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Study of Structural, Morphological and Compositional Properties of $Zn_{0.75}Cd_{0.25}Se$ Thin Films

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Abstract: The present investigation focuses on the II–VI semiconductor alloy zinc cadmium selenide ($Zn_xCd_{1-x}Se$), with a zinc composition of x = 0.75. $Zn_{0.75}Cd_{0.25}Se$ thin films having a nominal thickness of 1000 Å were fabricated on glass substrates using the vacuum deposition technique under a vacuum pressure of approximately 10^{-5} mbar. High-purity zinc, cadmium and selenium materials procured from Sigma-Aldrich were employed as the source materials for film preparation. The structural, morphological and compositional characteristics of the deposited $Zn_{0.75}Cd_{0.25}Se$ films were investigated. X-ray diffraction (XRD) analysis indicates the formation of a ternary semiconductor compound exhibiting both cubic and hexagonal crystalline phases, with the deposited films displaying polycrystalline characteristics. Scanning electron microscopy (SEM) was employed to examine the surface morphology and particle distribution of the films, while energy-dispersive X-ray analysis (EDAX) was used to investigate their elemental composition. The study provides insight into the structural, morphological and compositional characteristics of vacuum-deposited $Zn_{0.75}Cd_{0.25}Se$ thin films.

Key Words: ZnCdSe, Semiconductor Thin Films, Vacuum Deposition, X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray Analysis (EDAX), Surface Morphology.

I. INTRODUCTION

Zinc cadmium selenide ($Zn_xCd_{1-x}Se$) is a ternary semiconductor alloy formed by combining zinc selenide (ZnSe) and cadmium selenide (CdSe). The properties of this alloy, particularly its optical band gap, can be tailored by adjusting the relative concentrations of zinc and cadmium. Owing to its tunable band gap, ZnCdSe has considerable potential for applications requiring efficient absorption of solar radiation and improved resistance to photocorrosion [5].

$Zn_xCd_{1-x}Se$ belongs to the II–VI semiconductor family and has gained considerable attention in the field of advanced materials and semiconductor technology. It is generally reported as an n-type semiconductor with an optical band gap ranging approximately from 1.75 to 2.7 eV, depending on its composition [2,9]. Previous investigations have indicated that the lattice parameters of $Zn_xCd_{1-x}Se$ decrease progressively with increasing zinc concentration across the compositional range of x = 0 to 1 [7]. Both constituent compounds, CdSe and ZnSe, are known to crystallize in hexagonal wurtzite and cubic zinc-blende structures, depending on their composition and preparation conditions [2,8].

Polycrystalline zinc-incorporated cadmium selenide thin films have attracted research interest because of their potential applications in several electronic and optoelectronic devices. These include laser diodes, projection television display materials, nuclear radiation detectors and light-emitting diodes. Their favourable optical and electrical characteristics, together with their rapid response behaviour, also make them promising materials for photoluminescent, electroluminescent, photoconductive and photovoltaic applications [10,12].

Various techniques have been explored for the preparation of $Zn_xCd_{1-x}Se$ thin films, including electron-beam evaporation, molecular beam epitaxy, chemical bath deposition (CBD), electrodeposition, ion sputtering and vacuum deposition [9]. Among these approaches, vacuum deposition is particularly attractive because it provides a relatively convenient and economical method for producing thin films with quality comparable to that obtained through several sophisticated deposition processes [7].

In the present investigation, $Zn_{0.75}Cd_{0.25}Se$ thin films with a nominal thickness of 1000 Å were fabricated on glass substrates using the vacuum deposition technique. Although $Zn_xCd_{1-x}Se$ materials have been investigated in previous studies, systematic information concerning the influence of film thickness on their physical, chemical, electrical and optical characteristics remains comparatively limited [4]. Therefore, the present work focuses on investigating the structural, surface morphological and elemental characteristics of the deposited films using X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy-dispersive X-ray analysis (EDAX), along with Fourier-transform infrared spectroscopy (FTIR) and atomic force microscopy (AFM). The experimental findings are discussed to understand the characteristics of the prepared $Zn_{0.75}Cd_{0.25}Se$ thin films[2].

II. EXPERIMENTAL

A. Preparation and Deposition of $Zn_{0.75}Cd_{0.25}Se$ Thin Films

$Zn_{0.75}Cd_{0.25}Se$ thin films were fabricated using the vacuum evaporation technique. During the deposition process, a high vacuum of approximately 10^{-6} torr was established with the assistance of rotary and diffusion pumps [1]. The vacuum deposition system

was equipped with Pirani and pressure gauges for monitoring low-vacuum conditions up to 10^{-3} torr, while a Penning gauge was employed to measure higher-vacuum levels within the range of 10^{-2} to 10^{-6} torr [2].

Glass slides were selected as the supporting substrates. Before deposition, the slides were thoroughly cleaned to eliminate surface contaminants and impurities. The cleaned glass substrates were subsequently dried and mounted inside a Hind High Vac vacuum coating unit for thin-film deposition [1,7].

The source material, $Zn_{0.75}Cd_{0.25}Se$, was prepared in ingot form by combining high-purity zinc granules, cadmium granules and selenium powder in the required proportions. The constituent materials were heated together at elevated temperatures inside a quartz tube to obtain a homogeneous compound. Materials having a purity of 99.999%, supplied by Sigma-Aldrich, were used during the preparation process [5–8].

The synthesized $Zn_{0.75}Cd_{0.25}Se$ compound was subsequently ground into a fine powder using a porcelain dish. The powdered material was transferred into a molybdenum boat, which served as the evaporation source. The cleaned glass substrates were positioned above the evaporation source at a suitable fixed distance inside the vacuum chamber.

Throughout the deposition process, the evaporation rate was maintained between 0.2 and 0.6 Å/s [13,14]. The source temperature was varied within the range of 600°C to 1200°C to facilitate evaporation of the source material. Meanwhile, the substrate temperature was maintained at a comparatively low and stable level through continuous circulation of cooling water.

Thin films of $Zn_{0.75}Cd_{0.25}Se$ with different nominal thicknesses were deposited under nearly identical experimental conditions. The required film thickness was monitored and controlled using the digital thickness monitoring system incorporated into the Hind High Vac deposition unit [2,5]. For the present investigation, particular attention was given to the film having a nominal thickness of 1000 Å.

By optimizing the deposition conditions and preparation parameters, thin films with uniform surface coverage, good substrate adhesion and minimal porosity were obtained.

B. Characterization Techniques

The structural properties of the $Zn_{0.75}Cd_{0.25}Se$ thin film with a nominal thickness of 1000 Å were investigated using X-ray diffraction (XRD). The average crystallite size (D) was estimated from the diffraction peak broadening using the Scherrer equation [1,2]

$$D = 0.94\lambda / \beta \cos \Theta$$

Where λ the wavelength of X-ray, Θ is the Bragg's angle and D is the mean dimension of the crystallites.

The lattice parameter (a) for the thin film is determined by using the following expression [6,14].

$$\frac{1}{d^2} = \frac{H^2+k^2+l^2}{a^2}$$

The interplanar spacing'd' has been obtained by using Bragg's law [18]. The structure of the $Zn_{0.75}Cd_{0.25}Se$ film was evaluated by X-ray diffractometer using nickel filtered copper Kα radiation having wavelength λ=1.54060 Å, the formula is given as,

$$n\lambda = 2d \sin \theta$$

Where 'λ' is a wavelength of monochromatic X-rays, 'θ' is the angle between the incident beam and the planes (hkl), 'd' is lattice spacing, 'n' is the order of reflection (n = 1, 2, 3,…..)[10].

Dislocation density is calculated by using formula $\delta = \frac{1}{D^2}$

Micro strain of given thin film is also obtain by formula $\varepsilon_s = \frac{\beta \cos \theta}{4}$ (11)

The surface morphology and topographical characteristics of the $Zn_{0.75}Cd_{0.25}Se$ thin film were examined using scanning electron microscopy (SEM). This technique provides information about the surface texture, particle distribution, grain morphology and film growth characteristics [8]. The elemental constituents and their relative composition were investigated through energy-dispersive X-ray analysis (EDAX).

Fourier-transform infrared spectroscopy (FTIR) was employed to examine the infrared absorption characteristics and identify the characteristic vibrational features associated with the chemical constituents of the deposited thin film. Furthermore, atomic force microscopy (AFM) was utilized to investigate the two-dimensional and three-dimensional surface morphology and topographical features of the film, providing information about its surface structure and roughness characteristics [8,10].

III. RESULTS AND DISCUSSIONS

X – Ray Diffraction - The structural characteristics of the $Zn_{0.75}Cd_{0.25}Se$ thin film with a nominal thickness of 1000 Å were investigated using the X-ray diffraction (XRD) technique. The measurements were performed using Cu Kα radiation with a wavelength of 1.54060 Å. The interplanar spacing (d) corresponding to the observed diffraction peaks was calculated using Bragg's law for the known values of the diffraction angle (θ), X-ray wavelength (λ), and order of reflection (n). The Miller indices (hkl) were assigned by comparing the experimentally obtained diffraction data with the reference patterns available in the Joint Committee on Powder Diffraction Standards (JCPDS) database [1,8,10]. The diffraction pattern was recorded over a 2θ angular range of 5°–80°, with an operating voltage of 40 kV and a current of 40 mA.

The average crystallite size (D) was estimated from the full width at half maximum (FWHM) of the diffraction peaks using the Scherrer equation [1,11]. The value of β (FWHM) was reported as 0.615. The crystallographic characteristics of the deposited films were also considered in relation to the structural differences between CdSe and ZnSe. Since cadmium has a larger atomic radius than zinc, substitution of cadmium atoms by zinc atoms results in a reduction in the lattice parameter. Consequently, changes in the zinc concentration influence the diffraction peak positions and produce a shift in the XRD pattern towards higher 2θ values [10].

The diffraction peaks observed in the CdSe reference pattern are characteristic of the hexagonal wurtzite structure. The reflections corresponding to the crystallographic planes {100}, {002}, {101}, {102}, and {110} occur at 2θ values of 24.900°, 25.013°, 26.299°, 35.090°, and 41.960°, respectively, in accordance with JCPDS card No. 08-0459.

In contrast, the ZnSe reference pattern exhibits diffraction peaks associated with the cubic crystal structure. The reflections observed at 2θ values of 26.299°, 31.520°, 45.200°, 53.600°, and 65.840° are assigned to the {111}, {200}, {220}, {311}, and {400} families of crystallographic planes, respectively, corresponding to JCPDS card No. 19-0191 [2].

The formation of both cubic and hexagonal wurtzite phases has been reported in $Zn_{0.75}Cd_{0.25}Se$ thin films. The structural transformation associated with zinc incorporation has been described as a change from the hexagonal wurtzite phase in cadmium-rich compositions towards the cubic phase in zinc-rich compositions. The coexistence of wurtzite and cubic structures has also been reported for Zn-doped CdSe thin films [12].

The XRD patterns of crystalline Zn doped CdSe [**$Zn_{0.75}Cd_{0.25}Se$**] thin film is shown in Figure 1

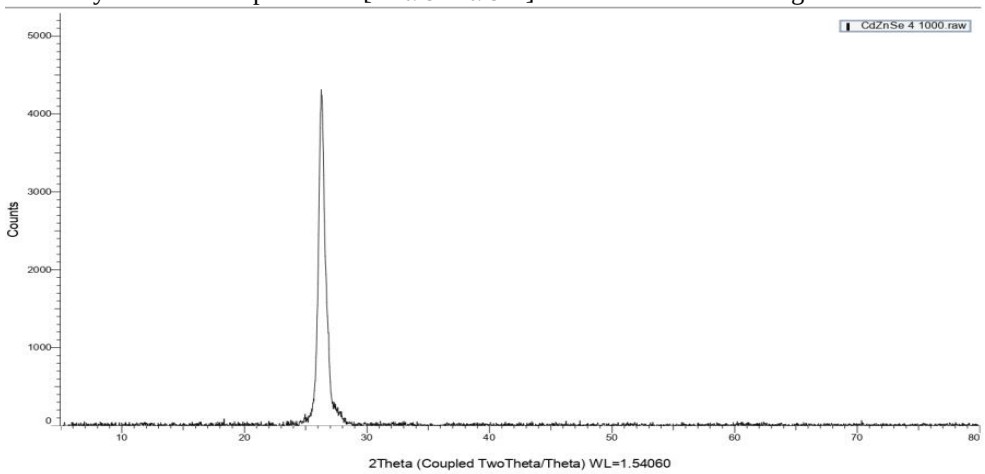

Fig. 1 : XRD of **$Zn_{0.75}Cd_{0.25}Se$** films of thickness 1000 Å

Table 1 & 2. X-ray diffractogram (XRD) **$Zn_{0.75}Cd_{0.25}Se$** sample of thickness 1000 A^0

[hkl] values from JCPDS data	d(Å) values from JCPDS data of cdse	Observed values of d(Å) **$Zn_{0.75}Cd_{0.25}Se$**	Observed (2ɵ)° values of peaks	intensity	Particle size D (nm)	Dislocation density δ ($\times 10^{15}$ lines/m^2)	Micro strain (ε_s)
100	3.574	3.57303	24.900	56	15.534	4.144	0.002331
002	3.557	3.55713	25.013	96	15.538	4.142	0.002330
101	3.386	3.38612	26.299	4255	15.577	4.121	0.002324
102	3.261	2.5547	35.090	47	15.909	3.951	0.002276
110	3.172	2.1517	41.960	42	16.246	3.789	0.002229

[hkl] values from JCPDS data	d(Å) values from JCPDS data of znse	Observed values of d(Å) **$Zn_{0.75}Cd_{0.25}Se$**	Observed (2ɵ)° values of peaks	intensity	Particle size D (nm)	Dislocation density δ ($\times 10^{15}$ lines/m^2)	Micro strain (ε_s)
111	3.386	3.38612	26.299	4255	15.577	4.121	0.002324
200	2.835	2.836	31.520	35	15.761	4.025	0.002297
220	2.004	2.005	45.200	42	16.431	3.704	0.002203
311	1.707	1.708	53.600	27	16.994	3.463	0.002130
222	1.635	1.635	56.150	22	17.192	3.383	0.002106

Scanning Electron Microscope - Scanning electron microscopy (SEM) is an effective technique for investigating the surface morphology and topographical features of $Zn_{0.75}Cd_{0.25}Se$ thin films. It provides valuable information about the film growth mechanism, as well as the shape, distribution, and size of the particles present on the deposited surface [2,6,11]. The SEM micrographs of $Zn_{0.75}Cd_{0.25}Se$ thin films with a nominal thickness of 1000 Å, deposited on glass substrates, are presented in Figure 3.

The morphological examination of the SEM micrographs reveals that the deposited film exhibits a relatively uniform surface with good adhesion to the glass substrate. The images further indicate the presence of very fine and closely distributed grains, which are difficult to distinguish individually and appear to be spread across the entire surface [11,12]. No visible cracks or major surface fractures are observed in the examined micrographs.

The SEM images also reveal particles with spherical and flower-like morphological features distributed over the film surface [8]. These surface features provide information about the morphology and growth characteristics of the deposited $Zn_{0.75}Cd_{0.25}Se$ thin film. The observed particle morphology is consistent with the crystalline growth characteristics reported for the deposited films [4].

The SEM characterization of the $Zn_{0.75}Cd_{0.25}Se$ thin-film samples was carried out at Kavayitri Bahinabai Chaudhari North Maharashtra University (KBCNMU), Jalgaon.

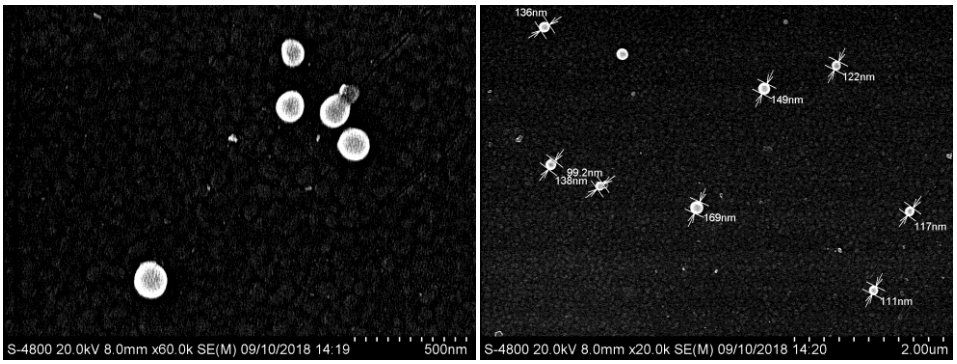

Fig 2: SEM pictures for $Zn_{0.75}Cd_{0.25}Se$ films (a)500 nm (b)2.0 µm

Energy-dispersive X-ray spectroscopy - The elemental composition of the Zn-doped CdSe ($Zn_{0.75}Cd_{0.25}Se$) thin film was examined using energy-dispersive X-ray analysis (EDAX), which confirms the presence of the constituent elements in the deposited material [10]. The EDAX results obtained for the films deposited on glass substrates indicate that the concentrations of cadmium and zinc are lower than their corresponding proportions in the starting material. In contrast, the selenium content remains approximately consistent with its initial stoichiometric proportion [10].

These compositional observations indicate a relatively higher proportion of selenium in the deposited $Zn_{0.75}Cd_{0.25}Se$ thin films. On this basis, the original study associates the selenium-rich composition with the n-type electrical character of the films [12–14].

Table 3 EDAX mass and atomic percentages of **Zn, Se** and **Cd**

Element		**$Zn_{0.75}Cd_{0.25}Se$**	
		Mass %	Atomic %
Zn	30	11.49	15.10
Se	34	59.09	57.80
Cd	48	35.43	27.10

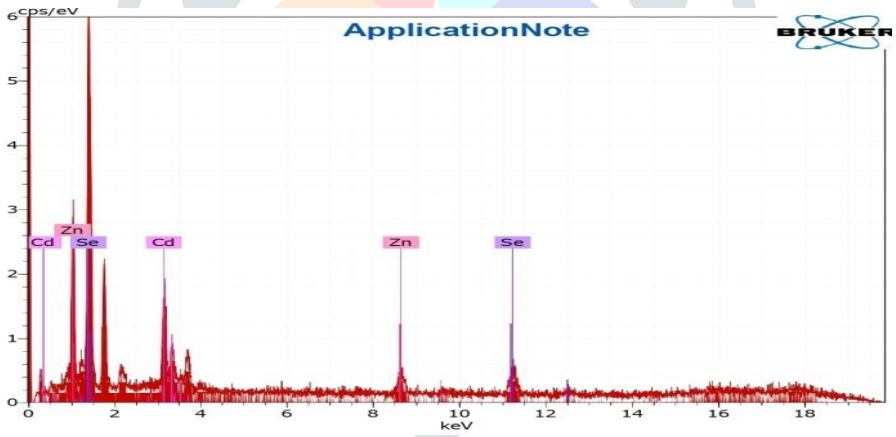

Fig 3:- EDAX spectra of **$Zn_{0.75}Cd_{0.25}Se$**

IV. CONCLUSION

The structural, morphological and compositional characteristics of the vacuum-deposited Zn-doped CdSe ($Zn_{0.75}Cd_{0.25}Se$) thin films with a nominal thickness of 1000 Å were investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy-dispersive X-ray analysis (EDAX).

The XRD investigation revealed that the deposited $Zn_{0.75}Cd_{0.25}Se$ thin films exhibit polycrystalline characteristics with diffraction features associated with both hexagonal wurtzite and cubic crystal structures. The reflections corresponding to the wurtzite phase were assigned to the crystallographic planes (100), (002), (101), (102) and (110), whereas the cubic phase exhibited preferred crystallographic orientations along the (111), (200), (220), (311) and (222) planes. The experimentally determined lattice parameters were found to be in close agreement with the corresponding reference data for CdSe and ZnSe available in the JCPDS database. These observations indicate that the deposited films possess crystallographic features associated with both constituent semiconductor materials.

The crystallite size estimated using the Scherrer equation was found to be in the range of approximately 15–17 nm. The calculated dislocation density (δ) and microstrain (εs) values were reported in the ranges of 3.383–14.144 and 0.002106–0.002334, respectively, for the investigated wurtzite and cubic structural features. These structural parameters provide information about the crystallite dimensions, lattice imperfections and internal strain present in the deposited films.

The SEM micrographs revealed relatively uniform film growth over the glass substrate, with no prominent surface cracks observed in the examined regions. The deposited material exhibited spherical and flower-like morphological features distributed across the surface. The estimated grain or surface-feature dimensions were found to vary from approximately 99 nm to 169 nm. The difference between the SEM-observed feature dimensions and the XRD-derived crystallite size suggests that the visible surface features may consist of several smaller crystallites or crystallite aggregates.

Furthermore, EDAX analysis confirmed the presence of the constituent elements in the $Zn_{0.75}Cd_{0.25}Se$ thin film. Strong characteristic signals corresponding to cadmium and selenium were observed in the EDAX spectrum, supporting the presence of these elements in the deposited material. The elemental analysis therefore provides additional evidence regarding the composition of the synthesized thin film.

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