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Deposition and characterization of CdS thin films by chemical bath deposition

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Abstract: Cadmium sulphide (CdS) thin films were deposited on glass substrate by chemical bath deposition (CBD). The bath-temperature of 80^{o}C and pH = 11 was maintained. The films were characterized by XRD, UV-visible spectrophotometer, Ellipsometer, SEM and Raman spectrum. The film-thickness of 391.1 nm was revealed by Ellipsometry. XRD confirmed the films to be in a mixed phase of hexagonal and cubic structure. UV-VIS spectral analysis yielded a band gap of 2.35 eV. The SEM micrograph exhibits uniform surface coverage and Raman spectrum of the films shows characteristic CdS peaks.
Key words: CBD; CdS thin films; XRD; SEM; Raman spectrum.

1. Introduction[1-4]

CdS is one of the most studied materials with a direct band gap of 2.42 eV at room temperature. CdS exists in two crystalline forms: hexagonal (wurtzite) Phase and cubic (zincblende) phase. CdS thin films can be obtained by vacuum evaporation, sputtering, electrochemical deposition, pulsed laser deposition and chemical bath deposition (CBD). CBD is a low cost method readily scalable to large-area deposition. Deposition and characterization of CBD-CdS thin films is presented in this paper.

2. Experimental[1-4]

A 250 mL capacity chemical bath was chosen. Ar grade chemicals (Sigma-Aldrich) were used. The bath temperature of 80^{0}C and pH of 11 were set. Microscopic glass slides (75 x 25 x 1.45 mm^{3}) were used as the substrate. Cadmium sulphate ($CdSO_4$) was used as a cadmium source and thiourea ($CS(NH_2)_2$) as the sulfur source. 2.5mL of aqueous solution of 1 M $CdSO_4$ was taken in the bath. 150 mL of 10 M ammonium hydroxide (NH_4OH) was added till the initially formed white precipitate of cadmium hydroxide $Cd(OH)_2$ in the bulk of the solution dissolved completely. The substrate was cleaned with distilled water, liquinox soap, soaked in dilute hydrochloric acid for one day, washed with ethanol, acetone and finally with distilled water and oven-dried for one hour. The substrate was dipped in the bath-solution with its plane inclined to the surface of the solution. To promote gravity-assisted deposition steadily (laminar flow) 10mL of 1 M thiourea solution was poured on the

substrate through a funnel. After deposition of one hour, the substrate was removed, cleaned and dried in air at room temperature. Adherent, transparent and yellow coloured CdS thin films were obtained.

2.1 Characterization techniques

The thickness of the films was measured using J. A. Woollam Co., Inc. M2000U ellipsometer. The X-ray diffractogram of the films was recorded by X-PERT PRO X-ray diffractometer using CuK_α radiation (λ = 1.54056 Å). The UV-VIS spectrum of the films was recorded by GBC-CINTRA 40 in the wavelength range 200-900 nm. The Raman spectrum (27°C) was recorded by HR800 (Horiba Jobin Yvon) using Ar laser (λ = 514 nm). Surface morphology of CdS thin films was observed in the SEM using FEI-Netherland Quanta 200.

3. Results and discussion

3.1 X-ray diffraction (XRD)

The XRD pattern of the films (Fig. 1) has a large number of peaks (111), (200), (220), (311), (222), (400) of the cubic phase (zinc blende) and peaks (100), (002), (101),(102), (110), (103), (112) of the hexagonal (wurtzite) phase (Polymorphism)[2]. The grain-size in the films estimated using Debye-Scherrer formula for (002) H reflection at 2θ=26.375° is 15.5 nm.

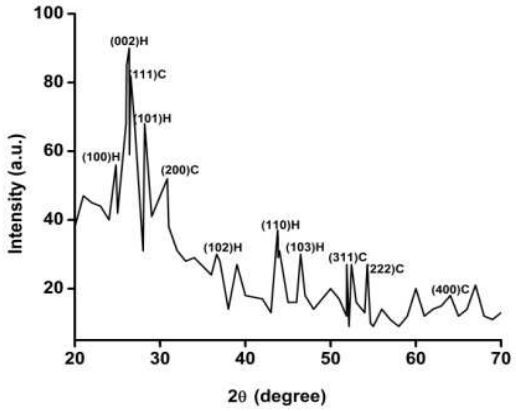

Fig. 1. XRD pattern of CdS thin films

3.2 UV-VIS spectrophotometer

UV-VIS spectrum shows the film to be transparent to 40% radiation for wavelength above 500 nm and more than 50% above 750 nm. The absorption edge is at 478 nm. The optical band gap is calculated using the formula $\alpha = \frac{A\left(h\nu - E_g\right)^{1/2}}{h\nu}$ where hν is the photon energy, E_g is the optical band gap of the material and A is a constant. The linear portion of the plot $(\alpha h\nu)^2$ vs hν extrapolated for $(\alpha h\nu)^2 = 0$ (Fig. 2) gives band gap value of 2.35 eV consistent with literature data[2].

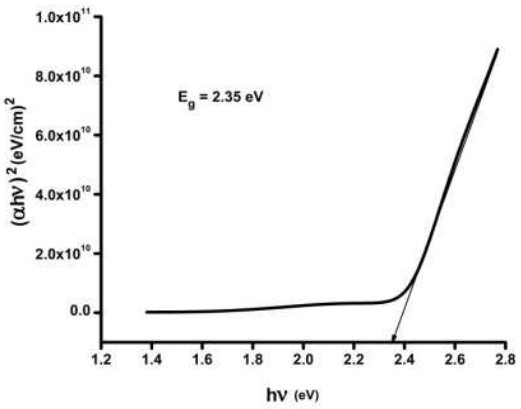

Fig. 2. Variation of $(\alpha h\nu)^2$ vs hν

3.3 Scanning electron microscope (SEM)

SEM micrograph of CdS thin films (Fig. 3) at magnification 40 Kx exhibits dense films with uniform surface coverage without cracks or pinholes. The clusters of grains (~300 nm) seen in the SEM are possibly due to a coalescence of small grains (~15nm) as evidenced by XRD data.

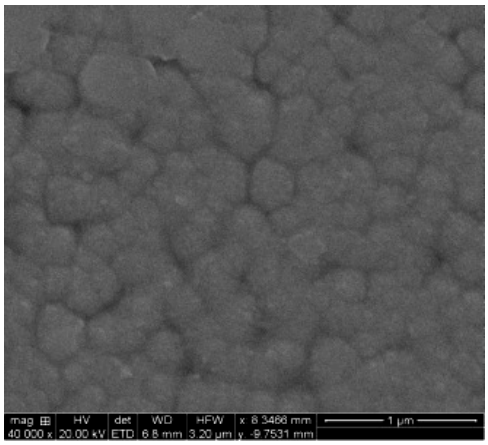

Fig. 3. SEM image of CdS thin films

3.4 Raman analysis

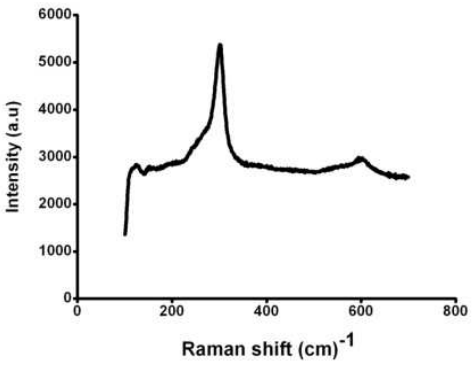

Fig. 4. Raman spectrum of CdS thin films

The Raman spectrum of CdS thin films (Fig. 4) reveals two Raman peaks corresponding to the multi-overtones of the longitudinal optical (LO) phonons. The wave number of first overtone of the longitudinal optical phonons (1LO) is 301cm^{-1} and second overtone of the LO phonons (2LO) is 602 cm^{-1} matching with the earlier report[4].

Discussion

The CdS thin films deposited in alkaline aqueous medium at optimised bath temperature have been observed to exhibit good crystallinity through the well defined sharp peaks in the XRD.The surface morphology based on SEM observation, shows a smooth surface with uniform surface-coverage with bottom dense layer and the top loose layer attributed to the two mechanisms viz. *ion by ion* and *cluster by cluster* operating in the film deposition. The optical band gap from the UV-VIS spectral data is found to be 2.35eV. The Raman spectrum exhibits the characteristic peaks of the CdS thin films.

Conclusion

The growth conditions for obtaining good quality CdS thin films have been optimized. Orientation of the substrate, growth temperature of 80^0 C and pH =11 has been found to be optimum. This work is of fundamental nature from the point of view of suitability for application of the CdS thin film as window material in heterojunction thin film solar cells.

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