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# Nanostructural Characterization Of Molar Dependent PVA Embedded Synthesized CdSe Thin Films

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***Abstract:***
*CBD (Chemical Bath Deposition) technique was used to synthesize CdSe thin films at molars 0.2M≤ b.≤0.8M on ultrafine micro-glass slides and silicon wafer substrates. XRD and FESEM techniques were used to study crystal structures and surface morphology of the films at different molar concentrations. The FESEM surface structures of the as grown CdSe thin films at different molarity showed formation of uniform distribution of CdSe –micro-particles without vacancies and transform into leave-like structures with increase of molarity from 0.2M to 0.4M and then into clusters as molars of the solution increase. The X-ray diffraction spectral analysis showed maximum peak intensity along (200)-:0.2M plane, (100)-0.4M, 0.6M and 0.8M reflection planes. The evaluated lattice parameters **a -** and **d** -values were matched with the JCPDS values. The pattern confirms CdSe cubic zinc blend structure. The grain sizes were calculated and found to exist between 20nm - 60nm where the size decreased with increase of molar concentrations. However, the dislocation density in the CdSe films were found to increase with molarity. The CdSe nanocrystalline filme were observed residual strained with 55.55 x $10^{-2}$ and enhanced residual stresses from 4.25-32.21GPa at 100% x-rays intensity with increase of molars.*

***Keywords:****Cadmium Selenide thin film, CBD, XRD, FESEM, nanostructure*

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## I. Introduction:

In the present 21st century, science and technology has evolved to bring about tremendous advancement and renovations in material science for the betterment of human society. Nanoscience is the study of materials' unique properties and behaviours at nanoscale 1-100nm (1nm=$10^{-9}$m) while nanotechnology is the application of the scientific knowledge to design and manufacturing of new products, devices for practical purposes. All these innovative advanced products available today depend on how the atoms in matters are arranged by manipulation at nanoscale. Therefore, investigation on nanostructures of materials and their characterization is indispensable work correlating to design and fabrication of new device and applications.

Cadmium selenide is binary bulk semiconducting compound in II-VI group and has a direct energy band gap in the range ( 1.70 – 1.80)eV [1,2] Thin films of CdSe find several potential applications in fabrication of thin film transistor, LEDs, photovoltaic Cells, LESER, [3,4,5]. A large number of scientists and researchers workers are found investigating on thin films of CdSe by several deposition techniques. However synthesis of cadmium selenide thin films at different molars by Chemical Bath Deposition (CBD) method is a rare case. In the present work, we prepare thin films of CdSe on micro glass substrates and Silicon wafer substrates at room temperature at different molar concentrations using high purity AR grade chemicals.

## II. Materials And Method:

In the synthesis process, we used high purity chemicals(i) Cadmium Chloride ($CdCl_2$) [ AR Grade Aldrich Sigma] for $Cd^{2+}$ - Cation Source, (ii)Sodium Solenosulphate ($Na_2SeSO_3$) → $Se^{2-}$ for anion Source, (iii) Trisodium Citrate [ $Na_3C_6H_5O_7$] as Reducing agent, (iv) Ammonium hydroxide ($NH_4OH$) as catalyst to adjust $p^H$ -value of the solution and (v) PVA for adhesive to substrates as well as for dispersing of CdSe micro – particles, in the following steps:

Stage-1.

i) We prepared equimolar solution of $CdCl_2$ at 0.2M in 100ml D.I. water by dissolving 4.027gm. and the resultant solution was stirred for 30mins.
ii) A few drops of $NH_3$ solution was added drop by drop in the precursor solution to adjust its pH value in the range 9-10 with constant magnetic stirring.

iii) 2wt.% PVA in 100ml D.I. water was prepared by dissolving 2gms. of PVA and stirred for 1hr. at 70$^0$C till PVA dissolves. Then 50ml of PVA solution was added to the precursor solution and stirred for 1hr. at 70$^0$C to reflux homogeneous solution.

Stage-2.

*Preparation of 0.4M sodium solenosulphate ($Na_2SeSO_3$) solution*:

i) We dissolved 2.524gm of sodium sulphite ($Na_2SO_3$) at 0.4M in 100ml DI water and 0.5gm of powder selenium was added to it, and the resultant mixture was refluxed at 70$^0$C for 1hr with constant stirring to yield 0.2M sodium solenosulphate ($Na_2SeSO_3$) solution.

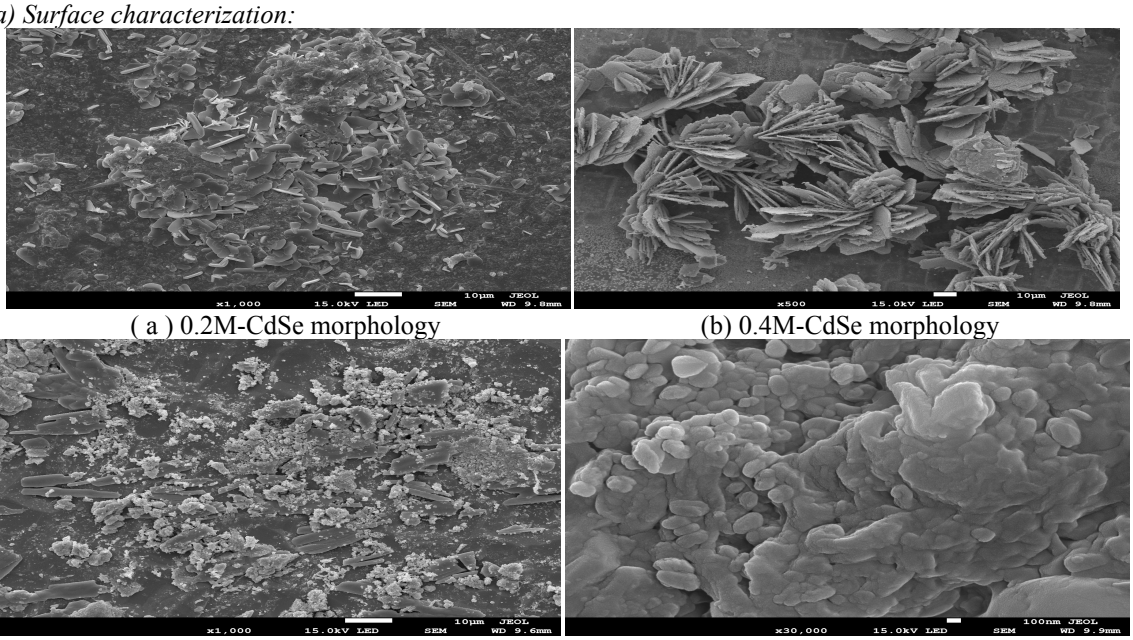
ii) We added 10ml trisodium citrate to the precursor solution, stirred and mixed the solution with the final precursor solution as in stage-1.

**iii)** Now, 5 number of properly etched and cleaned micro glass substrates or silicon wafer substrates wereclamped verticallyin the mixture solution for 48 hrsto adhereCdSe thin films on the substrates at 0.2M. Similarly, 0.4M, 0.6M, 0.8M and 1.0M CdSe thin films were systematically synthesized.

**iv)** The CdSe deposited substrates were annealed at 500$^0$C for three hours and kept overnight in electronic oven, withdrawn and rinsed gently in stream of DI running water to obtain fine CdSe thin films after removal of course unwanted particles.

## III. Results And Discussion

*3.(a) Surface characterization:*




( a ) 0.2M-CdSe morphology (b) 0.4M-CdSe morphology

( c ) 0.6M-CdSe morphology (d) 0.8M – CdSe morphology

**Figure 1. FESEM micrographs of selected molar depended CdSe films.**

The as deposited CdSe thin films at varied molars were scanned FESEM images for study of surface atomic micrographs as shown in Fig.1. (a, b, c & d). The analysis of the micrographs is observed that at 0.2M CdSe films, the particles in the film are resolved finely dispersed paddy seeds like structures without cracks or holes which are observed transformed into leaf-like structures in 0.4M CdSe films. The Figs. 1. ( c& d) show that the micro particles in the films are clustered and the clustered sizes of the CdSe particles are observed enhanced linearly with molars. The particle sizes in the films play crucial roles qualitatively and quantitatively, as will be measured from their spectral analysis.

*3.(b) XRD – spectral analysis:*

Figs. (2, 3, 4 & 5) represent the X-ray diffraction spectra of the as synthesized CdSe thin films at 0.2M, 0.4M, 0.6M and 0.8M at room temperature onto micro-glass substrates and annealed at 400$^0$C. The 0.2M CdSe XRD spectra showed the slow crystalline growth at 13$^0$ and 24$^0$ diffraction angles with corresponding twin reflection planes (100) and (110), while polly-crystalline growth with remarkable multifaceted X-ray diffraction planes (100), (110), (200), (211) and with some

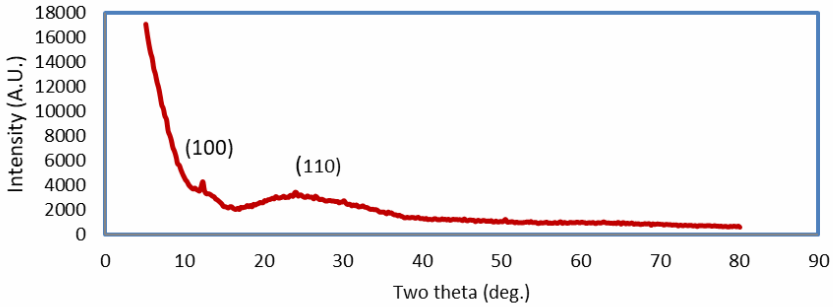



**Figure 2. XRD pattern of 0.2M of CdSe films.**

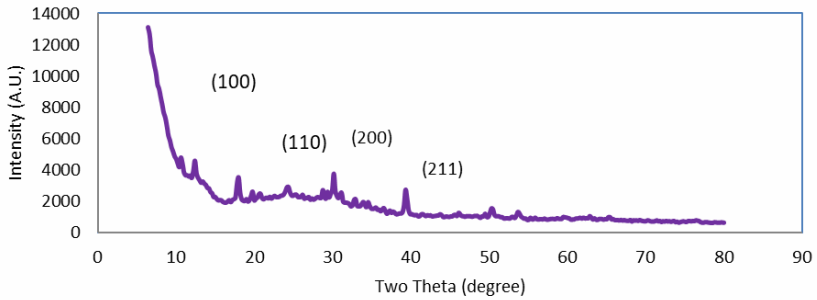



**Figure 3. XRD pattern of 0.4M CdSe films.**

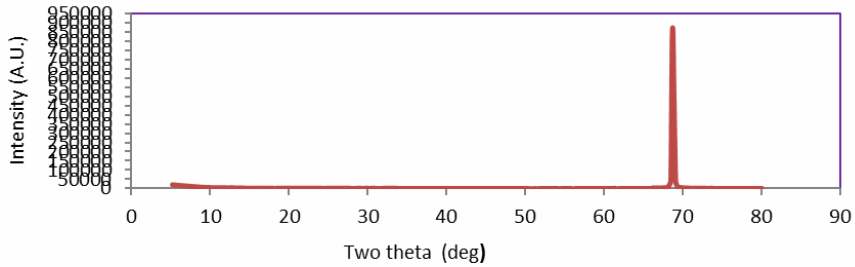



**Figure 4. XRD pattern of 0.6M CdSe thin film.**

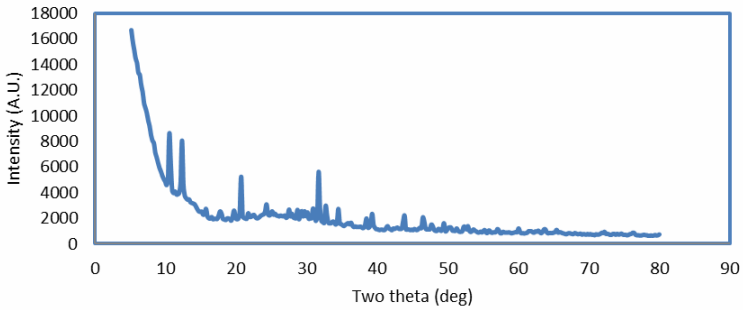



**Figure 5. XRD pattern of CdSe 0.8M.**

additional planes are observed in Fig. 3 in the 0.4M CdSe thin films.. The X-ray diffraction planes corresponding to the peak intensity in the spectra were calculated from the Bragg's relation [6, 7]

$$\mathrm{Sin}^2\Theta = (\lambda^2/4a^2) \times m \qquad (\because 2d\mathrm{Sin}\Theta = n\lambda) \qquad (1)$$

where $m = h^2 + k^2 + l^2$ and $\lambda = 1.54$Å for X-rays. The crystal lattice parameters **a** and ***d***–values were determined from the relation

$$a = (\lambda/2\mathrm{Sin}\Theta) \times m \qquad (2)$$

and

$$d = \lambda/2\text{Sin}\Theta \qquad (3)$$

**Table-1**. Evaluated lattice parameters at varied molars.

| Molars (M) | 2Θ (degree) | hkl-values | JCPDS $a_o$-value (Å) | $a_{cal}$-value (Å) | JCPDS $d$- value (Å) | $d_{cal}$-value (Å) |
|---|---|---|---|---|---|---|
| 0.2 | 1`3 | 100 | | 6.302 | | 6.802 |
| | 24 | 110 | | 5.237 | | 3.679 |
| | 11 | 100 | | 8.330 | | 8.033 |
| 0.4 | 20 | 110 | | 6.270 | | 4.434 |
| | 30 | 200 | | 5.950 | | 2.975 |
| | 39 | 211 | | 5.650 | | 2.307 |
| | 51 | 311 | | 5.932 | 1.820 | 1.789 |
| | 54 | 222 | 5.832 | 5.875 | | 1.696 |
| 0.6 | 69 | 411 | | 5.758 | | 1.359 |
| | 11 | 100 | | 8.415 | | 8.415 |
| 0.8 | 21 | 110 | | 5.975 | | 4.225 |
| | 24 | 111 | | 5.237 | | 3.704 |
| | 32 | 200 | | 5.587 | 2.130 | 2.794 |
| | 33 | 210 | | 6.062 | | 2.711 |
| | 38 | 211 | | 5.793 | 2.150 | 2.365 |
| | 44 | 220 | | 5.814 | | 2.056 |
| | 46 | 300 | | 5.912 | | 1.971 |

The crystal structures corresponding to the host samples at 0.2M, 0.4M, 0.6M and 0.8M were determined from the relation [8]

$$\text{Sin}^2\Theta_1/\text{Sin}^2\Theta_2 = (h_1^2+k_1^2+l_1^2)/(h_2^2+k_2^2+l_2^2) \qquad (4)$$

and were found to be f.c.c.cubic zincsulphide structures as shown in Table-2. The grain size or particle diameter in the films plays very important roles in nanoscience and technology relating to structural, optical, magnetic and opto electronic properties for fabrication of device and applications. The particle or grain sizes in the CdSe films at molars were determined fromthe Scherrerrelatioin [9, 10] at 100% intensity

$$D_{hkl} = k\lambda/\beta_{2\Theta} \text{ x } \text{Cos}\Theta \qquad (5)$$

where $\beta_{2\Theta}$ is the FWHM in the X-ray diffraction spectra measured in radians, Θ is the Bragg's angle, k is the shape factor whose value is taken as 0.94 and λ for X-rays is 1.54Å. The sizes of the grains were found to exist in the nanometer range 20nm to 60nm and observed to decrease with increase of molar concentrations (Table-3). Fig.6. shows thevariation of particle size vs. molar concentrations.

**Table-2**. Molar dependent CdSe crystal structures

| Molars | $h_1k_1l_1$ | $h_2k_2l_2$ | $2\Theta_1$ (degree) | $2\Theta_2$ (degree) | $\text{Sin}^2\Theta_1/\text{Sin}^2\Theta_2$ | $(h_1^2+k_1^2+l_1^2)/(h_2^2+k_2^2+l_2^2)$ | Crys. Stru. |
|---|---|---|---|---|---|---|---|
| 0.2M | 100 | 110 | 15 | 24 | 0.4 | 0.5 | Cub. (fcc) |
| 0.4M | 100 | 110 | 18 | 20 | 0.81 | 0.5 | Cub. (fcc) |
| 0.6M | No two adj. planes observed | | | | | | nil |
| 0.8M | 100 | 110 | 12 | 21 | 0.3 | 0.5 | Cub. (fcc) |

**Table-3.** Grain size, dislocation density, micro-stress and strain

| CdSe films | HWHM *(2Θ)* (degree) | Grain Size (D) (nm) | Dis. density *(δ) x 10¹⁵* lines/m² | Residual strains x $10^{-2}$ | *a*-value (Å) | Residual stress at 100% int. (S) (GPa) | Ave. residual stress (S) (GPa) |
|---|---|---|---|---|---|---|---|
| 0.2M | 0.276 | 30.15 | 1.10 | 55.55 | 5.710 | 4.25 | 3.96 |
| 0.4M | 0.288 | 28.90 | 1.20 | 55.53 | 5.830 | 6.14 | 2.56 |
| 0.6M | 0.138 | 60.30 | 0.28 | 55.52 | 6.320 | 31.49 | 3.05 |
| 0.8M | 0.394 | 21.10 | 2.25 | 55.54 | 6.390 | 32.21 | 4.01 |

***E = 42.5GPa, γ = 0.3 for CdSe material*

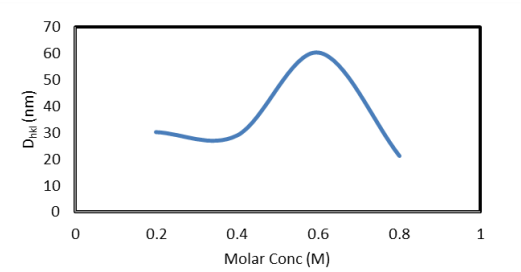



**Figure 6. Grain sizes vs. molar conc.**

*3.(c ) Dislocation density, residual strains and residual stress*

The intergrain crystalline states like dislocation density, residual stress and strains in the films were also studied which correlate the functional properties in electronic device and applications. Such dislocation density in the host CdSe films were calculated from the relation [11,12,13 ]

$$\delta = 1/D^2 \qquad (6)$$

in lines/$m^2$ where D is the particle diameter in the films. Fig. 7. Shows the variation of dislocation density vs. molar concentrations in the films.

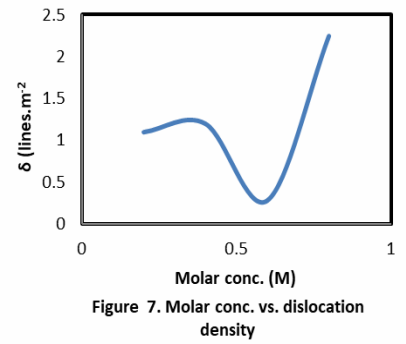



**Figure 7. Molar conc. vs. dislocation density**

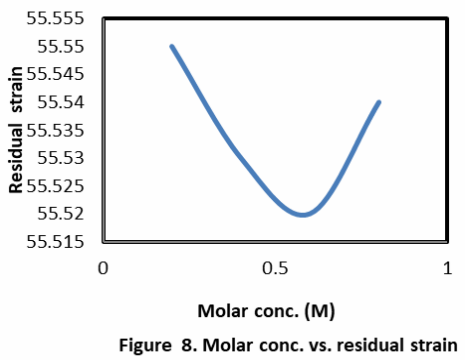



**Figure 8. Molar conc. vs. residual strain**

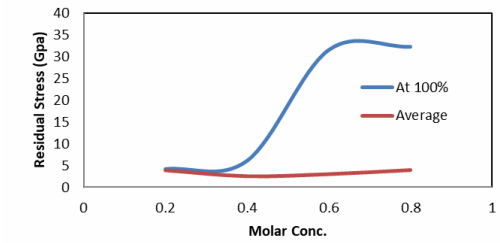



**Fig. 9. Molars vs. Residual Stress in CdSe films.**

The as grown semiconducting thin films under extreme care of experimentalconditions are naturally associated with various residual strains and stress on account of some physical uncontrollable factorslike fluctuations of lattice parameters and oxygen vacancies and thermal expansion co-efficients in the films [14 ]. The residual strains between lattice atoms were calculated from the relation [9]

$$\varepsilon = \beta 2\theta \text{ x } \text{Cot}\theta/4 \qquad (7)$$

The residual stress of the lattice atoms were also determined from [10]

$$S = E/2\gamma \text{ x } (a0 - a)/a0 \qquad (8)$$

where $a_0$ , for bulk material of CdSe, $a$ , for CdSe thin film, $E$, Young modulus of elasticity of the material = 42.5GPa and $\gamma$, Poisson ratio = 0.3 [11].The as deposited crystallined CdSe thin films are observed with undesirable residual stresses being comparatively higher at 100% X-ray peak intensity over the average values. The variation of residual stress vs. molar concentration in the CdSe thin films is shown in Fig. 8. Basically,

these residual stresses in the crystals are caused on account of non-uniform thermal expansion, mismatching materials or some plastic deformation or lattice defects during the process of synthesis and are expected to be minimized through controlled cooling

## IV. Conclusion

Molar dependent CdSe thin films grown by CBD technique are found to be crystallized with cubic zinc blend structures with uniform distribution of surface structures. The crystallinity is enhanced linearly with increase of molar concentrations. The grain sizes in the films are found to be nanocrystallite sizes between 20nm – 60nm. The films are found to exist with some crystal defects or dislocation density but controlled by undesirable residual stresses.

## Acknowledment

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