STRUCTURAL AND ELECTRICAL PROPERTIES OF LITHIUM DOPED ZINC OXIDE

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Abstract

Lithium doped zinc oxide (Zn_{1-x} Li_x O) compound is a transparent conducting oxide. According to the stoichiometric compositions, the high purity of zinc oxide and lithium oxide powders were mixed and grinded to obtain the lithium doped zinc oxide compound. This compound was prepared at pre-sintering temperature 800˚C for 2 h and final-sintering temperature 900˚C for 2 h by solid state method. The crystalline properties of lithium doped zinc oxide compound were investigated by X-ray diffraction (XRD). From XRD results, the crystal structure of this compound can be concluded hexagonal structure. And then the electrical properties of this compound were studied.

Key words: sample preparation, XRD result, resistivity and conductivity measurement

Introduction

A ceramic is a material that is neither metallic nor organic. It may be crystalline, glassy or both crystalline and glassy (Robynl. Johnson). Ceramics are favored for many sensors application because of their wide availability, low cost, and convenient fabrication. Ceramics materials are used in electronics because depending on their composition, they can be semiconducting, superconducting, ferroelectric, or an insulator. They have electrical, optical and magnetic properties of value in the computer and electronic industries (Isabelle Robinson, 2019). At room temperature, zinc oxide has a direct-band-gap 3.3eV. ZnO is a wide band gap oxide semiconductor with hexagonal crystal structure (Schmidt-Mende *et al.,* 2007-05-01). This material seems very promising for low-voltage and short wavelength electro- optical devices such as laser and light emitting diodes; and also, for another application such as ultraviolet absorber films, varistors and gas sensors (Boshra Ghanbari Shohany & Ali Khorsand Zak, 2020). ZnO nanostructures have found uses in environmental, technological and biomedical purposes including ultrafast optical functions, dye-sensitized solar cells, lithium-ion batteries (Zhang Lin Wang 2004). In this work, lithium doped zinc oxide powders have been synthesized by the conventional solid state reaction method. As prepared and heated powders were characterized by X-ray diffraction (XRD) method. The XRD result shows the structure, crystallite size and lattice parameters of this compound. The thermoelectric effects of pellet samples were investigated at various temperature of lithium (0.607g) doped zinc oxide (19.392g) samples had been calculated. And then the electrical properties of this compound were studied by the resistivity and conductivity measurement.

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Materials & Methods

1. Sample Preparation

First of all, 0.1 mole of Li_2O and 0.9 mole of ZnO were used to produce 1 mole of $Zn_{1-x}Li_xO$. $Zn_{1-x}Li_xO$ ceramic compound was prepared by using the lithium oxide and zinc oxide powder. These oxides were mixed according to their mix and weight the required amount of the samples was grind with a few drops of ethanol by using an agate motor for 1 h. And then, the required amount of the samples was grind adding a few drops of ethanol in the beaker. After that, the mixture powder was heated onto the hot plate with 100˚C by stirring with a glass rod for 30 minutes and then cooled at the room temperature. To obtain the homogeneous powder, the mixed powder was ground by ball milling machine. The mixture was pre-sintered at 800˚C for 2 h in an electrical furnace and then cooled down to room temperature.

2. Pellet Sample Preparation

The mixture powder was ground by an agate motor for 1 h. The powder was pressed into pellet by hydraulic pellet maker at a pressure of ~ 30 tons. The final-sintering was performed at 900˚C for 2 h in an electrical furnace. The dimension of sample was 1.53cm in diameter and 0.452cm in thickness. The phase formation and electrical properties of final-sintered pellet sample were investigated by using XRD, electrical resistivity and conductivity measurement. The process of the sample preparation has shown in Figure-1.

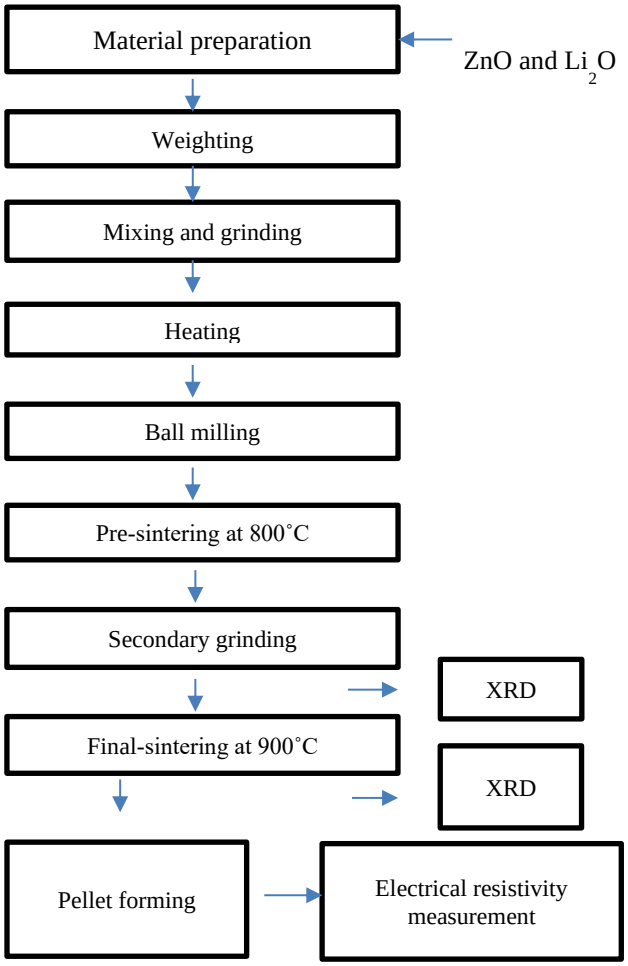

Figure-1 Process of sample preparation

Structural Analysis of XRD

Lithium doped zinc oxide ($Zn_{1-x}Li_xO$) sample has been prepared by solid state method. The phase formation of the pre-sintered sample was checked by using X-ray diffractometer. The XRD spectrum of the pre-sintered sample is shown in Figure-2. According to the XRD characterizations of the pre-sintered sample, it is confirmed that sample has been successfully formed hexagonal structure. The average crystallite size and average lattice parameter in Table-1 and Table-2.

The phase formation of the final-sintered sample has been checked by using X-ray diffractometer. The XRD spectrum of the final-sintered sample is shown in Figure-3. According to the XRD characterizations of the final-sintered sample, it is confirmed that sample has been successfully formed hexagonal structure. The average crystallite size and average lattice parameter in Table-3 and Table-4.

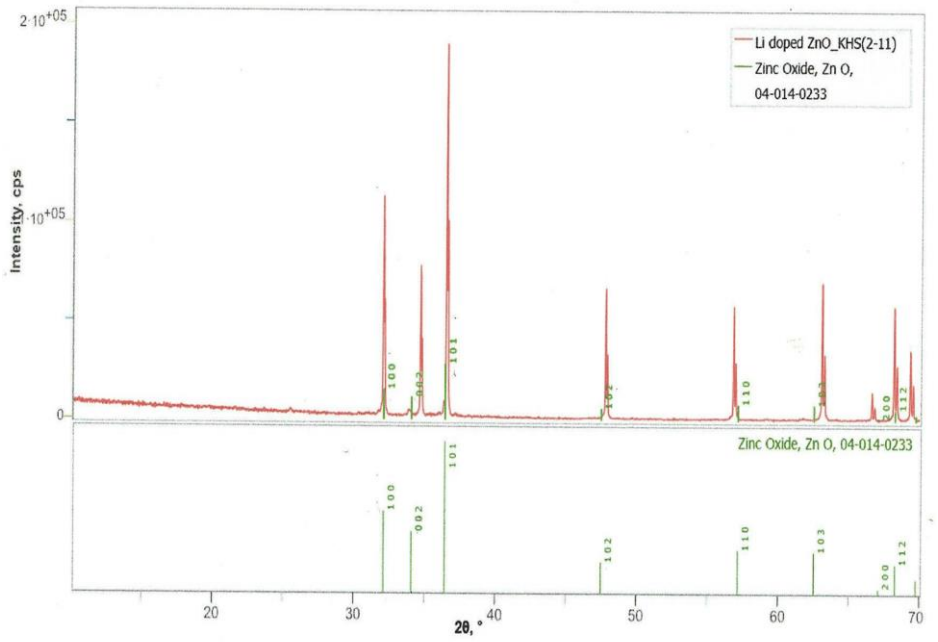

Figure-2 XRD diffractogram for pre-sintered Zn_{1-x} Li_x O powder

Table-1 Crystallite size of planes of Zn_{1-x} Li_x O powder

Plane	FWHM~B (deg)	Peak width B (rad)	2θ (deg)	Cosθ	Size D (nm)
100	0.159	0.0027	32.043	0.961	51.956
002	0.153	0.0026	34.699	0.955	54.377
101	0.160	0.0028	36.527	0.949	52.146
102	0.158	0.0027	47.806	0.914	54.963
110	0.160	0.0027	56.853	0.879	56.538
103	0.159	0.0027	63.106	0.852	58.793
200	0.159	0.0027	66.621	0.835	59.681
112	0.166	0.0028	68.195	0.828	57.943
Average crystallite size					55.799

Table-2 Lattice parameter of each plane of Zn_{1-x} Li_x O powder

Line	Interplanar spacing d (Å)	hkl	a(Å)	c(Å)
1	2.7909	100	3.223	-
2	2.5831	002	-	5.167
3	2.4689	101	3.22	5.2707
4	1.9010	102	3.166	5.198
5	1.6181	110	3.236	-
6	1.4720	103	3.092	5.1987
7	1.4026	200	3.239	-
8	1.3740	112	3.217	5.267
Average lattice parameter			3.1989	5.2203

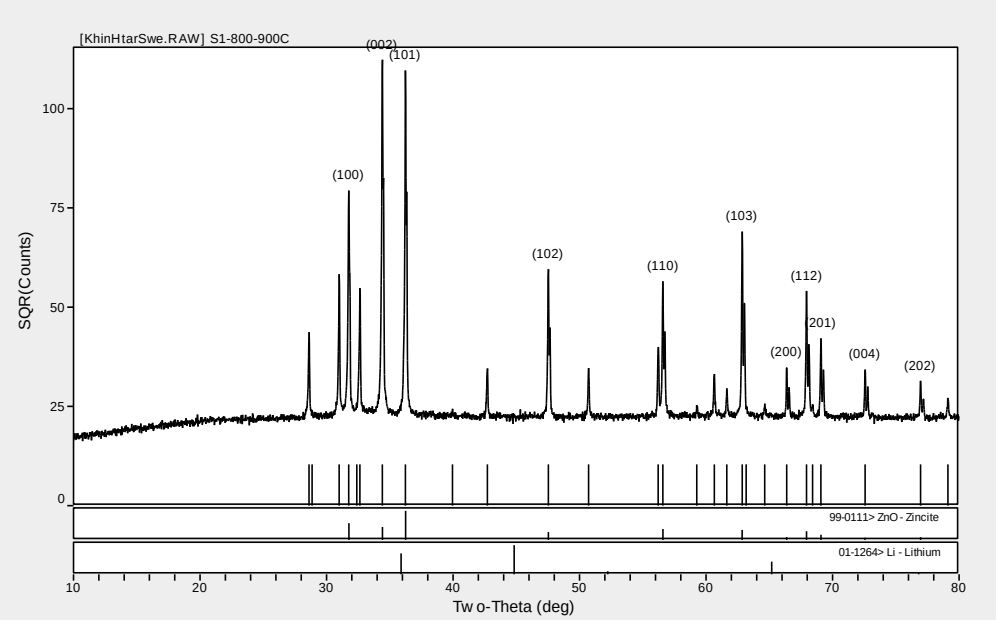

Figure-3 XRD diffractogram for final–sintered Zn_{1-x} Li_x O pellet

Table-3 Crystallite size of each plane of Zn_{1-x} Li_x O pellet

Plane	FWHM~B (deg)	Peak width B (rad)	2θ (deg)	Cosθ	Size D (nm)
100	0.122	0.0021	31.760	0.961	67.71
002	0.126	0.0021	34.417	0.955	66.08
101	0.160	0.0027	36.242	0.951	52.2
102	0.111	0.0019	47.536	0.915	78.49
110	0.114	0.0019	56.583	0.880	79.14
103	0.104	0.0018	62.859	0.853	89.52
200	0.106	0.0018	66.379	0.837	89.58
201	0.105	0.0018	69.082	0.842	91.85
Average crystallite size					76.8211

Table-4 Lattice parameter of each plane of Zn_{1-x} Li_x O pellet

Line	Interplanar spacing d (Å)	hkl	a(Å)	c(Å)
1	2.8151	100	3.2505	-
2	2.6036	002	-	5.207
3	2.4766	101	3.2401	5.1987
4	1.9112	102	3.2504	5.204
5	1.6252	110	3.2503	-
6	1.4772	103	3.2478	5.206
7	1.4071	200	3.249	-
8	1.3585	201	3.249	5.212
Average lattice parameter			3.2481	5.2055

Electrical Resistances Measurement

At first, the dimensions (thickness and diameter) of the sintered pellet sample were measured by Vernier-Caliper. The dimensions of the sample were 1.53cm in diameter and 0.452 cm in thickness.

Temperature dependent electrical resistances of sample were observed in the temperature range of 638K-703K. Photograph showing the experimental set up the temperature dependent electrical resistivity measurement is shown in Figure-4. Temperature dependent resistances of the sample were measured by using Lutron LCR-9073 digital meter. K-type thermocouple was used as the temperature sensor throughout the measurement. The copper block holder was heated by 1000 W heater with 500˚C.The electrical conductivity of the sample have been calculated by using formula, $\sigma = \frac{l}{RA}$.

Figure-4 Temperature dependent electrical resistances measurement

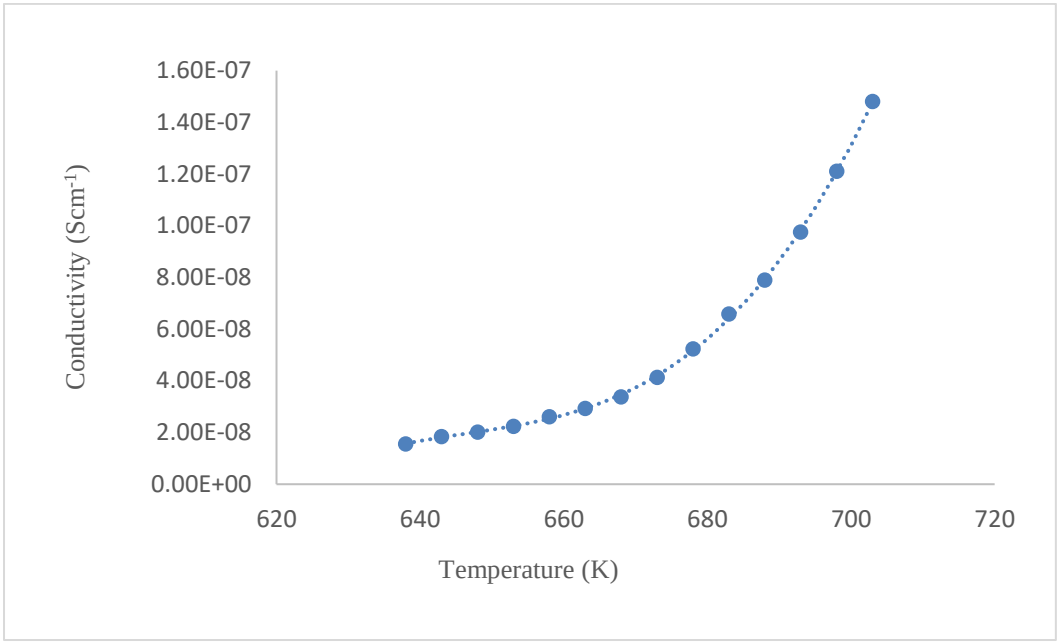

Figure-5 Plot of temperature dependent electrical conductivity curve of ($Zn_{1-x}Li_xO$) pellet

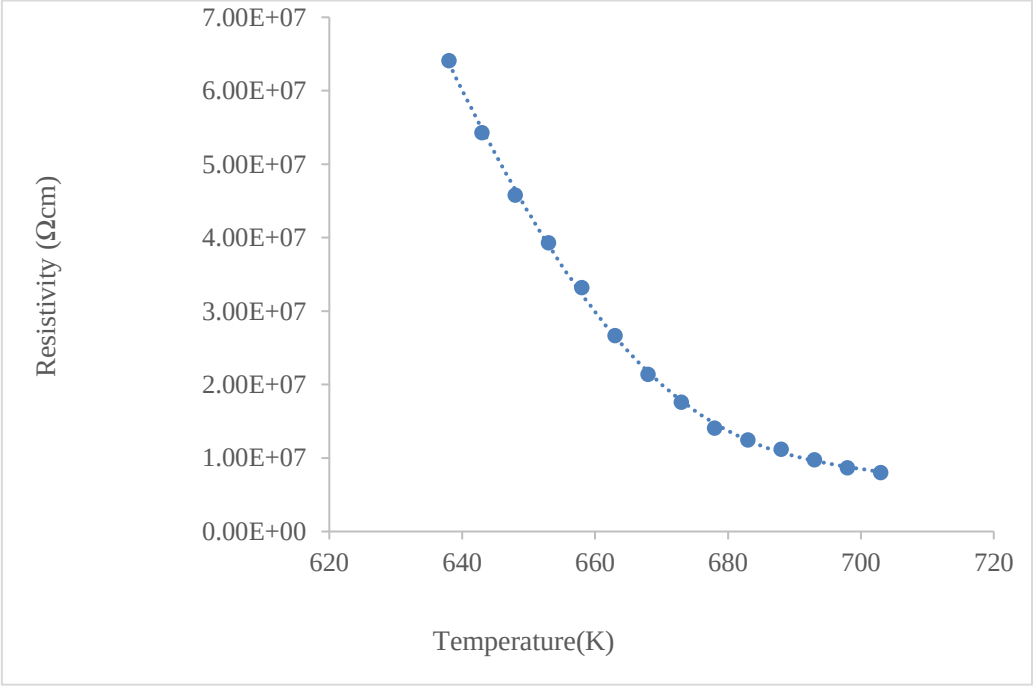

Figure-6 Plot of temperature dependent electrical resistivity curve of ($Zn_{1-x}Li_xO$) pellet

Discussion

Lithium doped zinc oxide (Zn_{1-x} Li_x O) powder has been prepared by solid state method in this result. The XRD investigation, the samples have been successfully formed typical hexagonal structure after the counter diffusion reaction of the metal oxides at pre-sintering temperature of 800˚C and final-sintering temperature of 900˚C. The average lattice parameter and average crystallite size have been calculated for further characterization.

Lithium doped zinc oxide ($Zn_{1-x}Li_xO$) powder can be presented of average lattice parameters and average crystallite size by a = 3.1989 Å, c = 5.22028 Å and D = 55.799 nm. Lithium zinc oxide ($Zn_{1-x}Li_xO$) pellet can be presented of average lattice parameters and average crystallite size by a = 3.2481 Å, c = 5.2055 Å and D = 76.8211 nm. By using XRD results were obtained hkl (100), (002), (101), (102), (021), (103), (220), (112).

Electrical conductivity of the lithium doped zinc oxide (Zn_{1-x} Li_x O) pellet sample has been received from measurement of resistances of the pellet sample. The electrical conductivity of the sample is found to increase with increasing temperature. At 638K (starting temperature), the resistivity of the sample is 64.185 $\times 10^6$ Ωcm (conductivity is 0.016 $\times 10^{-6}$ Scm^{-1}) and at 703K (end temperature), the resistivity of the sample is 8.02 $\times 10^6$ Ωcm (conductivity is 0.148 $\times 10^{-6}$ Scm^{-1}) respectively.

Conclusion

The main purpose of this result is to prepare and fabricate lithium doped zinc oxide ($Zn_{1-x}Li_xO$) powder and pellet by using solid state method. In theory, for an ideal hexagonal structure, $a = b \neq c$. According to their XRD results and calculations, the crystal structure of lithium doped zinc oxide ($Zn_{1-x}Li_xO$) compound can be concluded hexagonal structure and the ideal c/a ratio is 1.6. And then, the nano-size crystal structure has been investigated. Electrical conductivity of this sample increases as increasing temperature. The purpose of this paper, lithium doped zinc oxide compound can be used lithium-ion battery technology and semiconductor devices. In general, the electrical resistivity of the sample decreases with increasing temperature; it shows that the sample has semiconductor behavior.

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