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Influence of thickness on the structural and optical properties of cadmium selenide thin films

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ABSTRACT

The cadmium selenide (CdSe) thin films of thicknesses 1.31µm and 1.46µm were chemically deposited on well cleaned glass substrate at room temperature. The films are polycrystalline with hexagonal structure, confirmed by x-ray diffractogram. The optical spectra of cadmium selenide thin films were recorded in the wavelength range of 0.36µm and 1.10µm. The spectral absorption data shows that the films absorb in the ultra violet range of 0.36-0.45 microns and have low absorbance in VIS-IR regions of the spectrum. The films have average index of refraction of 2.2. The plot of α^2 versus h□ showed a direct band gap range of 1.50eV-1.75eV. The band gap is found to increase with increase in film thickness.

Keywords: Semiconductor, thin film, cadmium selenide, chemical bath, characterization, application.

INTRODUCTION

The growth and characterization of polycrystalline materials haveattracted much attention not only because of their exceptional properties [1, 2], but also due to their structural properties, thickness dependent properties, novel physical properties and potential applications [3, 4]. Presently, there has been an increase in research and development of II-VI semiconductor materials which are widely used in devices such as, optical fibres, solar energy collectors, optical instruments,and low cost solar cells, sensor and laser materials.Cadmium selenide, a group 11-VI compound semiconductorcan crystallize in two forms: a cubic form (c-CdSe) with sphalerite structure and a hexagonal form (h-CdSe) with wurtzite structure (5).Wurtzite is the low temperature phase, which transforms to sphalerite at 700-800˚C (6). Both phases can be obtained at room temperature in thin film form depending on the deposition conditions.CdSe films offer a larger number of applications in solid-state device technologies such as the target material of television cameras, microwave devices, switching devices, infrared detectors, diodes and Hall Effect devices. It has useful properties for optoelectronic devices, laser diodes, biomedical imaging and high efficiency solar cells.

A variety of techniques have been used to prepare CdSe thin films includingthermal evaporation (7-8), vacuum evaporation (9-10), electron beam evaporation(11), chemical bath deposition (12-14), electrochemical deposition (15-16)etc.They studied the regularities of electrochemicalformation of CdSe thin films on Ti surface and electro synthesis of CdSe films on Nickel substrate respectively (15-16).

In this work, chemical bath deposition technique has been chosen for deposition of CdSe thin films because it is a trouble-free and controllable technique. The present study is centred on the effect of thickness on the structural and optical properties of chemically deposited CdSe polycrystalline thin films. X-ray diffraction (XRD),UV–VIS-model of spectrophotometer, and Olumpus optical microscope (O.M) are used to characterize the samples. Optical constants, such as optical band gap, extinction coefficient, refractive index are evaluated from the optical spectra.

MATERIALS AND METHODS

Thin films of CdSe, were deposited by chemical bath deposition technique on a glass substrate at room temperature. Prior to deposition, the substrate were degreased in trioxonitrate (v), washed with detergent, rinsed in distilled water and dried in air. The deposition of CdSe thin films was based on the reaction between cadmium trioxonitrate (v) $Cd(NO_3)_2$and $SeSO_3$using$Na_2S_2O_3$ as the complexing agentand NH_3 was used to provide the alkaline medium needed for maximum growth and to increase the film adherence respectively. For deposition,5ml of 1M $Cd(NO_3)_2$ was complexed with 5ml of 0.5M $Na_2S_2O_3$. To this, 2ml of 0.1M $SeSO_3$ was added slowly to the reaction mixtures. The pH of the reaction baths was adjusted to 10.2 by addition of (5ml) ammonia and the volumes were made up to 50ml with distilled water. The cleaned glass substrates were vertically immersed into the chemical baths with the help of the synthetic foam. The reaction mechanisms for the growth are represented as follows:

$Cd(NO_3)_2 + Na_2S_2O_3 \Leftrightarrow [Cd(Na_2S_2O_3)]^{2+} + 2NO_3^-$
$[Cd(Na_2S_2O_3)]^{2+} \Leftrightarrow Cd^{2+} + Na_2S_2O_3$
$SeSO_3 + OH^- \Leftrightarrow HSe- + SO^{2-}_4$
$HSe- + OH^- \Leftrightarrow Se^- + H_2O$
$Cd^{2+} + Se^- \Leftrightarrow CdSe$

RESULTS AND DISCUSSION

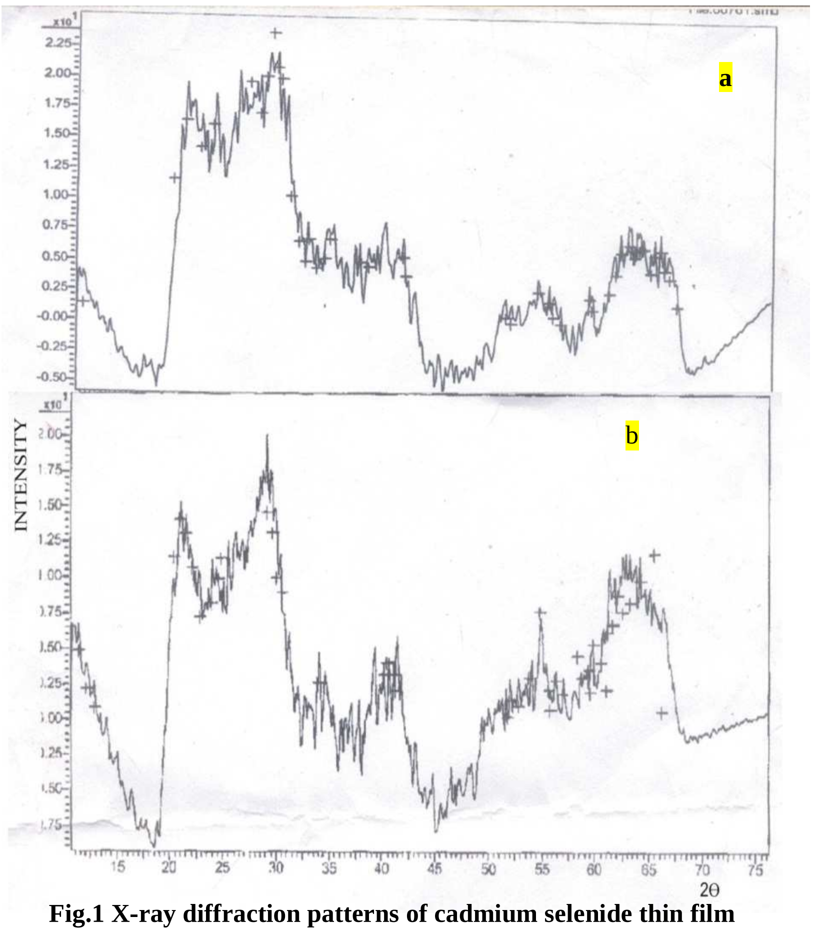

Fig.1 X-ray diffraction patterns of cadmium selenide thin film

Fig.1 is the x-ray diffraction patterns of cadmium selenide thin film prepared at a substrate temperature of 300K.The peaks in the patterns are identified as (101) and (110) planes of reflections of hexagonal structure (figure 1a) and(100), (002), (101) and (110) planes of reflections of hexagonal structure with composition CdSe (figure 1b). Increasing the film thickness from 1.49µm to 1.64µm intensified the characteristics peak of CdSe, hence the appearance of two other peaks in the XRD pattern (figure 1b) due to improvement of its crystallinity.XRD results point out that all the films are polycrystalline in nature and the grains are randomly oriented. The lattice constants from the XRD were found to be 4.299Å and c=7.01Å.The grain size was calculated from the XRD pattern usingDebye-Scherrerformula (17-18). The structural parameters of CdSe film in table 1 show variation in grain size from 3.76(Å)-3.88(Å) with thickness.The obtained CdSe films show the same crystalline aspects as those reported by (14) using other precursors.

Table 1: The structural parameters of CdSe film and thicknesses

Thickness, t (µm)	h k l	2θ (deg)	2θ (rad.)	FWHM(β) (rad.)	Lattice constant, a (Å)	Grain size, D (Å)
1.49	101	27.08	0.473	0.380	a=4.299,	3.76
	110	41.96	0.732	0.384	c=7.01	3.88
1.64	101	29.15	0.509	0.380	a=4.299,	3.77
	102	35.90	0.627	0.382	c=7.01	3.82
	110	40.21	0.702	0.384		3.84

Table-1 revealed that the thickness of the films increases as the crystallite size increases.

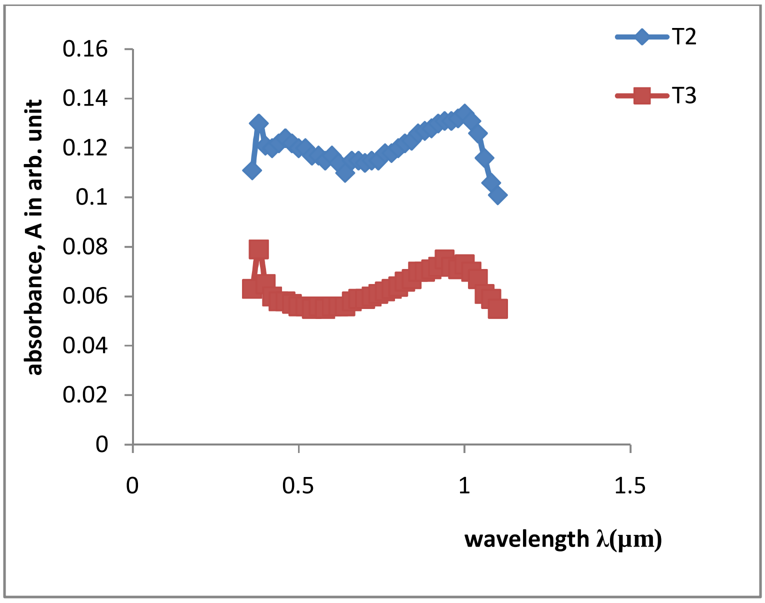

Fig-2 Absorbance spectra of 1.49µm and 1.64µm CdSe thin films.

The thicknesses of CdSe films were determined by the optical method as was described by (19).

The optical studies were investigated by measuring the absorbance and transmittance of CdSe films in the wavelength range of 0.36µm –1.10µm. The absorbance spectra of the samples are shown in figure 2. A careful look on the figure showed that the optical absorptions in the visible region are low. It is also seen that the absorption value in the ultraviolet region decreased with increase in the film thickness.

Figure 3 shows theUV-VIS-IR transmissionspectra of CdSe films having different thicknesses. The optical transmission in the visible region was high about 85% but decreased substantially at short wavelength.It clearly showed that the films are more transparent for short wavelengths as the film thickness increase due to the increase of light scattering on the surface of the films. However, increasing film thickness revealed a decrease of the transmission factor for short wavelengths. It is seen that the optical transmission is above85% for CdSe thin film with 1.64µm thick which decreased to 80% upon decreasing the thickness to 1.49µm. CdSe thin film could be useful as buffer layers for CGS solar cell

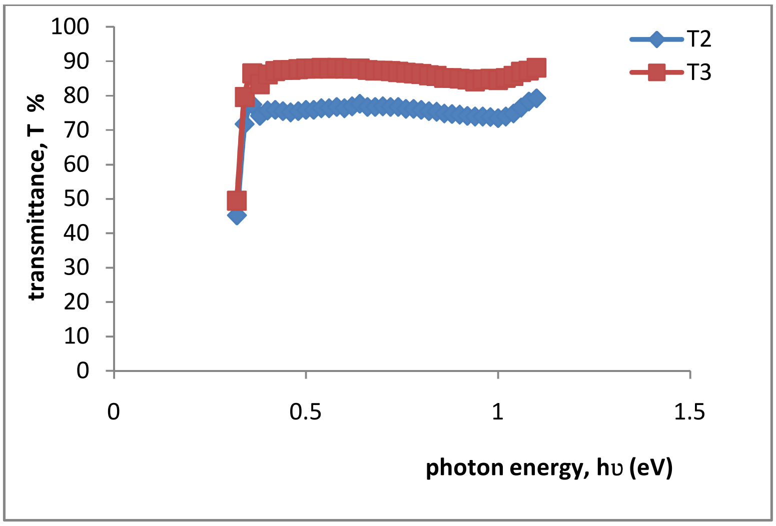

Fig-3 Transmittance spectra of 1.49µm and 1.64µm CdSe thin films.

Figure 4 gives the plot of absorption coefficient square versus photon energy for CdSe films. The figure revealed that the band gap of the deposited CdSe films of 1.49µm and 1.64µm thick are 2.50eVand 2.75eV respectively. The band gap of 1.64µm sample is very close to bulk value (~2.7eV) of CdSe film than that of other sample.It can be attributed to the improvement in the films crystallinity as supported by the XRD studies. In the case of film with 1.49µm thick, the band gap is less than the bulk value which can be attributed to the creation of allowed energy states in the band gap at the time of film preparation (20)

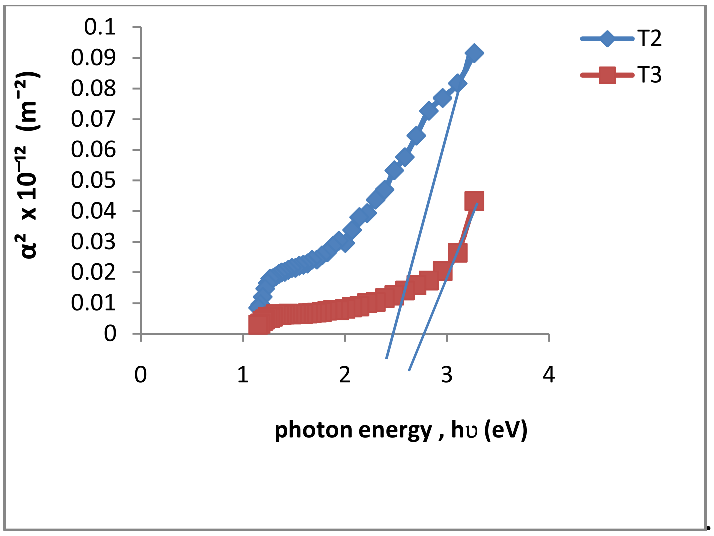

Fig-4 Plot of absorption coefficient square versus photon energy for 1.49µm and 1.64µmCdSe thin films.

Figure 5 is the plot of refractive index versus wavelength for 1.49µm and 1.64µm CdSe thin films. Thetwo samples show high refractive index in the same wavelength. It is observed in the two figures that the refractive index in all the samples have similar behavior in the entire spectral region. The values of refractive index at any wavelength were found higher in the case of thinner film. It can be seen that, for the two samples, as the wavelength is increased, the refractive index decreases gradually and later increased as it enters NIR region of electromagnetic spectrum. The high refractive index value makes this film a good material for photovoltaic application.

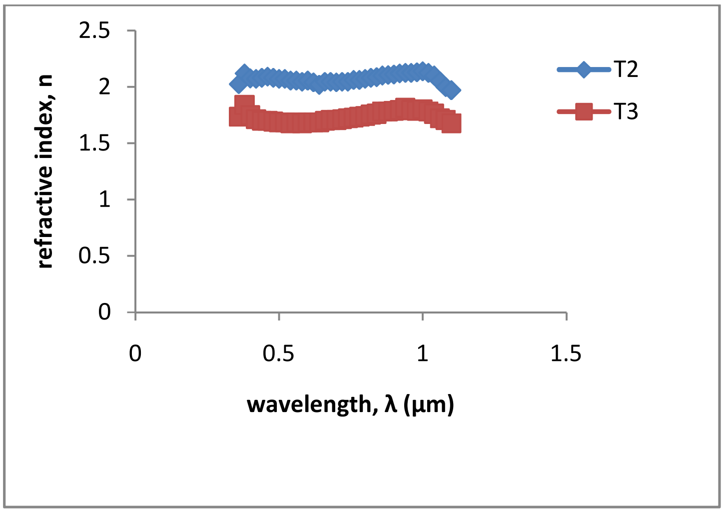

Fig-5 Plot of refractive index versus wavelength for 1.49µm and 1.64µmCdSe thin films.

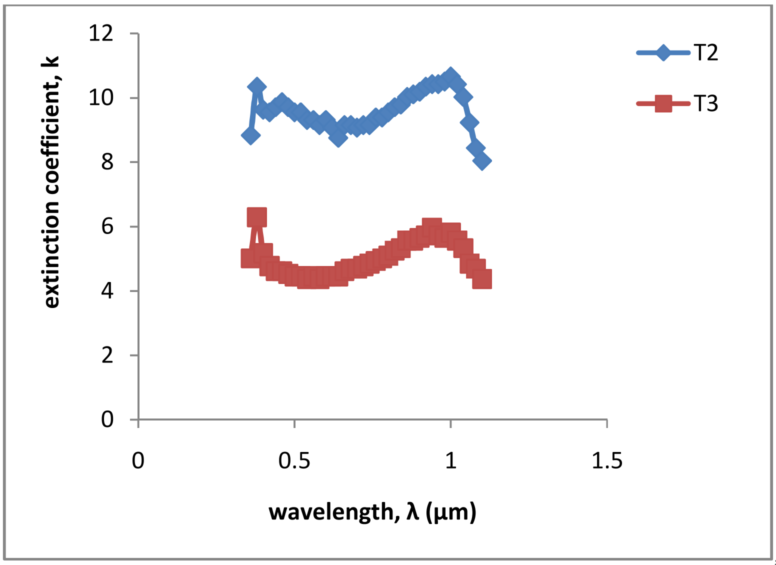

Fig-6 Plot of extinction coefficient versus wavelength for 1.49µm and 1.64µmCdSe thin films.

Graph of extinction coefficient as a function of wavelength for 1.49µm and 1.64µm of CdSe thin films is plotted in figure 6. The figure revealed that extinction coefficient decreases as film thickness increases

CONCLUSION

Various parameters related to optical properties were calculated for different thicknesses ofCdSethinfilm. Optical constants of CdSethinfilm are strongly dependent on the thickness of the films. Increasein band gap of the films with the increase of thickness has been attributed to the decrease of localizedstates in the band gap. The corresponding decrease in optical constant such as refractive index and extinctioncoefficient also decrease with increasing filmthickness.

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