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STRUCTURAL, MORPHOLOGICAL AND MOTT-SCHOTTKY CAPACITANCE ANALYSIS OF PEROVSKITE TYPE $SrTiO_3$, $CaTiO_3$ AND $BaTiO_3$ THIN FILMS ON ITO GLASS*

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Abstract

Phase-pure perovskite type $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ thin films are deposited on ITO coated glass substrate by using sol-gel process and spin-coating technique. The samples are studied by structural, morphological and electrical characteristics. The X-ray diffraction spectra of $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ thin films on ITO glass shows that the perovskite type cubic structures with preferred orientation along (110) plane. The surface morphological is investigated by scanning electron microscopy (SEM), which revealed the crystalline nature of the films. The lattice parameters, unit cell volume, crystallite size, dislocation density, strain and grain size are evaluated. Mott- Schottky capacitance analysis is adapted to determine the built-in voltage (V_{bi}) and doping density (N_A) of the perovskite thin film devices. The influence of the Schottky contact is studied for perovskite thin films devices, by using capacitance-voltage measurement at frequency 10 kH_z. Furthermore, the depletion region widths of the thin films devices are also evaluated.

Keyword: Perovskite type thin films, Sol-gel process, XRD, SEM, Mott-Schottky capacitance

Introduction

A thorough understanding of the device physics of perovskite-type solar cells is a crucial prerequisite for purposeful optimization of these devices and materials [Brabec C J et al 2011&2010, Clarke T M et al 2010,Blom P W M et al 2007, Deibel C et al 2010 and Glatthaar M et al 2007]. Stimulated by the study of capacitance/voltage (CV) measurements done on perovskite-type solar cells, there has been a recent debate about the correct band diagram of perovskite-type thin films solar cells and in particular about the relevance and magnitude of doping and contact barriers [Fabregat-Santiago F 2011 and Bisquert J et al 2011]. Mott-Schottky analysis is commonly used to determine the built-in voltage (V_{bi}) and doping density (N_A) of a semiconductor at Schottky and *p-n* junctions [Brabec C J et al 2011]. However, the method is not always straightforward. For example, when the analysis is applied to

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organic solar cells the parameters are frequency dependent, making it difficult to extract the true values [Brabec C J et al 2010]. Furthermore, sources of capacitance other than the depletion capacitance distort the capacitance-voltage (CV) response, resulting in values of V_{bi} and N_A that are larger than the actual values.

Other types of solar technologies also exhibit capacitive responses related to contact phenomena as the depletion layer capacitance commonly exhibited by inorganic and organic photovoltaic devices [Fabregat-Santiago F 2011]. Voltage-modulation of the depletion layer width (w) allows extracting relevant parameters as the absorber acceptor defect density (N_A) and built-in potential (V_{bi}) by means of capacitance-voltage Mott-Schottky (MS) analysis [Bisquert J et al 2011]. These two parameters can be used to derive experimentally-supported PSCs device models, and also constitute key information of variations in materials properties induced by device processing modifications.

Experimental

Firstly, the glass slides coated with indium tin oxide (ITO) were cleaned by acetone, HCl and deionized water. Secondly, the perovskite type $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ powder were mixed with 2-methoxyethanol solution by using sol-gel method. And then these pastes were coated on ITO conducting glass by using spin coating technique and annealed at 100˚ C for 30 minutes. The structure of prepared films were characterized by X-ray diffraction (RigakuMultiflex, Japan) with Cu K_α source (λ =1.54056 Å). The scanning electron microscopies were performed to analyze the surface morphology of the films. Capacitance Voltage measurements were performed using a $G^{\underline{W}}$InSTEK (LCR-8110G) at frequency 10 kHz and various applied voltage.

Results and Discussion

The crystallinity of the films was investigated using X- ray diffraction. The detailed structural characterizations exhibited the perovskite-type with cubic structure for all samples. Figure (1) shows the diffraction peak of $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ thin films on ITO glass.

The average crystallite size measured in direction perpendicular to the surface of the sample was calculated using Scherrer formula as shown in equation 1, where B represents a width measured in radians at intensity equal to half of the maximum intensity, θ_B is Bragg angle and k is the shape factor of the average crystallite.

$$t = \frac{k\lambda}{B\cos\theta_B} \tag{1}$$

Figure (2) shows the SEM micrograph of $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ thin films on ITO glass. From the SEM images, it can be seen that the particles are in spherical shape, fairly dense, crack-free and fine grain.

Mott-Schottky analysis probes the depletion capacitance at a Schottky or p-n junction which is determined by the width of the bias dependent depletion region. Hence the depletion capacitance "C" is also bias dependent and can be expressed as in equation 2, where, V is the applied bias voltage and V_{bi} is the built-in voltage.

$$\frac{1}{C^2} = \frac{2(V_{bi} - V)}{A^2 q \varepsilon_r \varepsilon_0 N_A} \tag{2}$$

The structural properties of $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ thin films on ITO glass are listed in Table 1.

Table 1: The structural properties of $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ thin films on ITO glass

Samples	***Maximum peak***	***Lattice constant "a"(Å)***	***Unit cell volume "V" (nm)^3***	***Crystallite size "t" (nm)***	***Dislocation density "□" (m)$^{-2}$***	***Strain "□"***
$SrTiO_3$/ITO glass	(110)	3.8839	0.0586	36.4677	7.5194×10^{14}	9.5049×10^{-4}
$CaTiO_3$/ITO glass	(110)	3.8092	0.0553	30.4817	1.0763×10^{15}	1.1372×10^{-3}
$BaTiO_3$/ITO glass	(110)	4.0116	0.0646	31.1411	1.0312×10^{15}	1.1311×10^{-3}

Figure (3) depicts the characteristics $1/C^2$ versus V plots for $SrTiO_3$, $CaTiO_3$ and $BaTiO_3$ thin films on ITO glass at frequency range 10 kHz. The so-called Mott-Schottky plot of $1/C^2$ versus applied DC voltage yields a straight line, whose slope yield the doping density and whose extrapolated intersection with the voltage axis yields the built-in voltage. The doping density is given by equation 3.

$$N_A = -\frac{2}{q\varepsilon_s A^2}\left(\frac{d(C)^{-2}}{dV}\right)^{-1} \tag{3}$$

The main parameters obtained from Mott-Schottky analysis for Perovskite-type thin film devices collected in Table 2.

Table 2: The main parameters obtained from Mott-Schottky analysis for Perovskite-type thin film devices

Samples	***V_{bi} (V)***	***N_A $(cm)^3$***	***W(cm)***
$SrTiO_3$/ITO glass	0.179	2.86×10^{16}	4.16×10^{-6}
$CaTiO_3$/ITO glass	0.370	5.03×10^{12}	5.71×10^{-4}
$BaTiO_3$/ITO glass	0.122	2.70×10^{14}	2.49×10^{-4}

Conclusion

Phase – pure perovskite type $SrTiO_3$,$CaTiO_3$ and $BaTiO_3$ thin films have been synthesized using sol-gel process and deposited on ITO coated glass substrate using spin-coating technique. The $SrTiO_3$/ITO glass, $CaTiO_3$/ITO glass and $BaTiO_3$/ITO glass, structures were studied by structural and microstructural characteristics. According to the XRD pattern, these films have perovskite type cubic structure. From the SEM investigation, the films crystallinity indicated that with large grain size. The average grain size was observed to be estimate of 0.79 μ m, 0.98 μ m and 0.75 μ m respectively.

Perovskite films thicknesses are 2.69 μ m for $SrTiO_3$/ITO glass, 10.66 μ m for $CaTiO_3$/ITO glass and 4.45 μ m for $BaTiO_3$/ITO glass respectively. The capacitance - voltage characteristics should be measured after applying reverse bias for several minutes at room temperature in order to obtain the true profile of shallow acceptors. Only under careful checking of the capacitance response, Mott-Schottky analysis can lead to meaningful and reliable parameter extraction to be properly used in device physical modeling.

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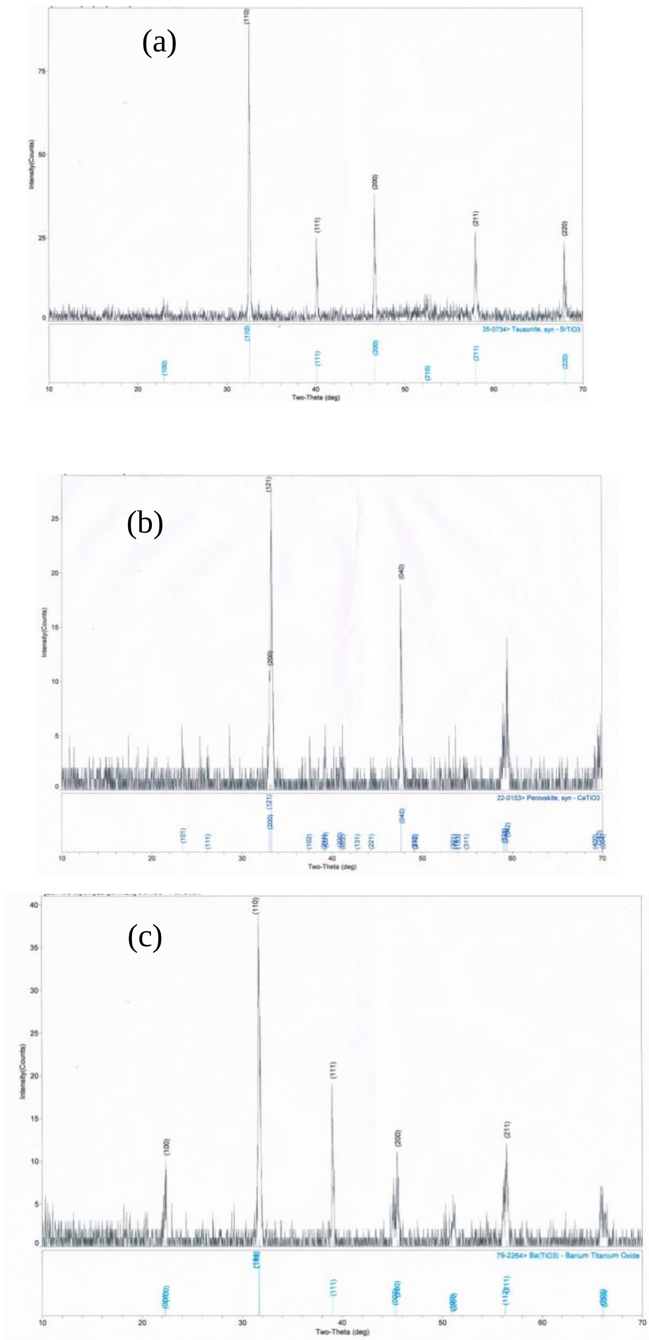

Figure 1: The diffraction peak of (a) $SrTiO_3$/ITO glass (b) $CaTiO_3$/ITO glass and (c) $BaTiO_3$/ITO glass thin fiml.

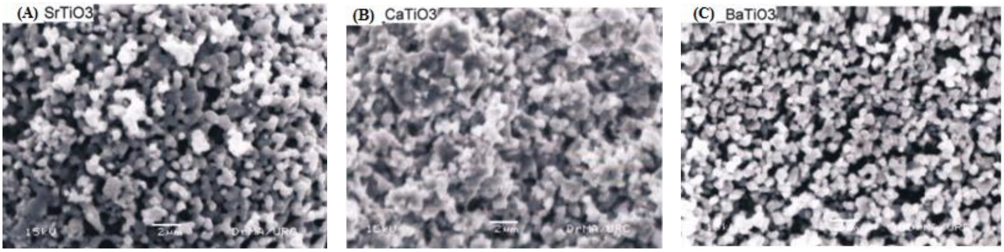

Figure 2: The scanning electron micrograph of (a) $SrTiO_3$/ITO glass (b) $CaTiO_3$/ITO glass (c) $BaTiO_3$/ITO glass thin film.

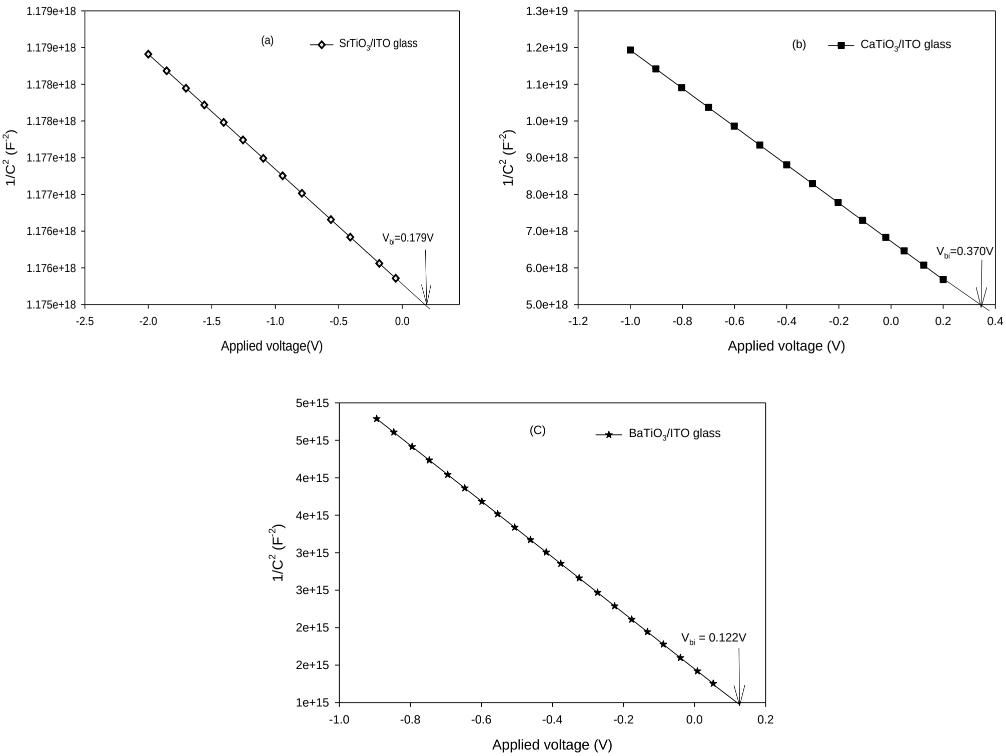

Figure 3: $1/C^2$ –V plots for Perovskite-type (a) $SrTiO_3$/ITO glass (b) $CaTiO_3$/ITO glass and (c) $BaTiO_3$/ITO glass thin film.

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