rg(r) = k^2u_0(r), \qquad (11)$$

The solution of equation is as equation (11).

$$A = \frac{Gb^{3}}{1 + k^{2}b^{2}} = \frac{Gb^{3}}{(1 + ikb)(1 - ikb)}$$
(12)

$$\mathbf{E}_{\mathbf{B}} = -\mathbf{B}_{0} \left\{ \sqrt{|\mathbf{S}|} \pm 1 \right\}$$
(13)

We can find bound state from equation (13).

For resonance state

$$E_{\text{Res}} = E_{\text{R}} - i\frac{\Gamma}{2} \tag{14}$$

$$E_{R} = B_{0}(S-1) \tag{15}$$

$$\frac{\Gamma}{2} = \pm 2B_0 \sqrt{S} \tag{16}$$

We calculated resonance states and level widths of $\Sigma^+\pi^-$ for various dynamical poles and strength parameters by using equation (15) and (16).

Resonance and Bound State in Coupled Channel

We consider two channels of $\overline{K}N$ (K⁻p) and $\pi\Sigma$ ($\pi^{-}\Sigma^{+}$) for simplicity. We employ a set of separable potentials with a Yukawa-type form factor, $\overline{K}N$ channel, 1, or the $\pi\Sigma$ channel, 2, μ_{I} and μ_{II} are the reduced mass of the channel 1 and 2.

$$-\frac{d^{2}}{dr^{2}}u_{I}(r) + (G_{I} + G_{III})r g(r) = k^{2}u_{I}(r),$$

$$-\frac{d^{2}}{dr^{2}}u_{II}(r) + (G_{II} + G_{III})r g(r) = (k^{2} - \Delta^{2})u_{II}(r)$$
Where, $g(r) = \frac{b}{r}e^{-\frac{r}{b}}, \quad \Delta^{2} = \frac{2\mu_{II}}{\hbar^{2}}(M_{p} + m_{k} - M_{\Sigma^{+}} - m_{\pi^{-}}) = 1.711 \text{fm}^{-2}$

$$k' = \sqrt{\frac{\mu_{II}}{\mu_{I}}}k = 1.609k$$
(17)

The coupled-channel equation for the radial wave functions, $u_1(r)$ and $u_2(r)$, of the present interaction model is written as follows:

$$\begin{cases} u_{I}(r) = \frac{(G_{I} + G_{II})b^{3}}{1 + k^{2}b^{2}}(e^{-\frac{r}{b}} - e^{ikr}) \\ u_{II}(r) = \frac{(G_{II} + G_{III})b^{3}}{1 - (k^{2} - \Delta^{2})b^{2}}(e^{-\frac{r}{b}} - e^{-\sqrt{\Delta^{2} - K^{2}r}}) \end{cases}$$
(18)

$$\begin{cases} G_{I} = -S_{I} \frac{G_{I} + G_{II}}{1 + k^{2}b^{2}} \frac{1 + ikb}{1 - ikb} \\ G_{III} = -S_{III} \frac{G_{II} + G_{III}}{1 - (\Delta^{2} - k^{2})b^{2}} \frac{1 - \sqrt{\Delta^{2} - k^{2}b}}{1 + \sqrt{\Delta^{2} - k^{2}b}} \\ G_{II} = -S_{III} \frac{G_{II} + G_{III}}{1 - (\Delta^{2} - k^{2})b^{2}} \frac{1 - \sqrt{\Delta^{2} - k^{2}b}}{1 + \sqrt{\Delta^{2} - k^{2}b}} \\ G_{III} = -S_{III} \frac{G_{I} + G_{III}}{1 + k^{2}b^{2}} \frac{1 + ikb}{1 - ikb} \\ \end{cases}$$

$$\begin{cases} S_{II} = \frac{1}{2} \frac{2\mu_{II}}{\hbar^{2}} \overline{V}_{0}^{I} b^{2} \\ S_{III} = \frac{1}{2} \frac{2\mu_{II}}{\hbar^{2}} \overline{V}_{0}^{I} b^{2} \\ S_{III} = \frac{1}{2} \frac{2\mu_{II}}{\hbar^{2}} \overline{V}_{0}^{I} b^{2} \\ S_{III} = \frac{1}{2} \frac{2\mu_{II}}{\hbar^{2}} \overline{V}_{0}^{I} b^{2} \\ \end{cases}$$

$$\begin{cases} (20) \\ S_{III} = \frac{1}{2} \frac{2\mu_{II}}{\hbar^{2}} \overline{V}_{0}^{I} b^{2} \\ S_{III} = \frac{1}{2} \frac{2\mu_{II}}{\hbar^{2}} \overline{V}_{0}^{I} b^{2} \\ S_{III} = \frac{1}{2} \frac{2\mu_{II}}{\hbar^{2}} \overline{V}_{0}^{I} b^{2} \\ \end{cases}$$

$$\begin{cases} (1 + \frac{S_{I}}{(1 - ikb)^{2}} \right\} \left\{ 1 + \frac{S_{III}}{(1 + \sqrt{\Delta^{2} - k^{2}b)^{2}} + S_{II} \right\} = \frac{S_{III}S_{III}}{(1 + \sqrt{\Delta^{2} k^{2}b})^{2}(1 - ikb)^{2}} \end{cases}$$

$$\end{cases}$$

For uncoupled case,

$$\left\{ (1 - ikb)^2 + S_I \right\} \left\{ (1 + \sqrt{\Delta^2 - k^2}b)^2 + S_{II} \right\} = 0$$
(22)

Resonance state for $S_I > 0$

$$E_{R} = \frac{\hbar^{2}}{2\mu_{I}}k^{2} = B_{0}^{(I)}(S_{I} - 1) - iB_{0}^{(I)}2\sqrt{S_{I}}$$
(23)

Bound state for $S_{II}\,{<}\,0$

$$E_{\rm B} = \frac{\hbar^2}{2\mu_{\rm II}} k^2 = \frac{\hbar^2}{2\mu_{\rm II}} \Delta^2 - B_0^{(\rm II)} (\sqrt{|S_{\rm II}|} - 1)^2$$
(24)

3.1 Numerical model A

We assumed that the range parameter of Yukawa type separable potential is to be $b = \frac{\hbar C}{M_B C^2} = 0.25 \text{fm}$, $M_B = 789 \text{MeV}/\text{C}^2 \sim \rho \text{meson mass}$ (25)

$$\begin{cases} B_0^{(I)} = \frac{\hbar^2}{2\mu_I} \frac{1}{b^2} = 2494 \text{Me}\overline{\text{V}} \\ B_0^{(I)} = \frac{\hbar^2}{2\mu_I} \frac{1}{b^2} = 963.2 \text{Me}\overline{\text{V}} \end{cases}$$
(26)

Bound state in channel II

$$BE_{II} = B_0^{(II)} (\sqrt{|S_{II}|} - 1)^2 = 27 \,\text{MeV} \sim \Delta(1405)$$
(27)

$$S_{II} = -1.363$$

$$E_{\rm B} = \frac{\hbar^2}{2\mu_{\rm II}} k^2 = (103 - 27) - 120 {\rm Me}\overline{\rm V}$$
(28)

$$k = 0.7042 - i0.09111 \text{ fm}^{-1}$$
⁽²⁹⁾

$$S_{I}S_{II} + 1.383S_{I} + 0.9239 S_{II} + 1.325 = C^{2}$$
(30)

If
$$S_I=0$$
, $S_{II} = -1.013$, $C^2=0.3891$

Resonance state in channel I.

$$f(z) = \left\{ (1 - ibz)^2 + S_I \right\} \left\{ 1 + b\sqrt{\Delta^2 - a^2 z^2} \right\}^2 + S_{II}(S_I) \right\} - C^2(Sz)$$
(31)

$$f'(z) = -2ib(1-ibz)\left\{1 + b\sqrt{\Delta^2 - a^2 z^2}\right)^2 + S_{II}\right\}$$
$$-2\left\{(1-ibz)^2 + SI\right\}(1 + b\sqrt{\Delta^2 - a^2 z^2})^2 \frac{a^2 bz}{\sqrt{\Delta^2 - a^2 z^2}}$$
(32)

$$Z^{(n+1)} = Z^{(n)} - f(z^{(n)})/f'(Z^{(n)})$$
(33)

We solved eq: (58) numerically by using FORTRAN CODE to obtain resonance energy of $\Sigma\pi$.

3.2 Numerical model B

1 ~

$$b = \frac{\hbar C}{M_B C^2} = 3.5 \text{fm}, \quad M_B = 56.4 \text{MeV} / \text{C}^2$$
 (34)

$$\begin{cases} B_0^{(I)} = \frac{\hbar^2}{2\mu_I} \frac{1}{b^2} = 12.7 \text{MeV} \\ B_0^{(II)} = \frac{\hbar^2}{2\mu_I} \frac{1}{b^2} = 4.91 \text{MeV} \end{cases}$$
(35)

Bound state in Channel II uncoupled

$$BE_{II} = B_0^{(II)} \left(\sqrt{|S_{II}|} - 1 \right)^2 = 27 MeV$$

$$S_{II} = -11.2$$
(36)

In this model, we solved eq:(58) numerically by using FORTRAN CODE to obtain potential strength and range parameters.

Results and Discussion

4.1 Resonance state for $\Sigma^+\pi^- \rightarrow \Sigma^+\pi^-$

We calculated resonance state for $\Sigma^+\pi^- \rightarrow \Sigma^+\pi^-$ by solving Schrodinger equation. The differential cross sections with different $\Sigma^+\pi^$ energies are obtained by changing strength parameters for fixed range parameters.

Firstly we calculated various differential cross-sections for various strength parameters at range parameter 2 fm, 3.5 fm and 5.0 fm. The results are shown in Figure (4.1), (4.2) and (4.3). It is observed that pole positions are varied with strength parameters. The various resonance states $\Sigma^+\pi^-$ are obtained from various strength parameters with dynamical-pole parameter 39.0MeV, 12.7 MeVand 6.2 MeV. The results are shown in table (4.1).



Figure(4.1): Various differential cross sections and energies of $\Sigma^+\pi^-$ for different strength parameters with fixed range parameter b=2 fm



Figure (4.2): Various differential cross sections and energies of $\Sigma^+\pi^-$ for different strength parameters with fixed range parameter b=3.5 fm



Figure (4.3): Various differential cross sections and energies of $\Sigma^+\pi^-$ for different strength parameters with fixed range parameter b=5 fm

	~ .		
Range Parameter	Strength	Resonance Energy	Level Width
b(fm)	Parameter (S)	E _R (MeV)	Γ (MeV)
2.0	-1	-77.95	-
	1.0	0	155.9
	3.0	77.95	270.03
	5.83	188.25	376.43
3.5	-1	-25.45	-
	1.0	0	50.91
	3.0	25.45	88.17
	5.83	61.47	122.91
5.0	-1	-12.47	_
	1.0	0	24.94
	3.0	12.47	43.20
	5.83	30.12	60.23
	10.0	56.12	78.88

Table (4.1): Resonance energies and level widths of $\Sigma^+\pi^-$ for various strength parameters and fixed range parameters for single channel

4.2 Resonance state and Bound State from coupled channel

We consider two channels of $\overline{K}N$ (K⁻p) and $\pi\Sigma$ ($\pi^{-}\Sigma^{+}$) for simplicity. We employ a set of separable potentials with a Yukawa-type form factor. The parameter sets of separable potential for bound state of K⁻p and resonance state of $\pi\Sigma$ are obtained by solving coupled channel. We constructed the numerical model A and model B for parameters of separable potential. The results are shown in the following table.

Table (4.2)	Resonance energies and l	evel widths of Σ	$\pi^+\pi^-$ for various
	strength and fixed range	parameters for	coupled channel

		Bound state in channel 2		Resona			
Our Model	Range Parameter b(fm)	Strength Parameters	Bound state energy of pK ⁻ (MeV)	Strength Parameters (coupled case)		Resonance energy of Σπ	Level Width Γ (MeV)
			(1.201)	SI	SII	(MeV)	
Α	0.25	-1.013	27.0	0.925	-0.642	76.0	40.0
						58.5	8450
В	3.5	-11.2	27.0	5.8	-11.14	76.0	40.0
						60.3	77.0

Conclusion

We investigated various differential cross sections with different $\Sigma^+\pi^-$ resonance energies at various strength and fixed range parameters for single channel. The resonance energy for range parameter 3.5 fm is 61.47 MeV and level width is 122.91 MeV. It is agreement with D. Jido et.al result [1]. The strength and range parameter sets of $\overline{K}N$ interaction for bound state of pK⁻ and resonance state of $\Sigma^+\pi^-$ are obtained on Λ (1405) resonance and bound state from $K^-p \rightarrow \Sigma^+\pi^-$ coupled channel calculation. We can construct our new model A and B for $\overline{K}N$ interaction. It is observed that separable potential is Yukawa type which can be solved analytically.

Acknowledgements

I would like to thank Dr Khin Swe Myint, Rector (Rtd), Emeritous Professor, Department of Physics, Mandalay University for stimulating and valuable discussions.

I am grateful to Dr Shwe Zin Aung, Professor and Head, Department of Physics, Monywa University for her advice and discussions.

References

Agakishiev. G et al. (HADES collaboration), Phys. Rev. C 87, 025201 (2013).

Akaishi. Y, Yamazaki. T, Obu. M and Wada. M, Nucl., Phys. A 835, 67 (2010).

Esmaili. J, Akaishi. Y and Yamazaki. T, Phys, Lett. B 686, 23 (2010).

Esmaili. J, Akaishi. Y and Yamazaki. T, Phys. Rev. C 83, 055207 (2011).

Hassanvand. M, Kalantari. S. Z, Akaishi. Y, Yamazaki. T, Phys. Rev. C 87, 055202 (2013); Phys. Rev, C 88, 019905 (E) (2013).

Hyodo. T and Weise. W, Phys. Rev. C 77, 035204 (2008).

Jido. D, Oller. J. A, Oset E., Ramos. A and Meibner. U.G, Nucl. Phys. A 725, 181 (2003)

Particle Data Group 2014, Olive. K. A et al., Chin. Phys. C 38, 090001 (2014).

PHOTOVOLTAIC PERFORMANCE OF MEH-PPV:PCBM POLYMER SOLAR CELLS WITH AN INTEGRATION OF ZINC OXIDE (ZnO) NANOPARTICLES

Thet Thet Naing¹ Nyein Wint Lwin² Than Zaw Oo³

Abstract

The poly (2-methoxy-5-(2-ethyl hexyloxy)-1, 4-phenylenevinylene) (MEH-PPV) films were prepared by spin coating technique. Introducing additive (ZnO nanoparticles (ZnO-NPs) of size ~ 250 nm) and the optical properties MEH-PPV polymer films were investigated by UV-vis of spectrophotometry. Following the polymer film characterization, the organic solar cells using MEH-PPV based light absorber layer were fabricated and the effect of additive (ZnO-NPs) on the power conversion efficiency of the devices was investigated. The "dichlorobenzene" device outperformed the devices with other three rival solvents and its efficiency is as high as 0.112%. Despite having higher absorption in active layer with ZnO-NPs, the efficiency of this modified device underperformed the reference device (without ZnO-NPs) which is attributed to the restricted charge carrier transport and morphological perturbation. The additive concentrations have a strong impact on optical and surface morphological properties of the photoactive polymer films and thus on the photovoltaic performance of the devices.

Keywords: MEH-PPV:PCBM solar cells, additive (ZnO-NPs)

Introduction

The worlds' energy consumption is being generated through the combustion of fossil fuels. The world is under the threat of global warming because of using fossil fuels such as coal and oil. Today, the reflections of global warming on daily life are seen as climate change. The fossil fuel resources are limited and costly. The finite supply of traditional fossil fuels (oil, natural gas, coal, etc.) underscores the urgency of searching for alternative energy sources. The need to develop inexpensive renewable energy sources stimulates scientific research for efficient, low-cost photovoltaic devices. Types of renewable energy technologies are solar energy, geothermal energy, wind energy, bioenergy, ocean energy and hydropower. Solar energy is one of the most promising, available, renewable energy sources of all.

¹ Dr, Lecturer, Department of Physics, Monywa University

² Dr, Associate Professor, Department of Physics, University of Distance Education

³ Dr, Associate Professor, Department of Physics, University of Mandalay

Photovoltaic (PV) cells convert solar energy into electrical energy. Solar cells are usually divided into three main generations. The first generation solar cells are mainly based on silicon (Si) wafers. The siliconbased photovoltaics have outstanding advantages in both efficiency and lifetime with power conversion efficiencies (PCE) in excess of 25%. Second generation solar cells are thin-film solar cells which include amorphous silicon (a-Si), and cadmium telluride (CdTe), and copper indium gallium selenide (CIGS). Their typical performance is 10-15%. Third generation solar cells are organic heterojunction solar cells, dye sensitized solar cells (DSSC) and organic/inorganic hybrid solar cells. Organic solar cells have received attention due to their low-cost, easy processability, low weight, and mechanical flexibility. Their power conversion efficiencies have increased considerably from 0.001% in 1975 to 1% in 1986 and more recently to 8.13% in 2010.

The power conversion efficiencies of organic solar cells are lower than inorganic (Si) solar cells. Several attempts have being implemented in order to achieve the higher device efficiency. Tailoring and controlling the morphology of photoactive layer and charge transport within the interpenetrating networks plays a crucial role in increasing the device performance. The general approach to enhance charge carrier transport in organic polymer materials is to increase the mesoscopic order and crystallinity. A nanoscale interpenetrating network with crystalline order is the desirable architecture for photoactive layer of organic solar cells. In addition, the electronic bandgaps of the materials in the photoactive layer should be tuned to harvest more light from the solar spectrum.

In addition, incorporating inorganic nanoparticles into conjugated polymer matrices is an area of current interest in the fields of optoelectronics and photovoltaics. This approach can take advantages of the beneficial properties of both materials: superior optoelectronic properties of conjugated polymers and high electron mobility of inorganic semiconductors which would result in an improved device performance. Moreover, polymers are technologically advantageous owing to the ease of flexibility of processing devices in solution. There have been reports on polymer-inorganic hybrid solar cells using zinc oxide (ZnO) nanoparticles. In a heterojunction between a polymer and a wide band gap semiconductor (e.g., MEH-PPV:PCBM/ZnO-NPs system), the electrons can diffuse from the polymer to the semiconductor. When the polymer is illuminated with photon of energy larger than band gap, electron-hole pairs are generated. The electrons are injected into the conduction band of the semiconductor and can move along the nanoparticles network . The nature of the charge transfer process depends on the optical properties of two materials as well as the surface properties of the nanoparticles. In short, selecting the appropriate solvent and introducing additives would be two strategies to modify the optical, electrical and morphological properties of the photoactive polymer layer, thereby modulating the photovoltaic performance of the polymer solar cells.

Experimental Details

This section details about (i) synthesis of ZnO-NPs and (ii) device fabrication and efficiency measurement.

Synthesis of ZnO-NPs

In the synthesis of ZnO nanoparticles, zinc acetate dihydrate $Zn(CH_3COO).2H_2O$ (2.95 g) was first dissolved in methanol (125 ml) and another solution of potassium hydroxide (1.57 g) in methanol (65 ml) was prepared by dissolving potassium hydroxide. This solution was added dropwise to the zinc acetate solution at 60 °C under vigorous stirring. After 2h and 15 min, nanoparticles started to precipitate and the solution became turbid. The heater and stirrer were removed after 2 h and 15 min. The ZnO nanoparticles settled at the bottom and the excess mother liquor was removed and the precipitate was washed twice with methanol (50ml). The ZnO nanoparticles powder was obtained. The experimental setup for synthesis of ZnO nanoparticle is shown in Fig. 1.

Device Fabrication and Efficiency Measurement

The fabrication steps for organic photovoltaic device are depicted in Fig. 2. The devices were fabricated on indium tin oxide (ITO) coated glass substrates which are used as the transparent electrodes. The indium tin oxide (ITO) glasses were cleaned by sequential ultrasonification in acetone, distilled

water and isopropyl alcohol (IPA) for 15 min consecutively and dried by nitrogen blow. Since ITO was coated throughout the glass substrate, etching had to be carried out to remove the ITO at the sides, leaving the only ITO in the center region as shown in Fig. 3(a). ITO surfaces were then treated by UV light in order to remove the organic contamination on the ITO surface. The ultrasonic cleaner and UV chamber used in our ITO cleaning processes are shown in Fig. 3(d).

For the fabrication of MEH-PPV:PCBM solar cells with additive (ZnO-NPs) concentrations (4 wt%, 6 wt%, 8 wt% and 10 wt%), the bulk heterojunction blend solutions of MEH-PPV:PCBM (1:2 wt%) were prepared in dichlorobenzene. A thin layer of poly (3, 4- ethylenedioxythiophene):poly (styrenesulfonate) or (PEDOT:PSS) (Sigma Aldrich) was spin-coated at 3000 rpm for 60 s on pre-cleaned ITO glass plates.

Then the PEDOT:PSS coated substrate was annealed at 100 °C for 15 min. Subsequently, MEH-PPV:PCBM photoactive layer was spun-coat at 1000 rpm for 60 s on the top of PEDOT:PSS layer. The active layer thicknesses were in the range of 80 nm-100 nm as determined by a surface profiler (Tencor Alpha-Step IQ). After annealing at 130 °C for 8 min, the devices were completed by deposition of cathode aluminum (Al) (~ 100 nm) through a mask by thermal evaporation at a pressure of 10^{-6} Torr. The device active area was around 0.07 cm². Fig. 4(a) shows thermal evaporator (NTE 1000) for the deposition metal (Al) cathode.

The I-V curves of the devices were recorded under illumination of light intensity (100 mW/cm²). The photovoltaic efficiency of organic solar cells were evaluated from the J-V characteristics of the device. It was measured using a computer-controlled digital source meter (Keithley 2420) with a Newport solar simulator (A.M. 1.5, 100 mW/cm²). Light intensity was calibrated with a National Renewable Laboratory (NREL)-calibrated monocrystalline Silicon solar cell. Fig. 4(b) shows the experimental setup for the efficiency measurement of OPV devices.



Figure 1:Experimental setup for synthesis of ZnO nanoparticles.



Figure 2: Fabrication steps for organic photovoltaic device.



Figure 3: Illustrations of (a) etched ITO pattern on glass substrate, (b) ultrasonic cleaner, (c) UV chamber and (d) fabricated OPVdevices.



(a)



Figure 4: (a) Thermal evaporator (NTE 1000) for the deposition metal (Al) cathode and (b) Experimental setup for the measurement of device efficiency (Newport Solar simulator and Keithley source meter).

Results and Discussion

This section discusses the effect of additive (ZnO-NPs) on photovoltaic performance of MEH-PPV:PCBM based organic solar cells.

Effect of Additive (ZnO-NPs) Concentration on Photovoltaic Performance of MEH-PPV/ZnO-NPs:PCBM Devices: Correlating the Properties and Performance

The device efficiencies of MEH-PPV:PCBM solar cells with additive (ZnO-NPs) concentrations (4 wt%, 6 wt%, 8 wt% and 10 wt%) were evaluated under A.M. 1.5 solar irradiation of intensity 100 mW/cm². The J-V characteristics of MEH-PPV:PCBM/ZnO-NPs devices are shown in Fig. 5(a) and the measured device parameters are listed in Table 1. A reference MEH-PPV:PCBM solar cell produced a power conversion efficiency (η) of 0.112% with fill factor (FF) of 26.40, open circuit voltage (V_{oc}) of 0.63 V and short-circuit current density (J_{sc}) of 0.67 mA/cm² which outperformed the MEH-PPV:PCBM device with ZnO-NPs.

The V_{oc} of the reference devices is 0.63 V and those of the devices with ZnO-NPs are 0.58 V, 0.49 V, 0.63 V and 0.71 V for ZnO-NPs concentrations of 4 wt%, 6 wt%, 8 wt% and 10 wt% respectively. Higher V_{oc} of 0.71 V is produced in the device with ZnO-NPs (10 wt%) while lower V_{oc} of 0.49 V in the device with ZnO-NPs (6 wt%). The J_{sc} of the devices with ZnO-NPs is lower than that of reference device $(67 \times 10^{-2} \text{ mA/cm}^2)$ despite having higher absorption in MEH-PPV:PCBM active layer with ZnO-NPs. There may be some ZnO-NPs induced disturbances in electron path way towards the electron collecting electrode which reduces the J_{sc} . Among the devices with ZnO-NPs, the ZnO-NPs concentration of 8 wt% yields a higher J_{sc} which is consistent with the absorption data (Fig. 5(b)) that the absorption of active layer with ZnO-NPs (8 wt%) is higher than those with other ZnO-NPs concentrations (2 wt%, 4 wt% and 10 wt%). Step height profile of MEH-PPV:PCBM photoactive layer is shown in Fig. 6(a). The thickness of the film is about 230 nm. The roughness profiles of MEH-PPV:PCBM without and with ZnO-NPs are shown in Fig. 6(b).

FF is sensitive to the morphology and series resistance of the device. A gradual decrease of FF with increasing ZnO-NPs concentration is ascribed to an increased roughness of the film surface (Table 1). The series resistances (R_s) of the devices are calculated from the J-V curves of the devices and tabulated in Table 2. It is found that the R_s increase with increasing ZnO-NPs concentrations which would result in the lower FF of ZnO-NPs incorporated devices. To sum up, the efficiency lowering in the modified devices (with ZnO-NPs) despite having higher absorption with ZnO-NPs can be attributed to the restricted charge carrier transport and perturbed morphology.



Figure 5: (a) J-V characteristics of the organic solar cells comprising MEH-PPV:PCBM/ZnO-NPs composite photoactive layer and (b) Absorption spectra of MEH-PPV:PCBM pure and MEH-PPV:PCBM/ZnO-NPs composite



Figure 6: (a) Step height profile of MEH-PPV:PCBM photoactive layer. The thickness is about 230 nm and (b) Roughness profiles for the MEH-PPV:PCBM films with and without ZnO-NPs.
MEH-PPV:PCBM Device	V _{oc} (V)	J _{sc} (mA/cm ²)	FF	PCE (%)
Without ZnO-NPs	0.63	67×10 ⁻²	26.40	11.20×10 ⁻²
With ZnO-NPs (4 wt%)	0.58	0.04×10^{-2}	22.81	0.01×10 ⁻²
With ZnO-NPs (6 wt%)	0.49	0.10×10 ⁻²	22.91	0.01×10 ⁻²
With ZnO-NPs (8 wt%)	0.63	7.19×10 ⁻²	16.99	0.77×10 ⁻²
With ZnO-NPs (10 wt%)	0.71	0.82×10^{-2}	11.68	0.07×10 ⁻²

 Table 1: Measured device parameters of pure MEH-PPV:PCBM and MEH-PPV:PCBM/ZnO-NPs solar cells.

Table 2: The series resistance (R_s) of the device and average roughness (R_a) of MEH-PPV:PCBM photoactive layer with and without ZnO-NPs.

MEH-PPV:PCBM Device	Average roughness R _a (nm)	Series resistance R_s (Ωcm^2)
Without ZnO-NPs	0.12	0.87
With ZnO-NPs (4 wt%)	0.22	15.62
With ZnO-NPs (6 wt%)	0.45	15.54
With ZnO-NPs (8 wt%)	0.66	18.18
With ZnO-NPs (10 wt%)	1.34	113.25

Conclusion

The additive "ZnO-NPs concentration of 8 wt%" provides the highest absorption intensity. Achieving the high optical absorption is requisite for photoactive layers in solar cells. This work involves the fabrication of organic solar cells using MEH-PPV/PCBM polymer blend film as photoactive layer. The effects of additive (ZnO-NPs) concentration on device efficiency were investigated. The device using "dichlorobenzene" produced the efficiency as high as 0.112% (open circuit voltage 0.63 V, short circuit current density 0.67 mAcm⁻² and fill factor 26.40). The obtained device efficiency was correlated to the properties of the photoactive films. Despite having higher absorption in active layer with ZnO-NPs, the efficiency of this modified device underperformed the reference device (without ZnO-NPs) which is attributed to the restricted charge carrier transport and morphological perturbation.

Acknowledgement

The author would like to thank Dr Thura Oo, Rector, Monywa University, for his invaluable guidance. The author gratefully thanks to Dr Thet Naing Oo and Dr Sein Sein Aung, Pro-Rectors, Monywa University, for their advice. The author also gratefully thanks Professor Dr Shwe Zin Aung, Head of Department, Department of Physics, Monywa University, for her permission and valuable suggestions.

References

- B. Chung et al., Appl. Phys. Lett. 55 (1989) 1741.
- C. J. Neef and J. P.Ferraris, Macromolecules 33 (2000) 2311.
- C. Tang et al., Appl. Phys. Lett. 91 (2007) 143.
- C. Ton-That et al., Solid State Mat. Sci. 6 (2002) 87.
- G. Zhang et al., Appl. Phys. Lett. 94 (2009) 143.
- J. Kim et al., J.Science 45 (2007) 222.
- K.Wu, "Master Thesis", McMaster University (2010).
- N. Shaheen et al., Appl. Phys. Lett. 78 (2001) 98.
- S. H. Yang, Adv. Mater. Sci. 15 (2007) 27.
- X. Wang et al., Front. Chem. Lett. 5 (2010) 45.

SINGLE-PARTICLE ENERGY LEVELS OF EVEN-EVEN SILICON ISOTOPE

Yin Mar Aung*

Abstract

In our research work, single particle energy levels of even-even silicon isotope ²⁸Si are calculated by using the phenomenological Woods-Saxon central potential with spin-orbit interaction. The Gaussian basis wave function is also used in our calculation. The average values of kinetic energy, potential energy and centrifugal energy are calculated. The neutron separation energy and the root-mean-square radius of ²⁸Si are also calculated. Our calculated shell spectra are similar as the prediction of the shell model. Moreover, the calculated last neutron separation energies are in good agreement with the experimental results.

Introduction

There are two basic types of simple nuclear models to investigate the characteristic of the nuclei. Nuclear models generally can be divided into independent particle models (IPM) in which the nucleons in discrete energy states are assumed, to move nearly independently in a common nuclear potential and the strong interaction (collective) models (SIM) in which the nucleons are strongly coupled to each other. The simplest SIM is the liquid drop model. The simplest IPM is also known the Fermi gas model (or) the shell model which is the basis of the semi-empirical mass formula.

The Shell Model

In nuclear physics, the nuclear shell model is a model of the atomic nucleus which uses the Pauli Exclusion Principle to describe the structure of the nucleus in terms of energy levels. The shell model is partly analogous to the atomic shell model which describes the arrangement of electrons in an atom, in that a filled shell results in greater stability. This observation that there are certain magic numbers of nucleons: 2, 8, 20, 28, 50, 82, 126 which

^{*} Dr, Lecturer, Department of Physics, Monywa University

are more tightly bound than the next higher number, is the origin of the shell model. The nuclear shell model explains the existence of magic numbers.

The energy levels are found by solving the Schrödinger equation for a single nucleon moving in the average potential generated by all other nucleons. Each level may be occupied by a nucleon, or empty. Some levels accommodate several different quantum states with the same energy, they are said to be degenerate.

Some nuclei are bound more tightly than others. This is because two nucleons of the same kind cannot be in the same state. So the lowest energy state of the nucleus is one where nucleons fill all energy levels from the bottom up to some level. The energy levels increase with the orbital angular quantum number l, and s, p, d, f ... symbols are used for l = 0, 1, 2, 3, The value of total angular momentum j and the multiplicity of the state is 2j+1.

Schrödinger equation and Interaction

In order to find the energy levels of a nucleus, Schrödinger equation is used. The time-independent Schrödinger equation for potential well is as follows.

$$\left[\left(-\frac{\hbar^2}{2M}\nabla^2\right) + v(\mathbf{r})\right]\Psi(\mathbf{r}) = \mathbf{E}\Psi(\mathbf{r})$$
(1)

The wave function $\Psi(\mathbf{r})$ can be expressed in terms of $R(\mathbf{r}) = \Theta(\theta)$ and $\Phi(\phi)$

$$\Psi(\mathbf{r}) = \mathbf{R}(\mathbf{r})\Theta(\theta)\Phi(\phi) \tag{2}$$

The angular part term,

$$\frac{M^2}{\sin^2\theta} - \frac{1}{\Theta(\theta)\sin\theta} \left[\cos\theta \frac{d\Theta}{d\theta} + \sin\theta \frac{d^2\Theta}{d\theta^2}\right] = l(l+1)$$
(3)

The Radial Part term is,

$$\frac{1}{R(r)} \left[2r \frac{dR(r)}{dr} + r^2 \frac{d^2 R(r)}{dr^2} \right] + \frac{2M}{\hbar^2} r^2 (E - V(r)) = l(l+1)$$
(4)

So, the radial part of Schrödinger equation is as follows.

$$-\frac{\hbar^{2}}{2M}\left[\frac{d^{2}}{dr^{2}}-\frac{l(l+1)}{r^{2}}\right]u(r)+V(r)u(r)=Eu(r)$$
(5)

The Gaussian basis wave function is used

$$\Psi(\mathbf{r}) = \mathbf{r}^{l+1} N \sum_{i} c_{i} e^{-(\frac{\mathbf{r}}{b_{i}})^{2}}$$
(6)

These linear equations can be solved by using Gauss elimination method which is the fundamental one for solving linear systems. And so norm matrix elements, kinetic energy matrix element and potential energy matrix elements, relative probability density and root-mean-square distance are analytically obtained by using Gaussian standard integral form. By diagonalzing the Hamiltonian matrix, the energy eigen-value is obtained with the help of FORTRAN PROGRAM.

Woods-Saxon Potential

The Dirac equation, which describes the motion of a spin ½ particle, has been used in solving many problems of nuclear and high-energy physics. Within the framework of Dirac equation, p-spin symmetry used to feature deformed nuclei, super deformation, and to establish an effective shell model.

The interactions between nuclei are commonly described by using Woods-Saxon potential that plays a great role in nuclear physics.

The form of the generalized Woods-Saxon potential is as follows.

$$V(r) = -\frac{V_0}{1 + e^{(r-R)/a}}$$
(7)

 $R=r_{_{0}}A^{\frac{1}{3}}$ is the nuclear radius where r_{0} = 1.25 fm and A is the mass number.

Typical values for the parameters are: $V_0 \approx 50 \text{ MeV}$, $a \approx 0.5 \text{ fm}$.

When using the Schrödinger equation to find the energy levels of nucleons subjected to the Woods-Saxon potential, it cannot be solved analytically, and must be treated numerically.

Normalization Constant

To solve the physical quantities of ²⁸Si nuclei, the normalization constant is calculated. The normalized condition is as follows;

$$\int_{0}^{\infty} \Psi^{*}(\mathbf{r}) \Psi(\mathbf{r}) d\mathbf{r} = 1$$
(8)

The normalized Gaussian basis wave function is defined as follows;

$$U(r) = A \sum_{i} c_{i} e^{-(\frac{r}{b_{i}})^{2}} r^{l+1}$$
(9)

$$A^{2} \sum_{i} \sum_{j} c_{i} c_{j} \int e^{-r^{2} (\frac{1}{b_{i}^{2}} + \frac{1}{b_{j}^{2}})} r^{2(l+1)} dr = 1$$
(10)

By using standard integral, the normalized constant is obtained.

$$A = \frac{1}{\left[\sum_{i} \sum_{j} c_{i} c_{j} \frac{(2L+1)!!}{2^{l+2}} \frac{1}{(\frac{1}{b_{i}^{2}} + \frac{1}{b_{j}^{2}})^{l+1}} \left(\frac{\pi}{\frac{1}{b_{i}^{2}} + \frac{1}{b_{j}^{2}}}\right)^{\frac{1}{2}}\right]^{\frac{1}{2}}}$$
(11)

In which normalized matrix element is

$$A_{ij} = \frac{(2l+1)!!}{2^{L+2}} \frac{1}{\left(\frac{1}{b_i^2} + \frac{1}{b_j^2}\right)^{l+1}} \left(\frac{\pi}{\frac{1}{b_i^2} + \frac{1}{b_j^2}}\right)^{l/2}$$
(12)

Kinetic Energy and Centrifugal Potential Energy

Kinetic Energy

The kinetic energy is calculated as follows;

$$\hat{T}(\mathbf{r})\mathbf{U}(\mathbf{r}) = \frac{\hbar^2}{2\mu} \left[\frac{d^2}{d\mathbf{r}^2} \mathbf{U}(\mathbf{r}) \right]$$
(13)

$$\hat{T}(\mathbf{r}) \mathbf{U}(\mathbf{r}) = \frac{\hbar^2}{2\mu} \mathbf{A} \sum_{i} \mathbf{c}_{i} e^{-(\frac{\mathbf{r}}{\mathbf{b}_{i}})^2} \left[l(l+1)\mathbf{r}^{l-1} - \frac{2}{\mathbf{b}_{i}^2} (2l+3)\mathbf{r}^{l+1} + \frac{4}{\mathbf{b}_{i}^4} \mathbf{r}^{l+3} \right]$$
(14)

Kinetic energy matrix element is as follows

$$T_{ij} = \frac{\hbar^2}{2\mu} A e^{-(\frac{r}{b_i})^2} \left[l(l+1)r^{l-1} - \frac{2}{b_i^2}(2l+3)r^{l+1} + \frac{4}{b_i^4}r^{l+3} \right]$$
(15)

Centrifugal Potential Energy

The centrifugal potential energy is follows

$$\hat{F}(r)U(r) = \frac{\hbar^2}{2\mu} \left[\frac{l(l+1)}{r^2} U(r) \right]$$
 (16)

By using wave function, the centrifugal potential energy is described as follows;

$$\hat{F}(r)U(r) = \frac{\hbar^2}{2\mu} \left[\frac{l(l+1)}{r^2} A \sum_{i} c_i e^{-(\frac{r}{b_i})^2} r^{l+1} \right]$$
(17)

The centrifugal potential matrix element is as follows;

$$F_{ij} = \frac{\hbar^2}{2\mu} \left[\frac{l(l+1)}{r^2} A e^{-(\frac{r}{b_i})^2} r^{l+1} \right]$$
(18)

Potential Energy

In our calculation the phenomenological Woods-Saxon Potential is used. The form of the generalized Wood-Saxon potential is as follows.

$$V(r) = \frac{-V_0}{1 + e^{(r-R_0)}/a}$$
(19)

In this equation $R_0 = r_0 A^{\frac{1}{3}}$ is the nuclear radius and A is the diffuse parameter. r_0 is the radii distance from the center. The potential strength depends upon the number of proton and neutron. It is represent by,

$$V_{0} = \left[50 - 32 \frac{N - Z}{A} \right] \text{ and the nuclear density, } \rho_{(r)} = \frac{1}{1 + e^{r - R/a}}.$$

Woods-Saxon potential including spin-orbit interaction is

$$V(r) = V_{W-S}(r) + V_{ls}(r)$$
(20)

The spin-orbit interaction is described as follows.

$$V_{ls}(r) = V_{so} \left(\frac{\hbar}{Mc}\right)^2 (l.s) \frac{1}{r} \frac{d\rho}{dr}$$

The total angular momentum is $\vec{J} = \vec{l} + \vec{s}$ and the spin of a nucleon is $\frac{1}{2}\hbar$.

For $j = l + \frac{1}{2}$, $l.s = \frac{1}{2}l$ $\therefore V(r) = V_{W-S}(r) + V_{ls}(r)$ (21) $V(r) = -V_0 \rho(r) + V_{ls}(r)$ $= \frac{-V_0}{1 + e^{r-R/a}} + V_{s0}(\frac{\hbar}{Mc})^2 (\frac{1}{2}l) \left[\frac{1}{r} \frac{e^{r-R/a}}{1 + e^{r-R/a}} \frac{1}{a} \right]$ For $j = l - \frac{1}{2}$, $l.s = -\frac{1}{2}(l+1)$ $\therefore V(r) = \frac{-V_0}{1 + e^{r-R/a}} - V_{s0}(\frac{\hbar}{Mc})^2 (\frac{1}{2}(l+1)) \left[\frac{1}{r} \frac{e^{r-R/a}}{1 + e^{r-R/a}} \frac{1}{a} \right]$ (22)

Probability Density and Root-Mean-Square Distance

To analyze the structure of the nuclei, the probability density and rootmean-square radius are calculated.

Probability Density

The probability density is follows

$$\int P(x,t)dx = \int_{r_1}^{r_2} \psi^*(x,t)\psi(x,t)dx$$
(23)

By applying the Gaussian wave function, the probability density is calculated.

Probability density =
$$A^2 \sum_{i} \sum_{j} c_i c_j \frac{(2l+1)!!}{2^{l+2}} \frac{1}{(\frac{1}{b_i^2} + \frac{1}{b_j^2})^{l+1}} \left(\frac{\pi}{\frac{1}{b_i^2} + \frac{1}{b_j^2}}\right)^{\frac{l}{2}}$$
 (24)

Root-Mean Square Distance

The root-mean square distance of a particle is as follows.

$$\langle \mathbf{r}^2 \rangle = \int \psi^* \mathbf{r}^2 \psi \, d\mathbf{r}$$
 (25)

By using normalized wave function, the root-mean square distance is described as follows.

$$\left\langle \mathbf{r}^{2} \right\rangle = \mathbf{A}^{2} \sum_{i} c_{i} \sum_{j} c_{j} \frac{(2l+3)(2l+3-2)!!}{2^{l+2} \times 2} \frac{1}{\left(\frac{1}{\mathbf{b}_{i}^{2}} + \frac{1}{\mathbf{b}_{j}^{2}}\right)^{l+1}} \frac{1}{\left(\frac{1}{\mathbf{b}_{i}^{2}} + \frac{1}{\mathbf{b}_{j}^{2}}\right)} \left(\frac{\pi}{\mathbf{b}_{i}^{2}} + \frac{1}{\mathbf{b}_{j}^{2}}\right)^{l/2}$$
(26)

Results and Discussions

The single-particle energy levels of ²⁸Si are calculated by using Gaussian basic wave function and the phenomenological Woods-Saxon potential including spin orbit interaction. The root-mean square radius and the last neutron separation energy of ²⁸Si are also investigated.

The calculated results of energy levels of ²⁸Si are shown in Table (1) and the corresponding energy shell levels are shown in Fig. (1). In this Fig. (1), the innermost level $1s_{1/2}$ among the calculated other levels has the highest binding energy and it has gradually decrease to $1f_{7/2}$ levels away from the ²⁸Si nucleus. The higher energy levels of $1s_{1/2}$ are split into two energy levels for same orbital angular momentum. The neutron separation energy of ²⁸Si is also calculated and it is 8.447744MeV and it is nearly equal to experimental results.

Finally, the single-particle energy levels of even-even silicon isotope ²⁸Si and ³⁰Si are calculated and are compared in Table (2).

Conclusion

In our research work, the ground state energy of the most abundance stable ²⁸Si are calculated by using phenomenological Woods-Saxon potential including spin-orbital interaction and the strength of the potential is 50MeV, $r_0 = 1.25$ fm and diffuse parameter a=0.53. It is found that Woods-Saxon potential provides a model for the properties of bound-state and continuum single-particle wave functions. Our calculated results are in good agreement with the experimental results.

Single-Particle State of ²⁸ Si	Total Energy (MeV)	Average Root-Mean Square Radius (fm)	Normalized Constant
$1s_{\frac{1}{2}}$	-36.243832	2.285874	32.9676497
1p _{3/2}	-25.328756	2.843373	21.2907179
1p _{1/2}	-22.553915	2.779176	7.974858
$1d_{\frac{5}{2}}$	-13.679509	3.329208	12.1807297
1d _{3/2}	-8.0593294	3.331005	13.880731
1f _{7/2}	-1.8267510	3.944157	2.687783

 Table 1: The Physical Quantities of ²⁸Si

Table 2: Energy levels of Even-Even Silicon Isotope

Energy States		Total Energy (MeV)			
		$^{28}_{14}$ Si	$^{30}_{14}$ Si		
s-state	s1/2	-36.243832	-36.76636		
p-state	p3/2	-25.328756	-26.12143		
	p1/2	-22.553915	-23.52642		
d-state	d5/2	-13.679509	-14.63793		
	d3/2	-8.0593294	-9.303161		
f-state	f7/2	-1.8267510	-2.730027		



Figure 1: Neutron single-particle energy levels of ²⁸Si

Acknowledgements

I would like to express our gratitude and sincere thanks to Rector Dr Thura Oo, Monywa University for their permission to do this work. I wish to thank Dr Shwe Zin Aung, Professor and Head, Department of Physics, Monywa University for her precious advice, discussions and guidance.

References

H. Frauenfelder and Ernest M.Henley, "Subatomic Physics", (1991).

https://en.wikipedia.org/wiki/Woods-Saxon potential.

TakaoTATI, Progress of Theoretical Physics, Vol.14, No.2, (1955).

W. Greiner, Joachim A. Maruhn, "Nuclear Models", (1995).

CALCULATION OF POTENTIAL ENERGY SURFACES FOR LIGHT NUCLEI IN β - γ PLANE

Khaing Pwint Wai¹, Nyein Wint Lwin²

Abstract

The nuclei having asymmetric shapes in their ground state have now become an interesting topic in both theoretical and experimental nuclear structure physics. In my present work, the deformations in neutron-rich light-mass nuclei are investigated by using self-consistent mean field approach. Using the constrained Skyrme Hartree-Fock+BCS method on the three-dimensional Cartesian mesh, we calculated the potential energy surfaces (PES) for some selected light nuclei (¹⁶O, ²²Ne and ²⁸Si) in $\beta - \gamma$ plane where β represents ellipsoidal quadrupole deformation and γ , the degree of axial asymmetry.

Keywords: light nuclei, Hartree-Fock + BCS method

Introduction

One of the major challenges in nuclear physics is the study of the nuclear structures of nuclei which can provide the precious information in nuclear theory. In the past decades, the relativistic and non-relativistic self-consistent mean-field approaches have been popular to study the structure of nuclei. In this report, we choose the non-relativistic mean field theory and calculate their potential energy surfaces to verify the shapes of ¹⁶O, ²²Ne and ²⁸Si nuclei.

The shape of a deformed nucleus can be parameterized by representing the nuclear surface via expansion of the spherical harmonics, $Y(\theta, \phi)$, as follow:

$$R(\theta,\phi) = R_0 \left(1 + \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta,\phi) \right)$$
(1)

where $R(\theta, \phi)$ denotes the nuclear radius in the direction (θ, ϕ) , λ indicates the order of the expansion, R_0 is the radius of a sphere containing the same

^{1.} Demonstrator, Department of Physics, Monywa University.

^{2.} Associate Professor, Department of Physics, Mandalay University of Distance Education.

total volume and $\alpha_{\lambda\mu}$ the expansion coefficients describe the variations of the nuclear shape with different multipolarity around the ground state.

In my calculation, the quadrupole deformation ($\lambda = 2$) which is the most important deviation from spherical shape is taken into account. For the case of pure quadrupole deformation, the Eq. 1 is given by

$$R(\theta,\phi) = R_0 \left(1 + \sum_{\mu=-2}^{2} \alpha_{2\mu} Y_{2\mu}(\theta,\phi) \right)$$
(2)

Such quadrupole shapes can either have axial symmetry, in which case one distinguishes elongated (prolate) and flattened (oblate) shapes, or the deformation can be without axial symmetry resulting in different elongations along the three axes of the system, referred to as triaxial shape.

There is a set of parameters introduced by Bohr [1] which corresponds to something like polar coordinates in space of $(\alpha_{20}, \alpha_{22})$ and is defined by

$$\alpha_{20} = \beta_2 \cos\gamma,\tag{3}$$

$$\alpha_{22} = \frac{1}{\sqrt{2}} \beta_2 \sin \gamma, \tag{4}$$

where the parameters β_2 and γ represent the deformation and non-axiality of the nuclear shapes, respectively.

The aim of this present work is to study the shapes of light nuclei (¹⁶O, ²²Ne, ²⁸Si) using self-consistent mean field approach. The structures of these nuclei will be investigated by calculating the potential energy surfaces in beta-gamma ($\beta - \gamma$) plane which can clearly show the structure of nuclei. Then Ev8 program which solves the Skyrme-Hartree-Fock+BCS problem using a 3-dimensional Cartesian mesh will be employed in this calculation [2].

Formalism

I. Hartree-Fock Equations with Skyrme Interaction

The aim of the Hartree-Fock method is to approximate the two-body Hamiltonian operator as an effective single-particle potential. The full manybody Hamiltonian can be written in terms of a one-body kinetic energy term and a two-body force as follows

$$H = \sum_{i=1}^{N} \hat{t}_{i} + \frac{1}{2} \sum_{i \neq j}^{N} \hat{V}(r_{i}, r_{j})$$
(5)

where the first term is the usual kinetic energy operator, and the second is the two-body force including the Coulomb interaction. The simplified expression for the Hatree-Fock equations is obtained

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \int d\mathbf{r}'\,\rho(\mathbf{r}')\,V(\mathbf{r},\mathbf{r}')\right)\varphi_i(\mathbf{r}) - \int d\mathbf{r}'\,\rho(\mathbf{r},\mathbf{r}')\,V(\mathbf{r},\mathbf{r}')\,\varphi_i(\mathbf{r}') = \varepsilon_i\,\varphi_i(\mathbf{r}). \tag{6}$$

This equation is known as the Hartree-Fock equation. The Hartree-Fock method is useful one because it gives an introduction to the solution of many-particle system and to the concepts of self-consistent field. In the following, the Skyrme approximation which can greatly reduce the number of integrations over single particle states will be discussed.

In non-relativistic approach, the most famous effective nucleonnucleon interaction is the Skyrme type which was performed by Vautherin and Brink [3] has been used for this work. In the Skyrme-Hartree-Fock approach, the total binding energy of the system is given by the sum of the kinetic and Coulomb energies as well as the Skyrme energy functional that models the effective interaction between nucleons [4].

The full Skyrme interaction can be shown in the form of the following equation,

$$E = E_{Coulomb} + E_{kin} + E_{Sk} . ag{7}$$

A Skyrme force that consists of central, spin-orbit and tensor interactions is given by

$$\widehat{V}_{sk}(\mathbf{r},\mathbf{r}') = \widehat{V}^{central}(\mathbf{r},\mathbf{r}') + \widehat{V}^{LS}(\mathbf{r},\mathbf{r}') + \widehat{V}^{tensor}(\mathbf{r},\mathbf{r}')$$
(8)

The Skyrme energy (E_{sk}) , is derived by evaluating,

$$E_{sk} = \frac{1}{2} \sum_{i,j}^{A} \int \phi_i^*(\mathbf{r}') \phi_j^*(\mathbf{r}') \hat{V}_{sk}(\mathbf{r},\mathbf{r}') \left(1 - \hat{P}_M \hat{P}_\sigma \hat{P}_q\right) \phi_i(\mathbf{r}) \phi_j(\mathbf{r}) d\mathbf{r} d\mathbf{r}' \Big|_{\mathbf{r}=\mathbf{r}'}$$
(9)

where \hat{P}_M is position exchange operator and \hat{P}_q is isospin exchange operator. Finally, the result of the Skyrme interaction is given by

$$E_{Sk} = B_{1}\rho^{2}(\mathbf{r}) + B_{2}\sum_{q}\rho_{q}^{2}(\mathbf{r}) + B_{3}\left\{\rho(\mathbf{r})\tau(r) - j^{2}(\mathbf{r})\right\} + B_{4}\sum_{q}\left\{\rho_{q}(\mathbf{r})\tau_{q}(\mathbf{r}) - j_{q}^{2}(\mathbf{r})\right\} + B_{5}\rho(\mathbf{r})\nabla^{2}\rho(\mathbf{r}) + B_{6}\sum_{q}\rho_{q}(\mathbf{r})\nabla^{2}\rho_{q}(\mathbf{r}) + B_{7}\rho^{\alpha}(\mathbf{r})\rho^{2}(\mathbf{r}) + B_{8}\rho^{\alpha}(\mathbf{r})\sum_{q}\rho_{q}^{2}(\mathbf{r}) + B_{9}\left[\rho(\mathbf{r})\nabla J(\mathbf{r}) + S(\mathbf{r}).(\nabla \times j(\mathbf{r})) + \sum_{q}\left\{\rho_{q}(\mathbf{r})\nabla J_{q}(\mathbf{r}) + S_{q}(\mathbf{r}).(\nabla \times j_{q}(\mathbf{r}))\right\}\right] + B_{10}S^{2}(\mathbf{r}) + B_{11}\sum_{q}S_{q}^{2}(\mathbf{r}) + B_{12}S^{2}(\mathbf{r})\rho^{\alpha}(\mathbf{r}) + B_{13}\rho^{\alpha}(\mathbf{r})\sum_{q}S_{q}^{2}(\mathbf{r})\rho_{q}^{\alpha}(\mathbf{r}) + B_{14}\left(S(\mathbf{r}).T(\mathbf{r}) - J^{2}(\mathbf{r})\right) + B_{15}\left(S(\mathbf{r})\nabla^{2}S(\mathbf{r})\right) + B_{16}\sum_{q}\left(S_{q}(\mathbf{r}).T_{q}(\mathbf{r}) - J_{q}^{2}(\mathbf{r})\right) + B_{17}\sum_{q}S_{q}(\mathbf{r})\nabla^{2}S_{q}(\mathbf{r})$$
(10)

The Skyrme interaction enormously simplifies the calculations with its zero-range form and has been very successfully used to describe the masses, charge radii and excited states of finite nuclei.

II. Constrained Hartree-Fock Method

The map of the energy surface as function of quadrupole deformation can be obtained by imposing constraints on the axial and triaxial mass quadrupole moments in the Hamiltonian. There can be many cases where it may be desirable to calculate other points on the energy surface. In this work, constrained Hartree-Fock (CHF) method is used to calculate the energy surface as a function of collective parameters of "q" such as quadrupole deformation. In this method, a wave function such as $|\Phi(q)\rangle$ is used to minimize the total energy under the constraint that a certain single particle operator $\langle \hat{Q} \rangle$ which has a fixed expectation value

$$\langle H' \rangle = \langle H \rangle - \lambda \langle \hat{Q} \rangle$$
, where $q = \langle \Phi | \hat{Q} | \Phi \rangle$. (11)

Results and Discussion

In this calculation, constrained quadrupole moment is added to the Hamiltonian to generate energy surfaces. The *Sly 4* parameter set is chosen for this calculation. Moreover, Ev8 code is used to solve the mean-field equations for the Skyrme energy density functional. In this code, the single particle wave functions are discretized on a 3-dimensional (3D) mesh to solve the mean-field equations.

A representation in terms of the deformation parameter (q) and the triaxiality angle (γ) is used to describe the shapes of nuclei. Their relationship can be represented by the following equations

$$q_1 = q\cos(\gamma) - \frac{1}{\sqrt{3}}q\sin(\gamma) \tag{12}$$

$$q_2 = \frac{2}{\sqrt{3}}q\sin(\gamma). \tag{13}$$

We select three light nuclei (¹⁶O, ²²Ne and ²⁸Si) and calculate their potential energy surfaces. In order to know the shapes of these nuclei, the calculated potential energy surfaces as the function of deformation parameters are depicted in the following figures.





Figure 1:The potential energy surfaces as the function of deformation parameter (β) for (a) ¹⁶O (b) ²²Ne and (c) ²⁸Si obtained with the *Sly4* parameter set.

For these calculations, we use the same symmetry axis for prolate and oblate configurations. The minimum energy located at the positive deformation parameter describes the prolate shape while the minimum energy with negative deformation parameter stands for the oblate shape. Fig. 1 (a) is the potential energy surface of ¹⁶O nucleus which shows the well deep spherical configuration of the magic number. Its ground state energy is predicted to have -128.29 MeV at the origin. As can be seen in Fig. 1(b), there is the deep energy minimum of prolate configuration for ²²Ne which has the ground state energy of -177.17 MeV at $\beta = 4.7$. In Fig. 1(c), the PES of ²⁸Si nucleus shows the oblate configuration with ground state energy (-243.29 MeV) and its quadrupole deformation is -0.38.

In order to investigate whether there is deviation from axial symmetry in these nuclei, it is necessary to calculate their potential energy surfaces in $\beta - \gamma$ plane.



Figure 2: The potential energy surfaces of (a) ¹⁶O (b) ²²Ne and (c) ²⁸Si in the $\beta - \gamma$ plane obtained with the *Sly4* parameter set.

To this end, we plotted the potential energy surfaces of three eveneven nuclei, ¹⁶O, ²²Ne and ²⁸Si in $\beta - \gamma$ plane as shown in Fig. 2. These contours are iso-energy lines, at every 0.2 MeV related to the ground state. In these figures, β represents the magnitude of deformation. The triaxiality angle $\gamma = 0^{\circ}$ corresponds to prolate shapes, whereas $\gamma = 60^{\circ}$ to oblate shape and triaxial for $0^{\circ} < \gamma < 60^{\circ}$. The potential energy surface (PES) for the ¹⁶O nucleus in the (β, γ) plane is plotted in Fig. 2(a). It has the minimum energy at the origin showing that it has the nature of spherically symmetric. Fig. 2(b) indicates ²²Ne nucleus is prolately deformed in its ground state minimum point which is located at $\gamma = 0$ axis. Similarly, the PES of ²⁸Si shows that it has the oblate minimum energy along $\gamma = 60$ axis as can be seen in Fig. 2(c). From these figures, we can conclude that these nuclei are axially symmetric.

Summary and Future Work

In this work, we have calculated the energy surfaces as a function of deformation parameter for some light nuclei, namely, ¹⁶O, ²²Ne and ²⁸Si. We also calculate the energy surfaces in $(\beta - \gamma)$ plane in order to check the deviation from axial symmetry in these nuclei. It is found that ¹⁶O nucleus has spherical shape as it can be expected and the other two nuclei ²²Ne and ²⁸Si have prolate and oblate shapes, respectively. No deviation from axial symmetry is found for these two deformed nuclei.

Recent experiments suggest that nuclei can have permanent triaxial shape. This new discovery motivates us to investigate the internal structure properties of the nuclei. We will investigate the existence of triaxial shapes in light nuclei by calculating the PES in $(\beta - \gamma)$ plane.

Acknowledgement

I would like to give my special thanks to the respectable person who contributed their effort and time for supporting to hold the seminar of Myanmar Academy of Arts and Science hosted by University of Yangon.

References

A. Bohr et al., Phys. 26 (1953) 14.

W.Ryssens et al., Computer .Phys. (2014) 187.

D. Vautherin and D. M. Brink, Phys. Rev. C 5 (1972) 626.

M. Bender et al., Rev. Mod. Phys. 75 (2003) 121.

E. Chabanat et al., Nucl. Phys. A 643 (1998) 441(E).

G.H. Bhat and J. A. Sheikh . Phys. Rev. C 91 (2015) 024319.

CONSTRUCTING A COUPLED CHANNEL $\overline{K}N-\pi\Sigma$ SEPARABLE POTENTIAL

Hnin Nu Aye¹, Thida Wint², Khin Swe Myint³

Abstract

The purpose of our research is to determine the KN potential parameters which reproduce the experimental binding energy and level width of $\Lambda(1405)$ resonance as well as the KN scattering parameter. $\Lambda(1405)$ has been interpreted as a $\overline{K}N^{1}$ quasi-bound state which is embedded in the $\pi\Sigma$ continuum. Particle Data Group (PDG) interpreted on the experimental finding of K⁻p bound state that $\Lambda(1405)$ is located around 1405MeV. Chiral dynamics claimed that there appears two poles in KN- $\pi\Sigma$ coupled channel system. The first pole is located around 1420MeV mainly coupled to \overline{KN} channel and the second pole is located around 1320MeV mainly coupled to $\Sigma\pi$ channel. The position of $\overline{K}N$ bound state is a still controversial issue. In order to get information about the \overline{KN} interaction, the parameter set 1 which satisfies the PDG data and the parameter set 2 which satisfies the Chiral model's result for single channel are constructed by solving the Schrödinger equation with Yukawa-type separable potential. For the coupled-channel system, ²the optical potential is constructed based on the Feshbath theory and the parameter set 1 and set 2 of the optical potential are investigated. In our research, we assumed that the range parameters Λ_1 and Λ_2 are the same and the interaction between $\pi\Sigma$ - $\pi\Sigma$: V₂₂=0. Our calculated scattering length is consistent with the empirical value at the mass of exchanged boson; 600MeV/c^2 for set 1 and 670MeV/c^2 for set 2. For the coupled channel system, the parameter set 1 are $\Lambda = 3.041 \text{ fm}^{-1}$, $S_{11} = -1.074$, $S_{12} = 0.707$ and $U_0 = -3.063 - i0.466 \text{MeV.fm}^3$ while the parameter set 2 are $\Lambda = 3.395 \text{fm}^{-1}$, $S_{11} = -0.890$, $S_{12} = 0.733$ and $U_0 = -2.476 - i0.428 \text{MeV.fm}^3$.

Keywords: quasi-bound state, the optical potential, \overline{KN} - $\pi\Sigma$ separable potential, $\Lambda(1405)$ resonance

Introduction

The study of the antikaon-nuclei has attracted a significant amount of attention in hadron and nuclear physics communities since over half a century ago. The properties of \overline{K} nuclei can be attributed to the bare $\overline{K}N$ interaction which is strongly attractive. According to a precise experiment of a kaonic

^{1.} Demonstrator, Department of Physics, University of Magway

^{2.} Lecturer, Department of Physics, University of Mandalay

³ Rector (Rtd.), Emeritus Professor, Department of Physics, University

hydrogen, it is suggested that the system of K⁻ and proton has a nuclear bound state which corresponds to I = 0 $\Lambda(1405)$ quasi-bound state lying at the energy 27MeV below the K⁻p threshold. $\Lambda(1405)$ was discovered in 1961 as a broad peak in the $(\pi\Sigma)^0$ invariant mass spectrum when the 1.15GeV/c K⁻ beam passes through a hydrogen bubble chamber, and was attributed to a baryon species with strangeness S = -1, spin-parity J^P =(1/2)⁻, and isospin I = 0. $\Lambda(1405)$ resonance has been interpreted as the quasi-bound state of $\overline{K}N$ embedded in $\pi\Sigma$ continuum. Particle Data Group (PDG) interpreted on the experimental finding of K⁻p bound state that it is located around 1405MeV. It also predicted that the binding energy of $\Lambda(1405)$ is (~27 MeV) below the KN threshold level and has a level width of 50.0 ± 2.0 MeV.

In contrast, chiral dynamics claimed that the $\Lambda(1405)$ is described by a superposition of two resonance states . One state located around 1420 MeV couples mainly to the \overline{K} N channel while the other one sitting around 1390 MeV with a 130 MeV width couples strongly to the $\pi\Sigma$ channel. In accordance with the chiral dynamics model, the binding energy ~15 MeV to 30MeV and width 50.0MeV of $\Lambda(1405)$ are obtained.

It is still a controversial issue about the position of KN quasi bound state whether $\Lambda(1405)$ or $\Lambda(1420)$. Therefore, investigating the parameter sets of $\Lambda(1405)$ is an interesting topic. In our research, the parameter set 1 for $\Lambda(1405)$ which satisfies the Particle Data Group's data and set 2 for $\Lambda(1420)$ which satisfies the Chiral Model's prediction were constructed.

Mathematical Formulation

Our purpose is to investigate the potential parameters of KN interaction which can produce the binding energy and decay width of $\Lambda(1405)$ as well as the scattering length of $\overline{K}N$ interaction. The potential parameters of $\overline{K}N$ system for single channel and the scattering length of $\overline{K}N$ interaction were calculated. Then, the optical potential for $\overline{K}N$ - $\pi\Sigma$ coupled channel system was constructed by using Fesbach Theory. In our calculation, the Yukawa-type separable potential was used.

1. Calculation of Two-Body System for Single Channel

In single channel, the Schrödinger equation of two-body system in terms of separable non-local potential operator can be expressed as:

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\vec{r}) + g(\vec{r})U_0\int d\vec{r}'g(\vec{r}')\psi(\vec{r}') = \frac{\hbar^2}{2\mu}\kappa^2\psi(\vec{r})$$
(1.1)

where $E = \frac{\hbar^2 \kappa^2}{2\mu}$; $\kappa = \text{complex wave vector}$

 $U_0 = \langle 0 | V | 0 \rangle$ = ground state potential

and $g(\vec{r}) =$ the Yukawa type form factor $= \sqrt{\frac{\pi}{2}} \frac{\tilde{\Lambda}^2}{r} e^{-\tilde{\Lambda}r}$; $\tilde{\Lambda} = \sqrt{N}\Lambda$ in which N = 1 for Yukawa-type, N = 2 for expotential-type , $N = \infty$ for Gaussian-type potential and so on.

Here, Λ is the range parameter which depends on the mass of exchanged boson particle, i.e., $\Lambda = \frac{m_B}{\hbar c}$.

Let
$$F = \frac{2S\Lambda^3}{A} \int_0^\infty dr' e^{-\Lambda r'} u(r')$$
 and $S = 2\pi^2 \frac{\mu}{\hbar^2} \Lambda U_0$ is the strength

parameter. Then, equation(1.1) becomes;

$$-\frac{d^2}{dr^2}u(r) + Fe^{-\Lambda r} = \kappa^2 u(r)$$
(1.2)

The solution with outgoing wave boundary condition is obtained by

$$\mathbf{u}(\mathbf{r}) = \mathbf{A} \left(\mathbf{e}^{-\Lambda \mathbf{r}} - \mathbf{e}^{\mathbf{i}\kappa \mathbf{r}} \right)$$
(1.3)

$$\left(\Lambda - i\kappa\right)^2 = -S\Lambda^2 \tag{1.4}$$

This is the relation between the strength parameter and the momentum which means the energy of the $\overline{K}N$ system.

For bound/virtual state, i.e., S<0, the relation between strength parameter and corresponding energy value is $\kappa^2 = -\Lambda^2 \left\{ \sqrt{-S} \pm 1 \right\}^2$,

$$E = -\frac{\hbar^2}{2\mu} \Lambda^2 \left\{ \sqrt{-S} \mp 1 \right\}^2 \left\{ \begin{array}{c} (-) \ bound \ state \\ (+) \ virtual \ state \end{array} \right.$$
(1.5)

For resonance state, i.e. S>0; $\kappa^2 = \left\{-i\Lambda \pm \Lambda\sqrt{S}\right\}^2$

$$E_{\text{Res}} = \frac{\hbar^2}{2\mu} \Lambda^2 (S-1) \mp i \frac{\hbar^2}{2\mu} \Lambda^2 .2\sqrt{S}$$
(1.6)

where, $E_{\text{Res}} = E_{\text{R}} - i \frac{\Gamma}{2}$ and $E_{\text{Res}} = \frac{\hbar^2 \kappa^2}{2\mu}$

$$E_{\rm R} = \frac{\hbar^2}{2\mu} \Lambda^2 (S - 1)$$
 (1.7)

$$\Gamma = \pm \frac{\hbar^2}{2\mu} \Lambda^2 . 4\sqrt{S} \begin{cases} (+) \text{ resonancestate} \\ (-) \text{ anti-resonancestate} \end{cases}$$
(1.8)

For scattering state, the wave function solution of equation(1.2) is

$$u(\mathbf{r}) = A\left(e^{-\Lambda \mathbf{r}}\sin\delta - \sin\left(\kappa \mathbf{r} + \delta\right)\right)$$
(1.9)

where A is the amplitude and δ is the phase shift. The scattering length of the

KN interaction can be derived as below:

$$\therefore a = -\frac{2S}{(1+S)} \cdot \frac{1}{\Lambda}$$
(1.10)

2. Construction of Optical Potential by Feshbach Theory

According to the Feshbach theory, the projection operators are P for channel I and Q for channel II.

$$PHP.P\psi + PVQ\frac{1}{(E-QHQ)}QVP.P\psi = E.P\psi$$
(2.1)

This is the channel I equation for coupled-channel system.

According to Feshbach theory, introducing the optical potential as;

$$U^{opt}(E) = PVP + PVQ \frac{1}{(E-QHQ)} QVP$$

Since $\langle \vec{k}' | U^{opt}(E) | \vec{k} \rangle = g(\vec{k}') U_0^{opt}(E) g(\vec{k})$ (2.2)
 $U_0^{opt}(E) = U_0^I + U_0^{I II} G_{II}(E) U_0^{II I}$ (2.3)

 $G_{II}(E)$ is a loop integral of channel II for coupled channel system and can be written as; $G_{II}(E) = \int d\vec{q} g(q) G_{II}(q,q) g(q)$

$$\therefore \mathbf{G}_{\mathrm{II}}(\mathbf{E}) = -2 \,\pi^2 \,\frac{\mu_{\mathrm{II}}}{\hbar^2} \,\Lambda \left(\frac{\Lambda}{\Lambda - \mathrm{i} \,\kappa'}\right)^2 \tag{2.4}$$

Then, the optical potential equation can be written as;

$$U_0^{\text{opt}}(\mathbf{E}) = U_0^{\text{I}} - \left(2\pi^2 \frac{\mu_{\text{II}}}{\hbar^2} \Lambda\right) U_0^{\text{I} \text{II}} \left(\frac{\Lambda}{\Lambda - i\kappa'}\right)^2 U_0^{\text{II} \text{II}}$$
(2.5)

$$U_{0}^{opt}(E) = U_{0}^{I} - \left(2\pi^{2} \frac{\mu_{II}}{\hbar^{2}}\Lambda\right) U_{0}^{III} \frac{\Lambda^{2} (\Lambda + i\kappa' *)^{2}}{(\Lambda - i\kappa')^{2} (\Lambda + i\kappa' *)^{2}} U_{0}^{III}$$
(2.6)

Since $\kappa' = \kappa'_R + i\kappa'_I$ and $\kappa'^* = \kappa'_R - i\kappa'_I$,

$$\operatorname{Re} U_{0}^{\operatorname{opt}}(E) = U_{0}^{\mathrm{I}} - \left(2\pi^{2} \frac{\mu_{\mathrm{II}}}{\hbar^{2}} \Lambda\right) U_{0}^{\mathrm{I} \mathrm{II}} \frac{\Lambda^{2} \left\{ \left(\Lambda + i\kappa_{\mathrm{I}}^{\prime}\right)^{2} - \kappa_{\mathrm{R}}^{\prime 2} \right\}}{\left\{ \left(\Lambda + i\kappa_{\mathrm{I}}^{\prime}\right)^{2} + \kappa_{\mathrm{R}}^{\prime 2} \right\}^{2}} U_{0}^{\mathrm{II} \mathrm{II}} \qquad (2.7a)$$

$$\operatorname{Im} U_{0}^{\text{opt}}(E) = -\left(2\pi^{2}\frac{\mu_{\text{II}}}{\hbar^{2}}\Lambda\right)U_{0}^{\text{III}}\frac{2\Lambda^{2}\kappa_{\text{R}}'(\Lambda+i\kappa_{\text{I}}')}{\left\{\left(\Lambda+i\kappa_{\text{I}}'\right)^{2}+\kappa_{\text{R}}'^{2}\right\}^{2}}U_{0}^{\text{IIII}}$$
(2.7b)

The above two equations are the real and imaginary parts of the optical potential for channel I, i.e., $\overline{K}N$ channel.

In addition, the potential parameter of the optical potential can be written as;

$$\mathbf{S}^{\text{opt}}(\mathbf{E}) = \mathbf{S}_{\text{I}} - \mathbf{S}_{\text{I}\,\text{II}} \left(\frac{\Lambda}{\Lambda - i\kappa'}\right)^2 \mathbf{S}_{\text{II}\,\text{I}}$$
(2.8)

$$\mathbf{S}^{\text{opt}}(\mathbf{E}) = \mathbf{S}_{\text{I}} - \mathbf{S}_{\text{I} \text{II}} \frac{\Lambda^2 (\Lambda + i\kappa' *)^2}{(\Lambda - i\kappa')^2 (\Lambda + i\kappa' *)^2} \mathbf{S}_{\text{II} \text{II}}$$

We get the real and imaginary parts of the strength parameter of that equation.

Re S^{opt}(E) = S_I - S_{III}
$$\frac{\Lambda^2 \left\{ \left(\Lambda + i\kappa'_I \right)^2 - \kappa'_R^2 \right\}}{\left\{ \left(\Lambda + i\kappa'_I \right)^2 + \kappa'_R^2 \right\}^2} S_{III}$$
 (2.9a)

Im S^{opt}(E) =
$$-S_{III} \frac{2\Lambda^2 \kappa'_R (\Lambda + i\kappa'_I)}{\{(\Lambda + i\kappa'_I)^2 + {\kappa'_R}^2\}^2} S_{III}$$
 (2.9b)

where, $E = \frac{\hbar^2}{2\mu_I} \kappa^2 = \frac{\hbar^2}{2\mu_{II}} {\kappa'}^2 - \Delta M$ and $\Delta M \approx 103 MeV/c^2$ is the threshold

mass difference. It is note that $\kappa = -\kappa$ if Im $\kappa < 0$ for channel I (\because Im $\kappa > 0$ for bound state) and $\kappa' = -\kappa'$ if Im $\kappa > 0$ for channel II (\because Im $\kappa < 0$ for virtual state). It is also assumed that $\Lambda_1 = \Lambda_2 = \Lambda$, $S_{12} = S_{21}$ and the potential of channel II $U_0^{II} = 0$. In constructing a phenomenological potential, to determine the parameters of the potential is very important. Thus, the strength parameters and scattering length of the optical potential for channel I in coupled-channel system.

By applying the potential parameter set 1 and set 2 which satisfy the PDG data and chiral group's data, binding energy and level width of $\Lambda(1405)$ were also numerically determined with the use of power inverse iteration method. Since the parameters are complex value, the real part of energy eigen value gives the binding energy of $\overline{K}N$ system and the imaginary part gives the level width of $\Lambda(1405)$ resonance, respectively.

Results and Discussion

In our research, the parameter set 1 for $\Lambda(1405)$ which satisfies the Particle Data Group's data and set 2 for $\Lambda(1420)$ which satisfies the Chiral Model's prediction are constructed. Firstly, the potential parameters for single channel are calculated by solving the Schrödinger equation with Yukawa-type separable potential. The scattering length of \overline{KN} interaction is also calculated.

According to the results of single channel calculation, the strength parameter set 1 are S = -1.527 - i0.233 and U = -3.063 - i0.466 while the strength parameter set 2 are S = -1.384 - i0.238 and U = -2.476 - i0.428.

To compute the potential parameters for the coupled-channel system, assuming that the exchanged particles of channel I and channel II are the same, i.e., $\Lambda_1 = \Lambda_2 = \Lambda$, and the interaction between $\pi\Sigma - \pi\Sigma$: $V_{22} = 0$ and varying the mass of boson exchanged particles, potential parameters and scattering length are obtained which are summarized in table 1 and table 2. We have selected the potential parameter set 1 and set 2 whose scattering lengths are consistent with the experimental scattering length is consistent with experimental value at the boson energy mass $m_B = 600 \text{ MeV/c}^2$ for parameter set 1 and at $m_B = 670 \text{ MeV/c}^2$ for parameter set 2. Our calculated results are summarized in table 3.

With the single channel potential parameter set 1 and set 2, binding energies and level widths of $\overline{K}N$ system are determined by solving the Schrödinger equation numerically with Gaussian basis treatment. To obtain the energy eigen value, power inverse iteration method is used. Our calculated results are compared with other theoretical and experimental results, which are illustrated in table 4. It is found that our calculated scattering length and energy are in good agreement with experimental and other theoretical results. Table 1: The parameters sets 1 for $\Lambda(1405)$ varying with the masses of exchanged bosons (BE = $27 MeV/c^2$, level width = $25.0 MeV/c^2$, $S_{12} = S_{21}$ and $S_{22} = 0.0$)

M _B (MeV/c ²)	Λ (fm ⁻¹)	S ^{opt}	S ₁₁	S ₁₂	U ₀ for channel I (MeV.fm ³)	$a^{I=0}_{\ \overline{K}N}$ (fm)
140.0	0.710	-3.943 -i1.629	-4.224	1.676	-33.900 -i14.010	-3.552 +i0.406
280.0	1.420	-2.249 -i0.608	-1.852	0.892	-9.665 -i2.615	-2.322 +i0.444
400.0	2.029	-1.827 -i0.383	-1.381	0.772	-5.498 -i1.151	-1.969 +i0.454
500.0	2.534	-1.644 -i0.290	-1.191	0.730	-3.958 -i0.698	-1.808 +i0.458
600.0	3.041	-1.527 -i0.233	-1.074	0.707	-3.063 -i0.466	-1.702 +i0.461
610.0	3.091	-1.518 -i0.228	-1.065	0.705	-2.995 -i0.450	-1.693 -i0.461
620.0	3.142	-1.509 -i0.224	-1.056	0.703	-2.929 -i0.434	-1.685 -i0.461
630.0	3.193	-1.500 -i0.220	-1.048	0.702	-2.865 -i0.419	-1.677 -i0.461
640.0	3.243	-1.492 -i0.215	-1.039	0.700	-2.805 -i0.405	-1.669 -i0.461
650.0	3.294	-1.483 -i0.212	-1.031	0.699	-2.746 -i0.392	-1.661 -i0.461
700.0	3.547	-1.446 -i0.194	-0.996	0.692	-2.486 -i0.333	-1.627 +i0.462
770.0	3.902	-1.403 -i0.174	-0.954	0.685	-2.192 -i0.271	-1.586 +i0.463
800.0	4.057	-1.386 -i0.166	-0.939	0.682	-2.085 -i0.250	-1.571 +i0.463
900.0	4.564	-1.341 -i0.145	-0.896	0.675	-1.793 -i0.194	-1.528 +i0.464

Experimental value of scattering length [5], $a^{I=0} = -(1.70 \pm 0.07) + i(0.68 \pm 0.04)$

522 -	. 0.0)					
$\frac{M_B}{(MeV/c^2)}$	Λ (fm ⁻¹)	S ^{opt}	S ₁₁	S ₁₂	U ₀ for channel I (MeV.fm ³)	$a^{I=0}_{\bar{K}N}$ (fm)
140.0	0.710	-3.202 -i1.792	-3.615	1.853	-27.526 -i15.402	-3.589 +i0.627
280.0	1.420	-1.977 -i0.689	-1.579	0.954	-8.499 -i2.964	-2.372 +i0.679
400.0	2.029	-1.658 -i0.439	-1.188	0.817	-4.989 -i1.322	-2.024 i0.692
500.0	2.534	-1.517 -i0.335	-1.033	0.770	-3.651 -i0.807	-1.864 +i0.697
600.0	3.041	-1.425 -i0.270	-0.937	0.745	-2.859 -i0.542	-1.759 +i0.700
650.0	3.294	-1.391 -i0.247	-0.908	0.736	-2.575 -i0.456	-1.719 +i0.701
660.0	3.345	-1.384 -i0.242	-0.896	0.735	-2.524 -i0.442	-1.712 +i0.702
670.0	3.395	-1.384 -i0.238	-0.890	0.733	-2.476 -i0.428	-1.704 +i0.702
680.0	3.446	-1.372 -i0.234	-0.884	0.732	-2.429 -i0.414	-1.698 +i0.702
690.0	3.497	-1.367 -i0.230	-0.878	0.730	-2.384 -i0.401	-1.691 +i0.702
700.0	3.547	-1.361 -i0.226	-0.873	0.729	-2.340 -i0.389	-1.685 +i0.702
770.0	3.902	-1.327 -i0.203	-0.839	0.721	-2.074 -i0.317	-1.644 +i0.703
800.0	4.057	-1.314 -i0.194	-0.827	0.718	-1.976 -i0.293	-1.629 +i0.703
900.0	4.564	-1.277 -i0.170	-0.792	0.711	-1.708 -i0.228	-1.586 +i0.704

Table 2: The parameters set 2 varying with the masses of exchanged bosons (BE = 15.0MeV/c^2 , level width = 25.0 MeV/c^2 , $S_{12} = S_{21}$, $S_{22} = 0.0$)

Experimental value of scattering length [5], $a^{I=0} = -(1.70 \pm 0.07) + i(0.68 \pm 0.04)$

	m _B (MeV/c ²)	Λ (fm ⁻¹)	S ^{opt}	S ₁₁	S_{12}	U ₀ for channel I (MeV.fm ³)
Parameter	600.0	3 0/1	-1.527	1.074	0 707	-3.063
set 1	000.0	5.041	-i0.233	-1.074	0.707	-i0.466
Parameter	670.0	2 205	-1.384	0.800	0.733	-2.476
set 2	070.0	5.595	-i0.238	-0.890	0.755	-i0.428

Table 3 : Our calculated results

 Table 4: Comparison of our calculated results and other theoretical and experimental results

	$\Lambda(\mathrm{fm}^{-1})$	a ^{I=0} (fm)	$\frac{\text{BE-i}\frac{\Gamma}{2}}{(\text{MeV})}$
Y. Akaishi and T. Yamazaki for Λ(1405) [6]	3.90	- 1.76 + i0.46	-27.0 - i20
Thida Oo for Λ(1405) [7]	3.91	- 1.67 + i0.42	-26.84 - i19.93
PDG for Λ(1405) [3]	-	-	$\sim -27.0 - i25.0 \pm 1.0$
Chiral prediction for $\Lambda(1420)$ [4]	-	-	~15 - i25.0
Experimental value of scattering length [5]	-	- (1.70 ± 0.07) + $i(0.68 \pm 0.04)$	-
Our calculated parameter set 1 for $\Lambda(1405)$	3.04	- 1.702 + i0.461	-26.76 - i24.84
Our calculated parameter set 2 for $\Lambda(1420)$	3.40	- 1.698 + i0.702	-14.77 - i24.80

Acknowledgements

Author gratefully acknowledges to Dr Khin Swe Myint, Rector (Rtd.), Emeritus Professor, Department of Physics, University of Mandalay, for her excellent advice, kindness and valuable discussion throughout this research.

Author also thanks to Professor Dr Lei Lei Win, Head of Department of Physics, Professor Dr Kalyar Thwe and Professor Dr Yee Yee Oo, Department of Physics, University of Mandalay, for their permission, and valuable discussion.

Author deeply expresses her gratitude to her supervisor, Dr Thida Wint, lecturer, Department of Physics, University of Mandalay, for her patience, kindness, excellent advice and continuous guidance throughout this research work.

References

- A.D. Martin, Nucl. Phys. B 179 (1981)33
- K.A. Olive et al., "Particle Data Group", Chin. Phys. C 38(2014)090001.
- M. Iwasaki et al., Phys. Rev. Lett. 78 (1997)3067;
- M. H. Alston et al., Phys. Rev. Lett 6 (1961) 698.
- Thida Oo, "PhD Thesis", University of Mandalay (2010)
- T. Hyodo, "Proceeding of Sendai International Symposium" (2008).
- T. M. Ito et al., Phys. Rev. C 58 (1998) 2366.
- Y. Akaishi, T. Yamazaki, Phys. Rev. C 65 (2002) 044005.

SYNTHESIS AND CHARACTERIZATION OF COPPER ZINC SULPHIDE (CuZnS₂) THIN FILMS

May Thawda Phoo¹, Nwe Wai²

Abstract

The Copper Zinc Sulphide (CuZnS₂) films were fabricated with and without complexing agents (EDTA and TEA) by chemical bath deposition method. Incorporation of complexing agents provided the higher optical absorption, lower band gap energy, and smoother surface of CuZnS₂ thin films. In addition, varying the concentration of precursor solution (0.5 - 1.5 M) and dipping time (24 - 72 hrs) the optical property and surface topography of thin films were investigated. The concentration (0.5 M) and dipping time (48 hrs) provided the lower band gap energy of 2.0 eV and RMS surface roughness of 0.93 µm which are key requirements for light absorber layer in solar cells.

Keywords: CuZnS₂, chemical bath deposition method, complexing agents, band gap energy

Introduction

A solar cell or photovoltaic cell (previously termed "solar battery"), is an electrical device that converts the energy of light directly into electricity by the photovoltaic effect, which is a physical and chemical phenomenon. It is a form of photoelectric cell, defined as a device whose electrical characteristics, such as current, voltage, or resistance, vary when exposed to light. Solar cells are the building blocks of photovoltaic modules, otherwise known as solar panels. Solar cells are described as being photovoltaic, irrespective of whether the source is sunlight or an artificial light. They are used as a photo detector (for example infrared detectors), detecting light or other electromagnetic radiation near the visible range, or measuring light intensity. The operation of a photovoltaic (PV) cell requires three basic attributes: (1). the absorption of light, generating either electron-hole pairs or exactions. (2) the separation of charge carriers of opposite types. (3) the separate extraction of those carriers to an external circuit.

The thin films technology has attracted much attention because of its unique size dependent properties and applications in the optoelectronic

¹ Demonstrator, Department of Physics, Magway University

² Lecturer, Department of Physics, Magway Uiversity

devices, solar cell, sensors and laser materials. The preparation of copper zinc sulphide (CuZnS₂) thin film by chemical bath deposition technique is currently attracting a great deal of attention as the technique is relatively simple and cost effective, has minimum material wastage, does not need sophisticated instrument and vacuum and can be applied in large area deposition at low temperature. The chemical bath deposition method uses a controlled chemical reaction to deposit a thin film. In typical experimental approach, the substrates are immersed in solution containing the chalcogenide source, metal ion and complexing. Copper Zinc Sulphide (CuZnS₂) thin film has absorb highly in the UV and near infrared wavelength. CuZnS₂ thin film can only allow visible radiation to be transmitted through the glazing system into the building if these films are used in coating the glazing. CuZnS₂ thin films can be called solar transmitting films (STF) such as films can also be used to anti-reflect solar radiation falling on and passing through solar collector glazing onto absorber plates in photo-thermal solar energy devices. The application of CuZnS₂ thin film are good materials for glazing system, poultry buildings, anti-reflection coatings, eyeglasses and solar cells fabrication[1].

Experiment

In the elementary state of my work, cleaning process totally play a vital role which includes four steps from washing with detergent and ending at cleaning stage with Isopropanol Alcohol (IPA). Firstly, we cleaned the glass substrates with ultrasonic cleaner in distilled water. Subsequently, it was being washed with acetone and IPA in order to ensure the cleaning purpose that can affect to my research. In making solution setup, 5 ml of Zinc chloride (ZnCl₂) and 5 ml of Copper chloride (CuCl₂) were measured, transferred into the beaker. The mixture was stirred for 10 minutes after which 10 ml Thiourea (NH₂)₂CS was added and stirred to have a homogeneous mixture. Addition of Thiourea formed a jelly – like solution, 5 ml of EDTA (Na₄ (C₁₀H₁₆N₂O₈)), 3 ml of TEA (C₆H₁₅NO₃) and 3 ml of Ammonia (NH₃) solution were added to the mixture. The solution was stirred for 15 minutes followed by addition of 20 ml of distilled water. The final solution was stirred to have a homogeneous mixture. At 6 hours, the film had no deposit. They were allowed to stand for 12 hours after which

deposition was noticed on the film. The remaining films were allowed to stand for 24 hours, 48 hours, 72 hours, The substrates were removed at the end of each time, dried in air at room temperature. They were then annealed at 672 K for 1 hour to obtain adherent copper zinc sulphide (CuZnS₂) transparent thin films.

Results and Discussions

The absorption spectrum of the Copper Zinc Sulphide (CuZnS₂) films were plotted Absorbance against wavelengths is presented in figure 1. The values are 0.39 at 300 nm for CuZnS₂ (with complexing agent) and 0.15 at 370 nm for CuZnS₂ (without complexing agent). The absorbance of copper zinc sulphide (CuZnS₂) thin film with complexing agents is higher than without complexing agents. This higher absorption may be due to the formation of more CuZnS₂ with better adhesion to the substrates under this condition.

The absorbance of the specimens plotted against wavelengths are presented in figure 2 It is observed that the spectral absorbance of the specimens vary with wavelength in similar manner, increasing rapidly from a value of about 0.20 at 280 nm to various maximum values of 0.4 at 355 nm for CuZnS₂ (0.5 M), 0.39 at 300 nm for CuZnS₂ (1.0 M) and 0.29 at 325 nm for CuZnS₂ (1.5 M) and then decreased to a minimum values of 0.27 at 550 nm for CuZnS₂ (0.5 M), 0.12 at 400 nm for CuZnS₂ (1.0 M) and 0.26 at 460 nm for CuZnS₂ (1.5 M). So, we can conclude that 0.5 M concentration of CuZnS₂ films gives the highest absorbance.



Figure 1: Absorbance (A) as a function of wavelength for Copper Zinc Sulphide (CuZnS₂) thin film





The changes of absorption of Copper Zinc Sulphide $(CuZnS_2)$ film on different dip time are wondered. So, the absorption spectrum of the Copper Zinc Sulphide $(CuZnS_2)$ films were plotted Absorbance against wavelengths is presented in figure 3. As shown in figure 3, we observed that 48 hours dip time CuZnS₂ film possessed the highest absorption peak while the 72 hours dip time CuZnS₂ film gave the lowest absorption peak. The absorption peak of 24 hours dip time CuZnS₂ film obtained the middle trend.

The graph of $(Ah\upsilon)^2$ against h υ are shown in figure 4. The band gap energy can be determined by extrapolation of $(Ah\upsilon)^2$ against h υ . The band gap energy value of Coppr Zinc Sulphide (CuZnS₂) thin film for without complexing agent is 2.1 eV. As a result, we observed that the copper zinc sulphide (CuZnS₂) film without complexing agents provided the lower band gap energy than the copper zinc sulphide (CuZnS₂) films.



Figure 3: Absorbance (A) as a function of wavelength for Copper Zinc Sulphide (CuZnS₂) thin film for different dip time



Figure 4: Plot of $(Ahu)^2$ vs hu for Copper Zinc Sulphide (CuZnS₂) thin film

The graph of $(Ah\nu)^2$ against h ν are shown in figure 5. The band gap energy can be determined by extrapolation of $(Ah\nu)^2$ against h ν . CuZnS₂ (0.5 M) increasing from a value is 1.7 eV to various maximum values 2 eV, CuZnS₂ (1.0 M) increasing from value is 2.5 eV to 2.7 eV and CuZnS₂ (1.5 M) increasing from value is 1.5 eV to 2.4 eV. The direct band gaps were extrapolated from the graph at $\alpha^2 = 0$, and the values obtained are 2eV for CuZnS₂ (0.5 M), 2.7eV for CuZnS₂ (1.0 M) and 2.1eV for CuZnS₂ (1.5 M).

The graph of $(Ah\upsilon)^2$ against h υ are shown in Figure 6. The band gap energy can be determined by extrapolation of $(Ah\upsilon)^2$ against h υ . CuZnS₂ (24 hrs) increasing from a value is 2.4 eV to various maximum values 2.7 eV, CuZnS₂ (48 hrs) increasing from a value is 1.8 eV to various maximum values 2 eV and CuZnS₂ (72 hrs) increasing from a value is 1.7 eV to various maximum values 2.3 eV. The direct band gaps were extrapolated from the graph at $\alpha^2 = 0$, and the values obtained are 2.7 eV for CuZnS₂ (24 hrs), 2 eV for CuZnS₂ (48 hrs), and 2.3 eV for CuZnS₂ (72 hrs).



Figure 5: Plot of $(Ah\upsilon)^2$ vs h υ for Copper Zinc Sulphide (CuZnS₂) thin film


Figure 6: Plot of $(Ahu)^2$ vs hu for Copper Zinc Sulphide (CuZnS₂) thin film

7 11 1	D I	• 41	•	1 1 7 1	$(\mathbf{n} \mathbf{n} \mathbf{n})$	41 * 0*1
I ONIA I ·	Rond a	on anarmae the	CONNER 7100	Guinhida	(1 n n n n n)	thin tilme
Laure L.	Danu 2	ad unu 2103 unu		Sulphiuc		111111 1111113

No	Туре	Band Gap Energy (eV)	Reference Band Gap Energy (eV)
1	Without Complexing agents	2.1	2.0 - 2.7
	With complexing agents	2.0	
2	0.5 M	2.0	
	1.0 M	2.7	
	1.5 M	2.1	
3	24 hrs dip time	2.7	
	48 hrs dip time	2.0	
	72 hrs dip time	2.3	

The topography of $CuZnS_2$ film was studied by using Atomic Force Microscope (AFM). The AFM images of the $CuZnS_2$ thin films grown on glass substrate are presented in Figure 7. Average roughness is the arithmetic average of the absolute values of the profile height deviations, within the sampling length. Root mean square average of the profile height deviations within the sampling length. The root mean square roughness value of $CuZnS_2$ thin films are 0.1714 µm for without complexing agent and 0.1321µm for with complexing agent.

The topography of $CuZnS_2$ film was studied by using Atomic Force Microscope (AFM). The AFM images of the $CuZnS_2$ thin films grown on glass substrate are presented in Figure 8. Average roughness is the arithmetic

average of the absolute values of the profile height deviations, within the sampling length. Root mean square average of the profile height deviations within the sampling length. The root mean square roughness value of $CuZnS_2$ thin films are 0.1321 µm for (0.5 M), 0.2043 µm for (1.0 M) and 0.1691 µm for (1.5 M). The roughness value of $CuZnS_2$ film was measured over the scanning areas (50.0 µm × 50.0 µm). The root mean square roughness value of $CuZnS_2$ thin film is 0.2043 µm.

The topography of CuZnS₂ film was studied by using Atomic Force Microscope (AFM). The AFM images of the CuZnS₂ thin films grown on glass substrate are presented in Figure9. Average roughness is the arithmetic average of the absolute values of the profile height deviations, within the sampling length. Root mean square average of the profile height deviations within the sampling length. The root mean square roughness value of CuZnS₂ thin film are 173.70 nm for 24 hrs, 93.25nm for 48 hrs and 80.30 nm for 72 hrs. The average roughness value of CuZnS₂ thin film are 135.0 nm for 24 hrs, 71.5 nm for 48 hrs and 55.9 nm for 72 hrs. The roughness value of CuZnS₂ film was measured over the scanning areas (30.0 μ m × 30.0 μ m). The root mean square roughness value of CuZnS₂ thin film is 80.30 nm.



(a)



(b)

Figure 7: Atomic force microscopy images of Copper Zinc Sulphide $(CuZnS_2)$ thin film (a) without complexing agent (b) with complexing agent



(a)



(b)



(c)

Figure 8: Atomic force microscopy images of Copper Zinc Sulphide $(CuZnS_2)$ thin film for different concentration (a) 0.5 M (b) 1.0 M (c) 1.5 M



(a)



(b)



(c)

Figure 9: Atomic force microscopic images of Copper Zinc Sulphide (CuZnS₂) thin film for different deposition time (a) 24 hrs (b) 48 hrs (c) 72 hrs

Conclusion

The Copper Zinc Sulphide (CuZnS₂) films were fabricated with and without complexing agents (EDTA and TEA) by chemical bath deposition method. The CuZnS₂ film with complexing agents provided the higher optical absorption and band gap energy than that film of without complexing agents. Therefore, different concentration (0.5 M, 1.0 M, and 1.5 M) and different dip time (24 hrs, 48 hrs, and 72 hrs) were studied with complexing agents. 0.5 M CuZnS₂ film and 48 hrs dip time CuZnS₂ films gave the highest absorption and lowest band gap energies and smoother surface in each other concentration and dip times. The root mean square (RMS) roughness of CuZnS₂ films for different concentrations increased with increasing concentration while the root mean square (RMS) roughness of those films decreased with increasing the deposition time. The concentration (0.5M) and dipping time (48hrs) provided the lower band gap energy of 2.0eV and RMS surface roughness of 0.93 μ m which are key requirements for light absorber layer in solar cells.

Acknowledgements

Author gratefully acknowledges to Rector Dr Khin Mg Oo, Pro-rector, Dr Win Soe, Magway University and Professor and Head Dr Nay Win Oo, Department of Physics, Magway University for their encouragement to do this research.

References

C.C.Uhuegbu et.al., Am.J.Sci.Ind.Res, 1 (2010) 397

C.C.Uhuegbu, Sol.Cells.Ind.Appl, 1 (2007) 1

C.C.Uhuegbu et.al., Turk.J.Phys, 32 (2008) 39

K.C.Preetha et.al., Mater.Sci.Eng, 73 (2015) 1

I.A.Ezenwa et.al., Eu.Open.Appl.J, 1 (2015) 1

https://en.m.Wikipedia.org/wiki/solar cells

www.allaboutvision.com/ lenses / anti-reflective.htm