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Study of crystal structure of vacuum evaporated ($Cd_{1-x}Zn_x$ Se) thin films by using X-Ray diffraction technique

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ABSTRACT

Thin films study of ternary alloys of II-VI group have directly or indirectly advanced many new areas of research in solid state physics and chemistry which are based on the phenomena uniquely characteristics of the thickness, geometry and structure of the films. X - ray crystallography is a tool used for determining the atomic and molecular structure of a crystal. The thin films of $Cd_{1-x}Zn_xSe$ alloy has been deposited onto highly cleaned glass substrates by using vacuum evaporation technique. The structural properties are characterized by using X-ray diffraction (XRD). All XRD patterns confirmed the preferred orientation and polycrystalline nature of as- deposited $Cd_{1-x}Zn_xSe$ thin films. The presence of sharp peaks in these XRD patterns confirmed the nature of the prepared materials. We have calculated d-values from Vegard's law. Internal strain and dislocation densities were also studied by X - ray diffraction patterns of vacuum-evaporated $Cd_{1-x}Zn_xSe$ thin films. The particles size of vacuum evaporated $Cd_{1-x}Zn_xSe$ thin films at x = (0,0.4,0.6,1) also calculated with the help of Debye-scherrer formula and found to be 11.34, 16.456, 16.40, and 16.831nm respectively.

Key words: polycrystalline semiconductors, structural properties, ternary alloys, vacuum evaporation.

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INTRODUCTION

The demand for development of smaller and smaller devices with high speed especially in new generation of integrated circuits requires advanced materials and new processing techniques suitable for Giga Scale integration (GSI) technology. Ternary alloys of II-VI group semiconductors prepared by using binary semiconductors can thus be grouped as a class of tailored and engineered materials in which energy band gap lattice parameters and other functional parameters could be continuously varied by selecting binary constituents and their relative compositions accordingly. Cadmium zinc-selenide [(CdZn)Se] is one of the important ternary materials for use in electroluminescent, photo luminescent, photoconductive and photovoltaic device applications because of its interesting size-dependent properties as well as a high stability and wide optical band gap which covers the maximum electromagnetic spectrum [1,2]. Thin films studies have directly or indirectly advanced many new areas of research in solid state physics and chemistry which are based on the phenomena uniquely characteristics of the thickness, geometry and structure of the films. The importance of coating and the synthesis of new materials for industry have resulted in a tremendous increase of innovative thin film processing technologies. Currently this development goes hand-in-hand with explosion of scientific and technological break-troughs in microelectronics, optics and nanotechnology [3]. These films are essential for multitude of production areas, such as thermal barrier coatings and wear protections, enhancing service life of tools and to protect materials against thermal and atmospheric influences [4, 5].

In fabrication, there are various techniques to fabricate a thin film. Thin Film synthesis techniques are mainly based on physical and chemical process as physical vapor deposition (PVD) and chemical vapor deposition (CVD) respectively. Thin films of (CdZnSe) have been obtained by chemical bath deposition (CBD) [6], vacuum evaporation [7, 8], molecular beam epitaxy [9], electron beam pumping [10] etc. Usually the process must be performed in vacuum or in controlled atmosphere to avoid interaction between vapor & air and to increase the mean free path for better adhesion of the film material to the substrate. PVD technique is used for the deposition of metals, alloys and also many compounds. It involves the evaporation or sublimation of the material in vacuum by thermal energy and allowing the vapor stream of the charge to condense on a substrate so as to form a continuous thin film of desired thickness [11, 12]. In order to obtain a better film, vacuum provides better conditions. It increases mean free path and so better adhesion of the film is achieved. The grain size of the atoms also increases and the film formed will be a better film. X-ray crystallography has been fundamental in the development of many scientific fields. In its first decades of use, this method determined the size of atoms, the lengths and types of chemical bonds, and the atomic-scale differences among various materials X-ray Diffraction uses only short wavelength X-rays in the range of a few angstrom to 0.1 Angstrom (1 keV - 120 keV). Because the wavelength of the X-rays is comparable to the size of atoms, they are ideally suited for probing the structural arrangement of atoms, crystalline, grain size, lattice parameters and effective strain in a wide range of materials [13-15].

METHODOLOGY:

The thin films of $Cd_{1-x}Zn_xSe$ alloy at different composition (x= 0, 0.4, 0.6,1) have been deposited by using vacuum evaporation technique (Vacuum Coating Unit Model 12A4). The fine powders of different $Cd_{1-x}Zn_xSe$ ($0 \leq x \leq 1$) compositions have been used as a starting material for deposition. The limiting compositions (x=0 and x=1.0) are the case of binary Case and ZnSe compounds as the composition at x=0 and x=1 gives CdSe and ZnSe binary system respectively and used directly for evaporation. Thin films of these compositions of $Cd_{1-x}Zn_xSe$ alloy have been deposited onto highly cleaned glass substrates by using vacuum evaporation technique. The substrate was cleaned in aqua-regia, washed in distilled water, acetone and isopropyl alcohol (IPA). The structural properties of $Cd_{1-x}Zn_xSe$ ternary system have been characterized by using Bruker, D8 Advance XRD unit.

X-rays are ideally suited for probing the structural arrangement of atoms, crystallinity, grain size, lattice parameters and effective strain in a wide range of materials because the wavelength of the X-rays is comparable to the size of atoms. The variation of peak position with sample orientation can be utilized to deduce the information regarding the internal strain of the sample. The particle size is calculated from the Scherer's formula as given below

$$D = \frac{0.94\lambda}{\beta cos\theta} \qquad \text{.....................(1)}$$

The strain (ε), dislocation density (δ) and lattice parameter of the films is calculated by the help of the equation (2), (3) and (4).

$$\varepsilon = \left[\frac{\lambda}{Dcos\theta} - \beta\right]\frac{1}{tan\theta} \qquad \text{.....................(2)}$$

$$\delta = \frac{1}{D^2} \qquad \text{.....................(3)}$$

$$\frac{1}{d^2} = \frac{h^2 + K^2 + l^2}{a^2} \qquad \text{.....................(4)}$$

$$c_{hex} = \left(\frac{4}{3}\right)^{\frac{1}{2}} \times a_{cub} \qquad \text{.....................(5)}$$

$$a_{hex} = \left(\frac{1}{2}\right)^{\frac{1}{2}} \times a_{cub} \qquad \text{.....................(6)}$$

$$c_{hex} = (1.633)\ a_{hex} \qquad \text{.....................(7)}$$

RESULTS AND DISCUSSION

The crystallinity and phase of the vacuum evaporated $Cd_{1-x}Zn_xSe$ thin films deposited on to highly cleaned glass substrates have been done by using an X-ray diffraction with CuKα radiation in the 2θ range of 20° to 80°. XRD samples were taken at room temperature. These patterns confirmed the formation of alloy $Cd_{1-x}Zn_xSe$ system. The presence of sharp peaks in these XRD patterns confirmed the nature of the prepared materials.

The XRD patterns of vacuum evaporated CdSe thin films (figure 1.1) reveales that x-ray diffraction patterns have a strong and highly intense peak having 2θ value about 25.368°with cubic (111) crystalline plane as well as hexagonal phase depicting the polycrystalline nature of the thin film. The particles size was found to be 11.34 nm.

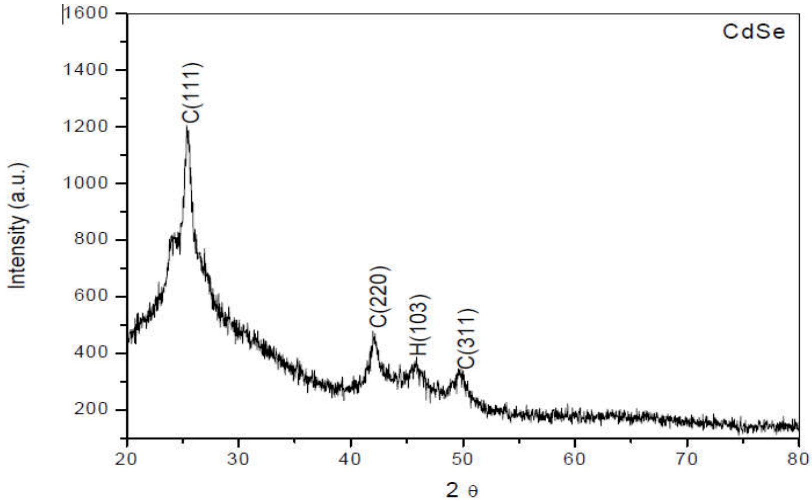

Figure 1.1: XRD patterns of vacuum evaporated CdSe thin films

The XRD pattern of vacuum evaporated $Cd_{0.6}Zn_{0.4}Se$ thin films are shown in figure 1.2. The XRD pattern has a strong and highly intense peak at 2θ value about 26.127° with cubic (111) crystalline plane, which shows that film is highly oriented to this plane. There are some another peaks of low intensity as compared to first dominating peak also appear having 2θ value 27.81°, 36.192°, 43.221°, 47.011°, 51.141°, and 65.826° corresponds to H(101), H(102), C(220), H(103), C(311) and H(203) plane. XRD pattern reveales that the vacuum evaporated thin film of $Cd_{0.6}Zn_{0.4}Se$ deposited onto highly cleaned glass substrate have cubic as well as hexagonal phase depicting the polycrystalline nature of the thin film. The particles size was found to be 16.456 nm.

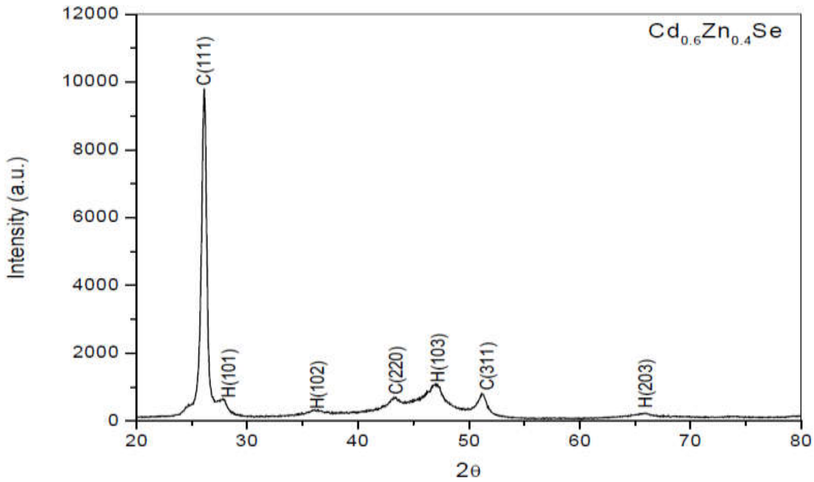

Figure 1.2: XRD pattern of vacuum evaporated $Cd_{0.6}Zn_{0.4}Se$ thin films

The XRD pattern of vacuum evaporated $Cd_{0.4}Zn_{0.6}Se$ thin films are shown in figure 1.3. The XRD pattern reveales that, x-ray diffraction patterns have a strong and highly intense peak having 2θ value about 26.556° with cubic (111) crystalline plane, which shows that film is highly oriented to this plane. There are some another peaks of low intensity as compared to first dominating peak also appear having 2θ value 44.079°, and 52.093° corresponds to C(220) and C(311) plane. XRD pattern revealed that the vacuum evaporated thin film have cubic phase depicting the crystalline nature of the thin film. The particles size was found to be 16.40 nm.

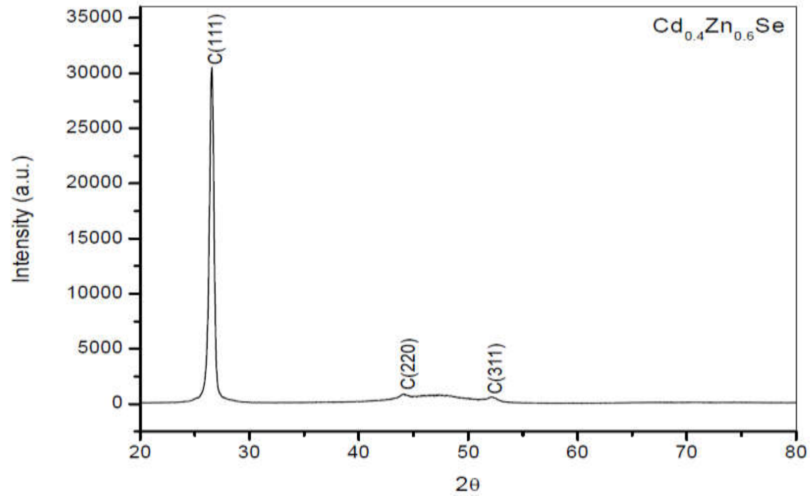

Figure 1.3: XRD pattern of vacuum evaporated $Cd_{0.4}Zn_{0.6}Se$ thin films

The XRD pattern of vacuum evaporated ZnSe thin films shown in figure 1.4 reveales that, x-ray diffraction patterns have a strong and highly intense peak having 2θ value about 27.216° with cubic (111) crystalline plane, which shows that film is highly oriented to this plane. There are some another peaks also appear having 2θvalue 45.36° and 52.395° corresponds to C (220), and C (311) plane. XRD pattern revealed that the vacuum evaporated thin film of ZnSe deposited onto highly cleaned glass substrate have cubic phase depicting the crystalline nature of the thin film. The particles size of ZnSe thin films also calculated with the help of Debye-Scherrer formula and found to be 16.831 nm

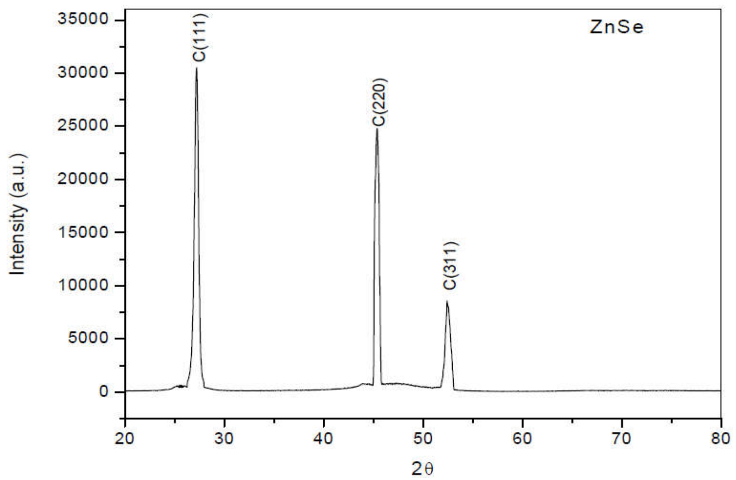

Figure1.4: XRD pattern of vacuum evaporated ZnSe thin films

spite of above structural properties, some other micro structural parameters such as internal strain and dislocation density were also studied by X-ray diffraction patterns of vacuum evaporated $Cd_{1-x}Zn_xSe$ thin films. The calculated values of strain, dislocation density and lattice parameters of vacuum evaporated $Cd_{1-x}Zn_xSe$ thin films are calculated with the help of equations (4), (5), (6) and are shown in Table 1

Table 1: Calculated values of strain, dislocation density and lattice parameters of vacuum evaporated $Cd_{1-x}Zn_xSe$ thin films

Composition	Bragg's angle θ	Planes	Particle size = (D) (nm)	Effective strain = $\varepsilon x10^{-3}$ lin^{-2} m^{-4}	Dislocation density = δ x 10^{15} (lin/m^2)	Lattice Parameters (Å)
Case	12.684	C(111)	11.34	8.6	7.7	
	20.548	H(110)	11.684	5.5	7.3	a_{cub} = 60.08
	22.93	H(103)	12.012	4.5	6.9	a_{hex} = 4.3
	27.795	H(112)	13.956	4.6	5.1	c_{hex} = 7.01

$Cd_{0.6}Zn_{0.4}Se$	13.635	C(111)	16.456	6.76	3.6	a_{cub} = 5.9 a_{hex} = 4.17 c_{hex} = 6.82
	13.90	H(102)	23.80	6.76	1.7	
	18.096	H(102)	18.781	5.0	2.8	
	26.61	C(220)	17.602	3.5	3.2	
	23.515	H(103)	11.898	4.8	7.06	
	25.57	C(311)	12.264	4.0	6.6	
	32.913	H(203)	17.328	2.4	3.3	
$Cd_{0.4}Zn_{0.6}Se$	13.278	C(111)	16.40	7.0	3.7	a_{cub} =5.8
	22.039	C(220)	17.294	2.7	3.3	
	26.046	C(311)	15.074	2.8	4.4	
ZnSe	13.608	C(111	16.837	5.8	3.5	a_{cub} =5.656
	22.683	C(220)	15.766	3.8	4.0	
	26.197	C(311)	14.120	4.3	5.0	

The particles size of vacuum evaporated $Cd_{1-x}Zn_xSe$ thin films at x = (0,0.4,0.6,1) also calculated with the help of Debye-scherrer formula and found to be 11.34, 16.456, 16.40, and 16.831nm respectively.

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