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Preparation And Characterization Of Znse Thin Film For Photovoltaic Applications

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Abstract:

ZnSe thin films are prepared by thermal evaporation of nanocrystalline ZnSe particles synthesized using solvothermal process. These are prepared on corning 1737 and ITO coated glass substrate under high vacuum. Structural properties investigated with X- ray diffraction show that the films are polycrystalline with zinc blende structure. Morphological and compositional analyses are performed using atomic force microscopy and scanning electron microscopy. Optical properties of the films are investigated using UV-vis-NIR measurement. The optical band gap is determined from the transmission data and is obtained as 2.75 eV. The electrical conductivity measurements are performed in both coplanar and sandwich geometry under high vacuum.

Keywords: *Crystallites, X-ray diffraction, Zinc compounds, Semiconducting II-VI materials.*

Introduction

Zinc Selenide (ZnSe) is a relatively wide direct band gap (2.7eV) II-VI compound semiconductor. Due to its advantageous properties for certain applications, it has been widely utilized in various opto-electronic devices such as thin film solar cells, green-blue light emitting diodes, lasers, photo-luminescent and electro-luminescent devices, etc [1-2]. There are several techniques for synthesizing high quality thin films including thermal evaporation, metal-organic chemical vapour deposition, electro-deposition, spray pyrolysis, pulse laser deposition, atomic layer deposition, sputtering, etc. Among these, thermal evaporation technique is one of the simplest methods for preparing high quality polycrystalline ZnSe thin film. In this paper we report the thin film preparation from nanocrystalline ZnSe particles using thermal evaporation technique. Nanocrystalline ZnSe particles are synthesized by solvothermal route using mixed solvent of hydrazine hydrate, ammonia and de-ionized water. Structural and opto-electronic properties are investigated on the prepared thin film for photovoltaic applications.

Experimental Technique

ZnSe thin films were deposited on corning 1737 and ITO coated glass by thermal evaporation of nanocrystalline ZnSe powder under high vacuum. The nanocrystalline sample was kept in the molybdenum boat and heated by supplying sufficient current to evaporate the material. The substrate temperature was set at 200^{o}C using PID temperature controller and chromel-alumel thermocouple fitted on the substrate holder.

X-ray diffraction (XRD) analysis was carried out on both the synthesized powder and thin film samples using CuKα radiation and was measured in 2θ range of 20^{o} – 65^{o}. The spectral transmittance of the films was recorded as a function of wavelength in the wavelength range of 200 – 3000 nm using UV-Vis-NIR spectrophotometer (Shimadzu UV 3101PC). FESEM and AFM in non-contact mode were used to study the thin film surface morphology. The conductivity of the film was measured by two probe method in vacuum using Keithley 6430 source-meter. Silver paste was used for making ohmic electrical contact to the thin film sample.

Results And Discussion

Plot of XRD intensity vs 2θ for the synthesized nanocrystalline ZnSe powder and the prepared thin film sample are shown in figure 1. The powder XRD shows three broad peaks corresponding to (111), (220) and (311) planes of zinc blende structure of ZnSe. The XRD of the prepared thin film however shows only one sharp peak corresponding to (111) plane of ZnSe zinc blende structure. This shows the thin film growth is along this direction only. Using Debye Sherrer's formula $L = \frac{K\lambda}{\beta \cos\theta}$, the grain size in the film is calculated as 22 nm. The obtained lattice constant (*a)* from Bragg's formula and the associated relation of lattice constant *'a'* and *d*-spacing is 5.66$\AA$. This slightly deviates from the bulk lattice constant *a* = 5.618 Å. This indicates that the crystallites of the film are under strain, which may be due to the change in nature and concentration of the native defects. The lattice strain is calculated using $\varepsilon = \frac{\beta \cos\theta}{4}$ and dislocation density is also calculated using $\delta = \frac{15\beta \cos\theta}{4aL}$ [3]. The lattice strain is obtained as 1.65×10^{-3} and the dislocation density is 1.99×10^{15} lines per m^2.

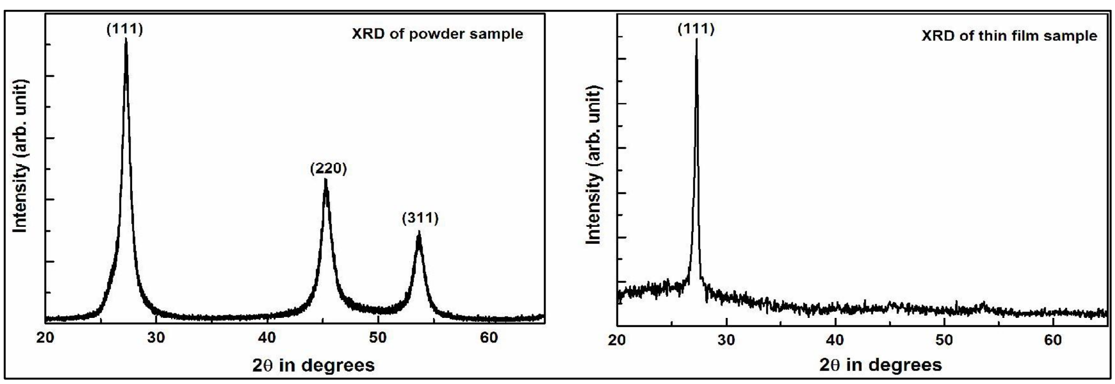

Figure 1: XRD of the synthesized powder sample and the prepared thin film sample

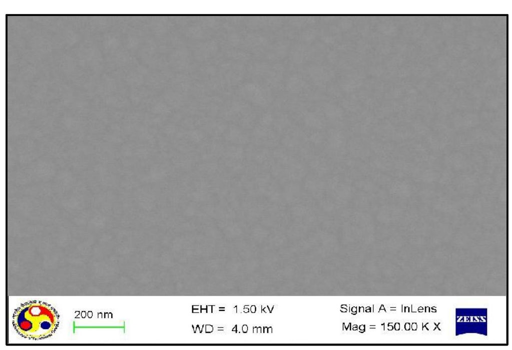

Figure 2: FESEM image of the thin film sample.

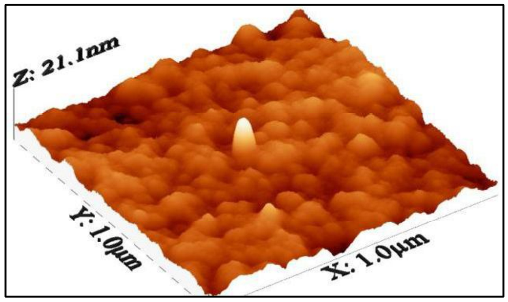

Figure 3: AFM image of ZnSe thin film sample.

The FESEM image of the thin film sample is shown in figure 2. The films are deposited uniformly throughout the surface without any cracks, serious defects or voids formation. The film surface is not perfectly smooth with formation of grains with sizes varying over a wide range. AFM image is shown in figure 3. The measurement is done in non-contact mode over 1 µm x 1 µm sample dimension. The AFM measurements show that the as deposited film possesses good quality surface with average roughness of 1.55 nm.

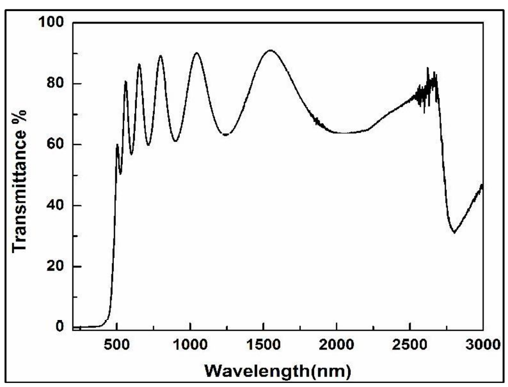

Figure 4: Transmittance spectra of ZnSe thin film

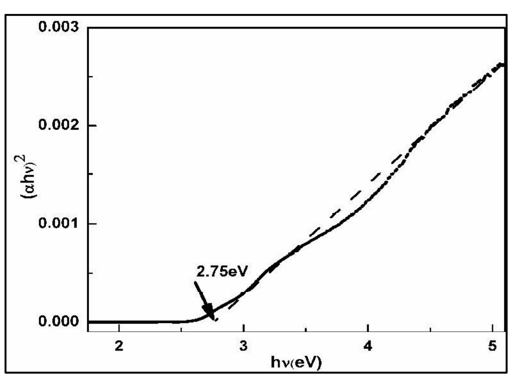

Figure 5: Plot of $(\alpha h\nu)^2$ vs hν of ZnSe thin film

The transmittance vs wavelength plot is shown in figure 4. The transmittance spectrum reveals a high transmission of 83 – 91 % in the near infrared region (≥ 600 nm) and a low transmission of less than 40% in the visible region at wavelength below 475 nm. It has maximum transmission at 1549 nm with decreasing transmission towards visible region. The as prepared thin film is therefore highly transparent in near IR region and has high absorbance in the visible region below 475 nm. Thin film interference pattern with oscillatory behavior is observed for wavelength ranging from 500 nm to 3000 nm, where the film is transparent. The optical constants are obtained from the interference fringes using the method developed by R. Swanepoel [4]. The thickness calculated from the fringes is about 715 nm. The refractive index at 600 nm is calculated as 2.51. The refractive index remains almost constant in the wavelength range of 560 nm to 1044 nm and it decreases almost rapidly after that. This dispersion behavior deviates from Cauchy's relation, which is a first order approximation and is in agreement with the reported data [5]. The absorption coefficients are calculated for wavelength in the absorption region (< 560 nm) and the optical band gap is determined by studying the dependence of absorption coefficient (α) on the photon energy (hν). The relation between absorption coefficient and photon energy for direct and indirect band gap semiconducting materials are described by the following relations:

$\alpha h\nu = A_1\left(h\nu - E_g^d\right)^{1/2}$, for direct allowed transition -------- (1)

$\alpha h\nu = A_2\left(h\nu - E_g^i\right)^2$, for indirect allowed transition -------- (2)

where $A_1$and A_2 are constants. E_g^d and E_g^i are direct and indirect band gap respectively. The plot of $(\alpha h\nu)^2$ verses $h\nu$ of the ZnSe thin film is shown in figure 5. Towards higher photon energy in the absorption region, the plot is linear indicating direct band gap behavior as described by equation (1). Extrapolation of the linear portion of the curve to $(\alpha h\nu)^2 = 0$ gives the optical band gap value for the deposited film. The evaluated optical band gap of the prepared ZnSe thin film is 2.75 eV, which is slightly higher than the bulk value. This slight increase may be due to quantum confinement effect

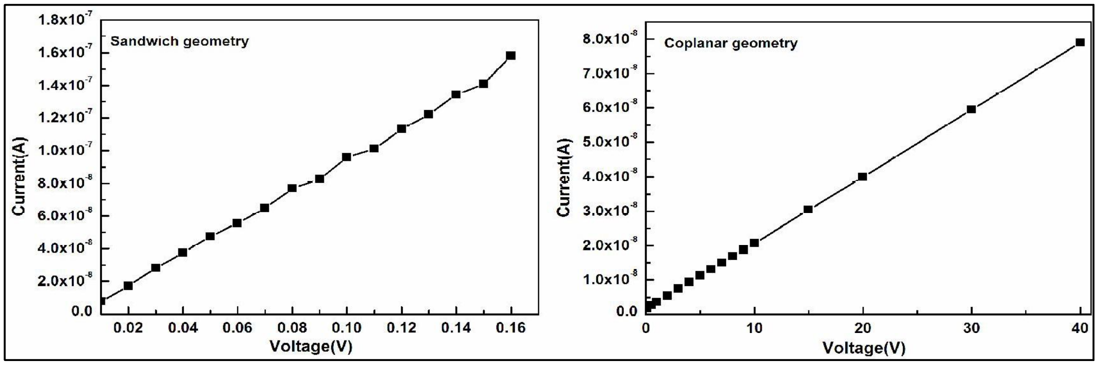

Figure 6: I-V plot for sandwich geometry and coplanar geometry.

The measured DC I-V for the thin film samples are plotted for both sandwich geometry and coplanar geometry and are shown in figure 6. Both plots exhibit linear I-V indicating ohmic conduction in the measurement range. The conductivity of the samples is therefore calculated using ohms law. For both measurements the DC conductivity obtained is about $6 \times 10^{-6} \Omega^{-1} cm^{-1}$, which matches with reported literature [6].

Conclusion

Good quality ZnSe thin film was successfully deposited on both corning 1737 and ITO coated glass substrates using simple thermal evaporation technique in high vacuum at about 10^{-6} mbar pressure. The deposited film has a good crystallinity with cubic zinc blende structure and it has a preferential growth along [111] direction. Calculation of the lattice constant however shows slight deviation from bulk value, which is an indication of the presence of strain and defects in the thin film layer. The investigation of the optical behavior of the thin film sample shows high transmission in the NIR region with good absorption in the visible and UV region. The calculated optical band gap of the film is 2.75 eV and it has high refractive index of 2.51 at 600 nm. The DC conductivity was measured and it is found to be $6 \times 10^{-6} \Omega^{-1} cm^{-1}$. These properties indicate that the films can be used as a buffer layer in the fabrication of thin film heterojunction solar cell and other optoelectronic devices.

Reference

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