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Structural, morphological and optical properties of CdS thin film prepared by perfume atomizer

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Abstract: Nanocrystalline cadmium sulfide (CdS) thin film was deposited on glass substrate by relatively simple, quick and cost effective perfume spray atomizer method at the temperature 350^0C. A further study has been made for structural, surface morphological and optical properties of the film using X-ray diffraction (XRD), scanning electron microscopy (SEM), and optical absorption method. The deposited CdS thin film exhibited hexagonal phase with optical band gap (Eg) of 3.0 eV. SEM images confirmed that films of smooth surface morphology and nanocrystalline nature with fine crystallites.
Keywords: Nanocrystalline thin films, cadmium sulphide, Band gap, X-ray diffraction, morphological and optical properties.

I. INTRODUCTION

Cadmium sulfide (CdS) is wide band gap material belongs to II-VI group compound materials. Its band gap varies from 2.1 - 2.4 eV, depending upon the composition. The CdS thin films have been used in applications such as field effect transistors, light emitting diodes [3-4], optical window solar cells [1-2], photocatalysis and biological sensors [5-6] optical coding, optical data storage and sensing [7], nonlinear integregated optical device [8]. In recent years there has been growing interest in developing techniques for preparing semiconductor nanoparticles and thin films because the properties in nano form differ significantly from those of their bulk counter parts. Therefore there is much interest in physical properties of nanometer size (20-80nm) semiconductor materials due to their novelties; their properties are different and often superior to those coarse grained polycrystalline materials and also amorphous alloys of same composition [9-10]. In addition to increased strength, hardness, enhanced diffusivity, improved quality, roughness, reduced elastic modulus, higher thermal exapansion coefficient, lower thermal conductivity and superior soft magnetic properties [11]. Much effort has been made to control the size, morphology and crystallinity of CdS thin film. In past many researchers have been deposited CdS thin films by both gas phase and liquid phase methods. Gas phase deposition method includes vacuum evaporation [12], flash evaporation, activated reactive evaporation (ARE), sputtering and chemical vapor deposition (CVD) [13] whereas liquid phase include electrodeposition [14], chemical bath deposition (CBD) [15-17] and spray pyrolysis methods. Among them, perfume spray pyrolysis is well known d for simple and cost effective method for depositing large area of semiconductor thin films.

Many researchers have deposited CdS thin film by spray pyrolysis method. In this paper, we report perfume spray method for the synthesis of nanocrystlline CdS thin film on the glass substrate. The deposition condition for CdS thin film was optimized to get good quality, well adherent films onto glass substrate. The as deposited film was characterized for structural, surface morphological and optical technique.

II. EXPERIMENTAL DETAILS

CdS thin film was prepared using spray pyrolysis by a simple perfume atomizer. Cadmium chloride as cadmium source and thiourea as sulfur source. 0.2 M of cadmium chloride ($CdCl_{2)}$ and 0.2M of thiourea were taken with D.I water and they were striated for 1 hour as spray solution. For deposition, 50 ml solution was sprayed through perfume bottle on to the preheated (350 °C) glass. Before the start of the deposition process, the glass plate was cleaned with chromic acid and acetone and then ultrasonically cleaned with de-ionized water in order to remove the contaminants if any on the surface and to improve the adhesiveness of the films. The experiment was repeated three times keeping the spray interval as 5s. Thickness of the deposited films was measured by weight difference method. After measuring the thickness, they were subjected to micro structural, morphological and optical studies using X-ray diffraction (XRD) and scanning electron microscope (SEM). XRD study was carried out using X'pert PRO (PANalytical) diffractometer with CuKα radiation (k = 0.15405 nm) in steps of 0.1 over the 2θ range of 20° – 80°. Hitachi S-3000H model SEM was used to study the crystallite size and morphology of the grown CdS thin film. For the SEM studies, the samples were coated with Au using JFC-1100 model sputter instrument. Optical transmission study was also carried out using Perkin Elmer Lambda 35 spectrophotometer in the wavelength range of 300–1100 nm. Figure 1 show the simple spray pyrolysis setup.

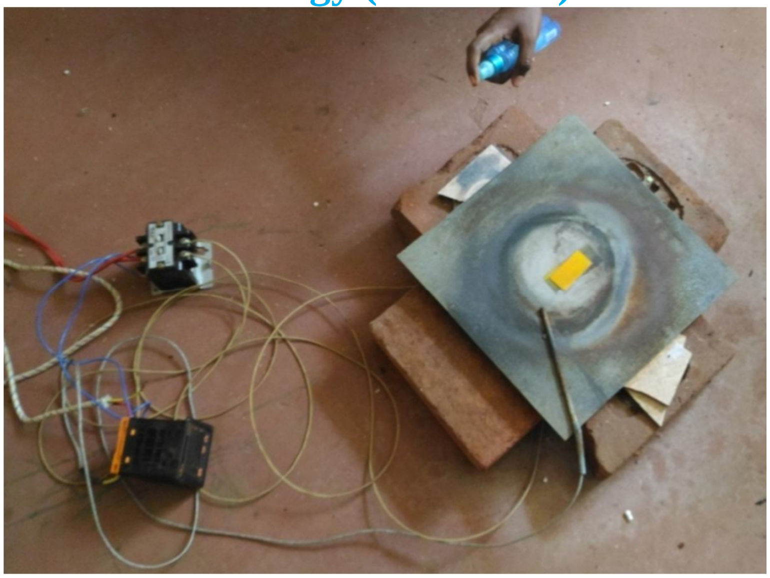

Figure 1 Simple Spray Pyrolysis technique

III. RESULTS AND DISCUSSION

A. Thickness Measurement

Thickness is the most important film parameter, which controls the film properties. Hence, precise knowledge of the film thickness is necessary for the intensive study of the properties of thin films. Thickness of the prepared film was estimated using weight method. The well-cleaned glass plate is weighted in a high precision microbalance. After the deposition the coated glass plate is weighted. The difference in weight gives the mass of the deposited film "m". The area over which the film deposited is measured as "A". The standard value of density "ρ" has been taken and the thickness is calculated using the expression.

$$t = m/ (A\rho) \text{ (microns)}$$

Where, t – is the thickness of the film, m – is the weight difference (Mass of the film), A – is the area of the film and ρ – is the density of the film. The thickness of the prepared CdS film was 540 nm.

B. XRD Analysis

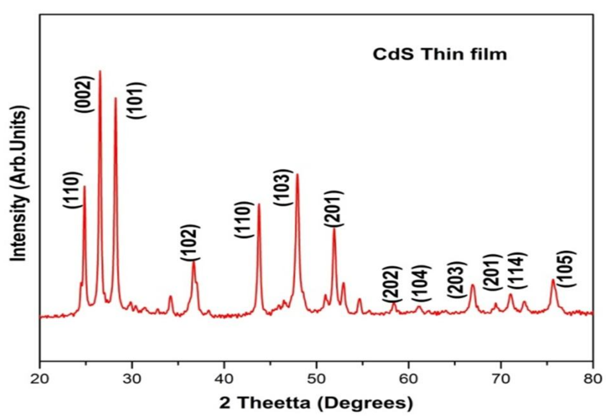

Figure 2 The X-ray diffraction patterns for pure CdS thin film

Figure 2 shows the X-ray diffraction pattern of the spray deposited CdS thin film. The XRD pattern obtained correlate well with standard JCPDS (41-1049) data. Good agreement between the observed (3.35366 A^0) and standard *d*' (3.35643 A^0) values suggests that the material deposited was CdS with hexagonal structure. The predominant peak at 26.5576^0 indicates that CdS is preferentially oriented along (002) plane. Crystallite size (D) was calculated using Debye - Scherer's formula [18 - 20].

$$D = \frac{k\lambda}{\beta Cos\theta}$$

Where D is the crystallite size, the constant 'k' is the shape factor = 0.94, 'λ' is wavelength of X-rays (1.5406 ÅCuK_α) 'θ' is the Bragg's angle and 'β' is FWHM. The calculated crystallite size using Debye - Scherer's formula is 52.81 nm.

The dislocation density (δ) is the reciprocal of the square the crystallite size (D). The calculated value for the dislocation density is $3.4040 \times 10^{14}/m^2$. The micro strain (ε) of the film can be calculated using the formula.

$$\varepsilon = \left(\frac{\lambda}{DCos\theta} - \beta\right)\frac{1}{\tan\theta}$$

The micro strain estimated to have a $12.38 \times 10^{-4}/m^2$. The grain was also calculated using the Willamson – Hall equation [21].

$$\beta\cos\theta = \frac{k\lambda}{D} 2\ \varepsilon\sin\theta$$

The calculated grain size using the Willamson – Hall equation is 56.08 nm.

C. Morphological Analysis

Scanning electron microscopy is a convenient tool to study the surface morphology of micro, nano-materials as well as thin films. Figure 3 shows the SEM image of CdS thin film. The SEM micrographs were recorded at 1000 kV with magnification 10000. The film had small uniformly spherical grains and nearly uniform grains sizes spread throughout the surface and also some void and vacancies are there. Though a smooth morphology was achieved some smaller particles agglomerated randomly.

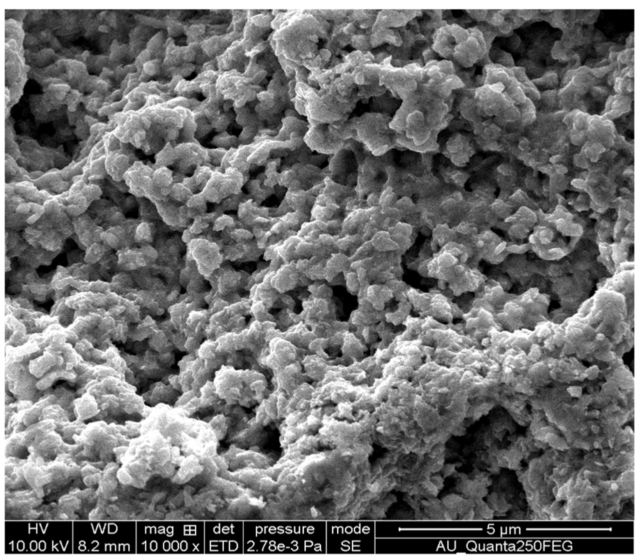

Figure 3 SEM micrograph of CdS thin film

D. Optical Analysis:

1) *UV-Visible Spectroscopy:* The optical transparency of the CdS thin film fabricated by simplified spray pyrolysis technique is show in figure 4. The percentage transmission takes very low wavelength region (λ<500 nm) which is the spectral region of edge absorption. In this region the incoming photons have sufficient energy to excite electrons from the valence band to conduction band and thus these photons are absorbed within the material to decrease the transmission. The maximum transmission was found in the wavelength region (λ>500 nm). Figure 5 shows the variation of $(\alpha h\nu)^2$ with the photon energy for CdS thin film deposited on glass substrate. The absorption coefficient (α) and incident photon energy (hν) can be related as

$$\alpha = \frac{A(h\nu - E_g)^m}{h\nu}$$

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where A is a constant and E_g is the band gap of the material. The values of m depends upon the type of the transition; which may have values 1/2, 2, and 3/2 corresponding to the allowed direct, allowed indirect, and forbidden direct transitions respectively. From the above equation, it is clear that the plot of $(\alpha h\nu)^2$ versus hν (Figure 5), will indicate a divergence of an energy value, E_g where the transition takes place. The values of optical band gap energies E_g were obtained by extrapolating the straight portion to the hυ axis at (αhυ) = 0. In all the cases, the relation is linear in the absorbance region. It is due to the direct band-to-band transition. The band gaps energy was found to be 3.0 eV for CdS thin film.

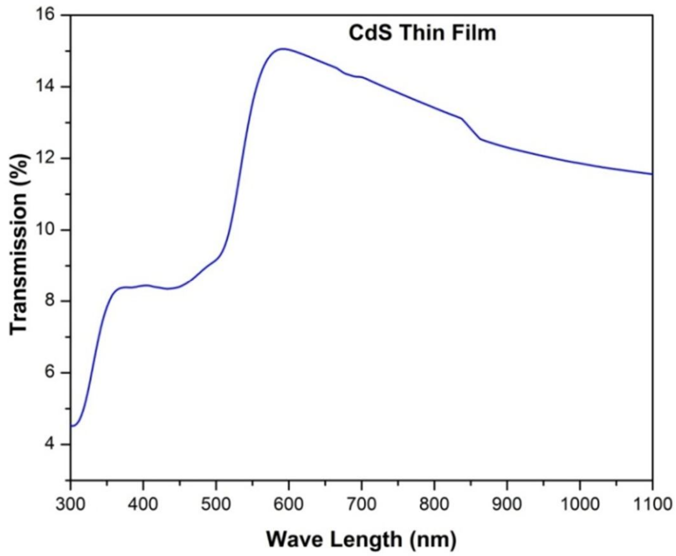

Figure 4 Transmission spectra of CdS thin film

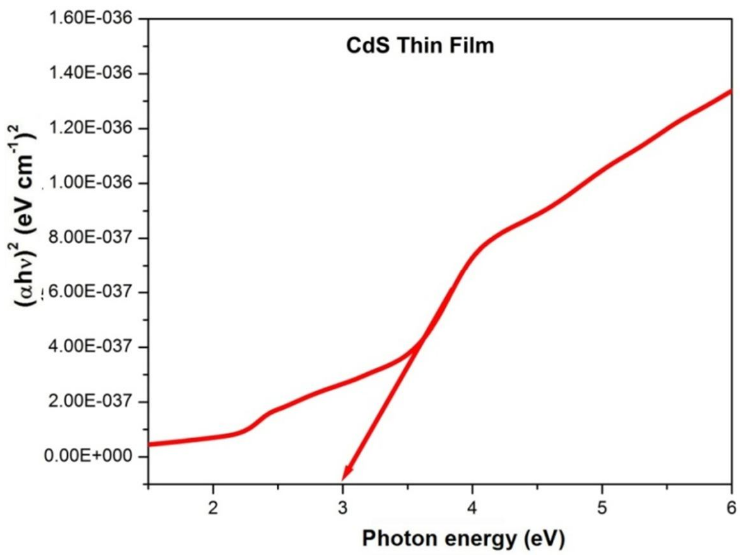

Figure 5 Tauc's plot of CdS thin film

IV. CONCLUSION

CdS thin films were fabricated by cost effective perfume atomizer using spray pyrolysis method. XRD studies show that the prepared film had hexagonal structure having preferential orientation along (0 0 2) plane. Crystallite size, Dislocation density and micro strain values are calculated from XRD. The surface morphology study reveals the presence of uniformly sized spherical grains distributed over the surface. The optical band determined from the transmittance spectra was found to be equal to 3.0 eV.

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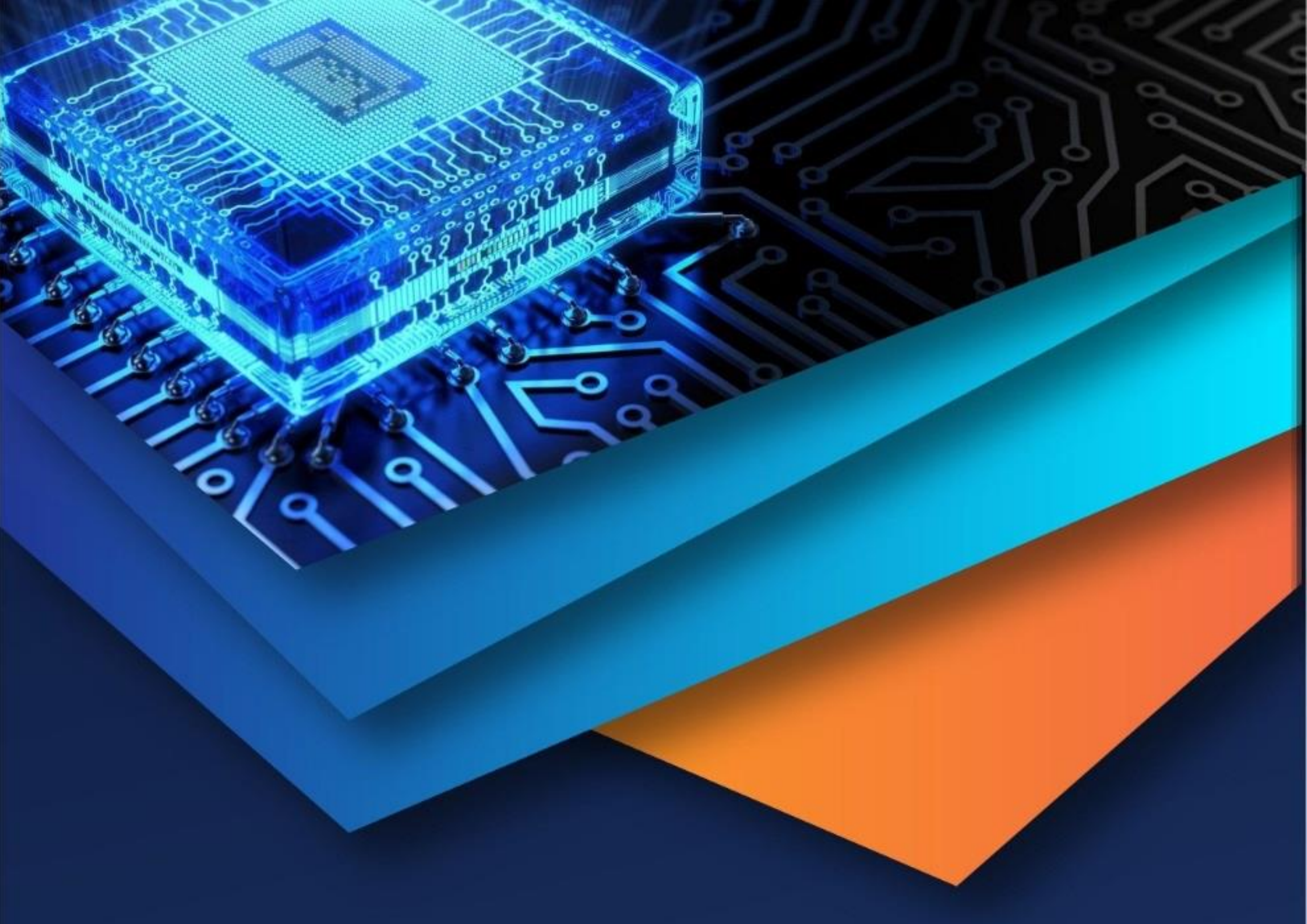

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