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Influence of substrate temperature on the structural, optical and electrical properties of CdS thin films deposited by thermal evaporation

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ABSTRACT

CdS thin films were deposited onto glass substrates at three different temperatures (20, 100 and 200 °C) by vacuum thermal evaporation at 10^{-5} Torr using pure crystal as evaporated targets. The effects of substrate temperature on structural, electrical and optical properties were studied. Structural analysis using X-ray diffraction (XRD) and scanning electronic microscope (SEM) revealed that the films are polycrystalline in nature with a hexagonal wurtzite structure having (002) plane as the preferred orientation. The crystalline size (D), dislocation density (δ), strain (ε) and texture coefficient $TC(hkl)$ were calculated. All the films have high optical transmittance (>80%) in the visible range. The optical band gap values are found to be in the range of (2.3–2.43 eV) and found to decrease with increase in substrate temperature. DC electrical conductivity was carried out at room temperature indicating a very low electrical conductivity.

1. Introduction

Cadmium sulfide, CdS is a (II–VI) compound semiconductor, because of its wide and direct band gap (2.42 eV) at room temperature, good optical transmittance, low resistivity and easy ohmic contact it has found potential applications [1] In particular, thin films of n-type CdS are widely used as a window layer in heterojunction realization of p-type CdTe and CuInSe solar cells. Hence, a large number of studies have been carried in order to produce CdS thin films of this material with suitable optoelectronic properties for photovoltaic applications. For this purpose several properties are required of the CdS films:

(1) Relatively high transparency, not too thick to favor the absorption in the CdTe or CuInSe absorber layer. (2) Not too thin to avoid the short circuiting. (3) Relatively large conductivity to reduce the electrical solar cells losses and higher photoconductivity to not alter the solar cell spectral response [2]. Several techniques have been used to prepare CdS thin films namely: vacuum evaporation [3], spray paralysis [4], electro deposition [5] and chemical path deposition [6]. Among these, vacuum evaporation technique is a well established technique for the preparation of uniform films with good crystallinity. The physical properties of the films prepared by vacuum evaporation technique depend on many factors such as film thickness, substrate temperature and deposition rate [7]. Furthermore, the crystallites and impurities incorporated during the deposition process strongly affect the electrical, structural and optical properties of the deposited films. It is well known that CdS thin films can exist in either cubic or hexagonal phase or as a mixture of both the phases depending on the deposition condition. In the present study, CdS thin films are deposited by vacuum evaporation at different substrate temperatures and the films are characterized by several techniques such as X-ray diffraction, Transmission Electron Microscopy and optical transmittance. Also the effect of substrate temperature on the structural, electrical properties and optical properties is discussed.

2. Experimental details

Cadmium sulfide thin films were prepared by evaporating pure crystal onto well-cleaned glass substrates from a molybdenum boat. The evaporation was made using a conventional vacuum coating unit (Edwards E306) at a vacuum of 10^{-5} Torr. The films were grown at substrate temperatures of 20, 100 and 200 °C. The structural properties have been examined by the X-ray diffraction

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Table 1
XRD data of CdS thin films deposited at different substrate temperatures.

Substrate temp.	2θ (°)	*d* (Å) from XRD results	*d* (Å) from SEM images	*d* (Å) JCPDS	*hkl* plans	*a* (Å) values observed	*c* (Å) values observed	*a* (Å) JCPDS	*c* (Å) JCPDS
T = 20 °C	30.92	3.3584		3.3567	002	4.147	6.735	4.136	6.713
	64.49	1.6776		1.6782	004				
T = 100 °C	30.99	3.3506		3.3565	002	4.144	6.732	4.136	6.713
	32.89	3.1615		3.1601	101				
	56.39	1.8947		1.8977	103				
T = 200 °C	30.79	3.376	3.363	3.3565	002	4.142	6.730	4.136	6.713
	32.8	3.175	3.153	3.161	101				
	56.21	1.903	1.889	1.8977	103				
	64.33	1.684			004				

Table 2
Structural parameters of CdS thin films deposited at different substrate temperatures obtained from 002 peaks.

Substrate temp.	2θ (°)	$\beta \times 10^{-3}$ (rad)	*D* (nm)		δ ($\times 10^{15}$) lines/m^2	*N* ($\times 10^{15}$)	Thickness of films (nm) (*t*)	ε ($\times 10^{-4}$)	*TC* (*hkl*)
			From XRD results	From TEM images					
T = 20 °C	30.99	4.013	43	42	34.29	7.71	1600	5.126	3.194
T = 100 °C	30.99	4.36	39	36	9.032	6.096	600	5.569	3.006
T = 200 °C	30.79	5.06	38	36	2.699	5.668	200	6.464	2.995

method (XRD) (Diano PW 1370, CoKα Ni filter, radiation, λ = 0.1793 nm) and Scanning Electron Microscopy (model JEOL-JSM-T840). The optical properties were measured by the (UV–VIS-NIR) double beam spectrophotometer (JASCO-V570 model) in the wavelength range of 400–2500 nm at room temperature. The electrical resistivity of the films was measured by the Van der paw technique at room temperature. For this purpose silver paint electrodes of 2 mm length at 2 mm separation were painted on the samples in a coplanar configuration. The current was measured using an (HP4140B) Pico ammeter/Dc voltage source. Surface morphological study has been carried out on deposited films using Transmission Electron Microscope model (JEOL 1230 of magnification 300,000).

3. Results and discussion

3.1. Thickness measurement

Film thickness (t) is an important parameter in the study of film properties. The thickness of CdS films was measured with the help of a weight difference method employing a sensitive electronic microbalance, in this method the substrate was weighted before (m_1) and after the deposition (m_2) and the thickness of the films was obtained using the formula.

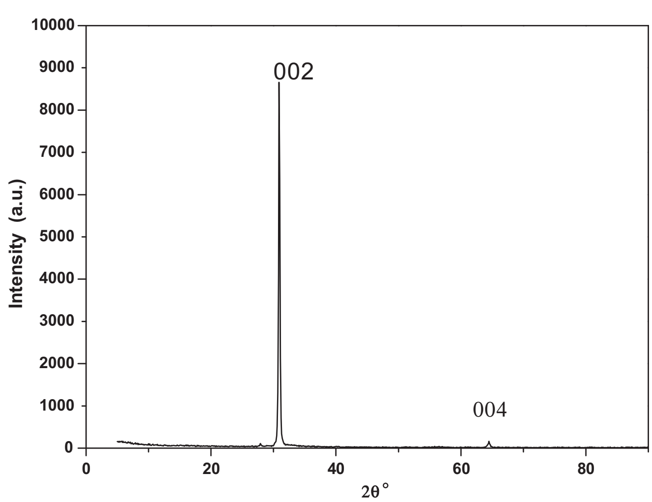

Fig. 1. XRD of CdS film grown at substrate temperature 20 °C.

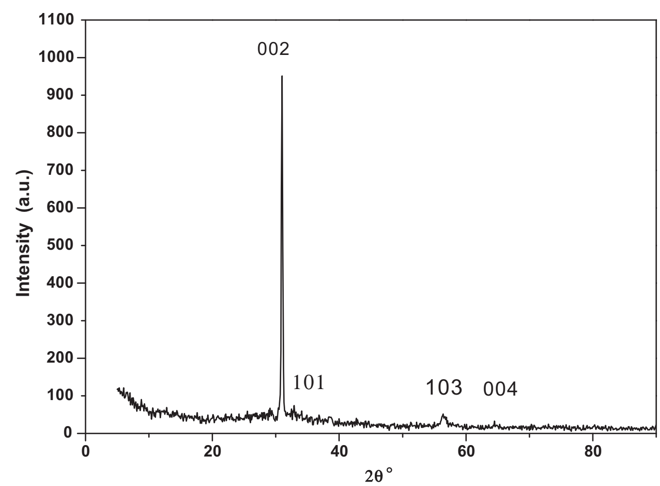

Fig. 2. XRD of CdS film grown at substrate temperature 100 °C.

$$t = m_2 - m_1/\rho A \quad (1)$$

where ρ is the density of the film material (g/cm^2) and (A) is the area of the film (in cm^2). Thickness of films is shown in Table 2. It is noted that film thickness decreases from 1600 to 200 nm with a rise in substrate temperature. The possible reason for the increase in the thickness with decreasing substrate temperature could be the decreasing back diffusion upon a further decrease in the substrate temperature affecting the deposition rate.

3.2. X-ray diffraction studies

Figs. 1–3 shows the XRD pattern of vacuum-evaporated films deposited at substrate temperatures of 20, 100 and 200 °C. The XRD patterns were recorded in 2θ intervals from 20° up to 90° with the step 0.1°. As seen, it is clear that the films are polycrystalline in nature. Also it is seen that all samples show a predominant peak at

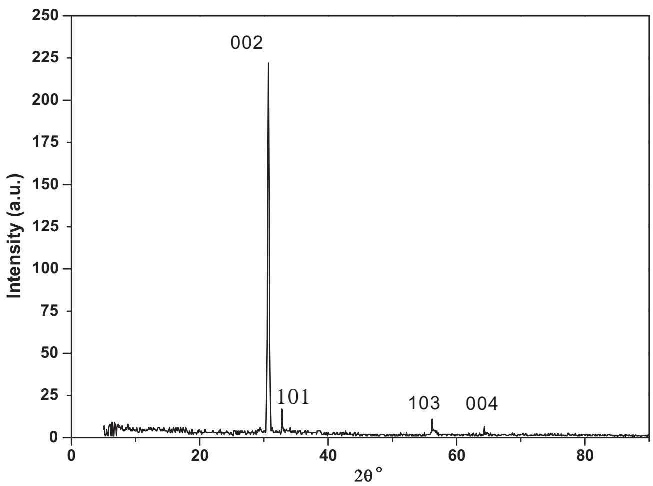

Fig. 3. XRD of CdS film grown at substrate temperature 200 °C.

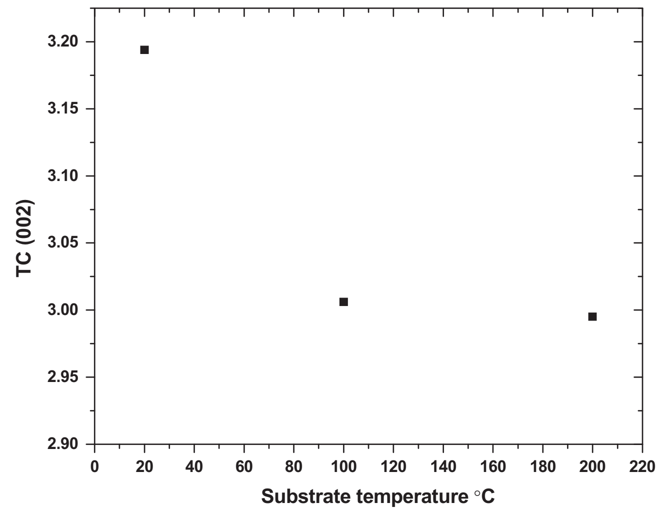

Fig. 6. Variation of the texture coefficient (TC_{002}) with the substrate temperature.

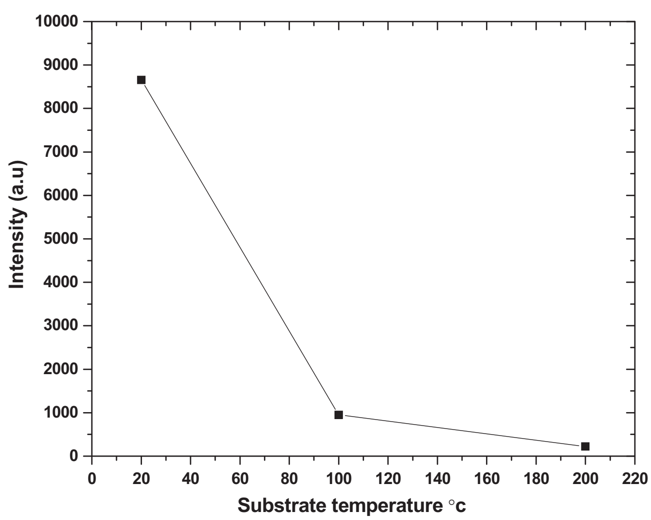

Fig. 4. Intensities of the (002) diffraction peak in the XRD patterns of films as a function of substrate temperature.

$2\theta = 30.9°$ which can be assigned to the (002) plan, which corresponds to CdS hexagonal plane (002), or cubic plane (111). But,

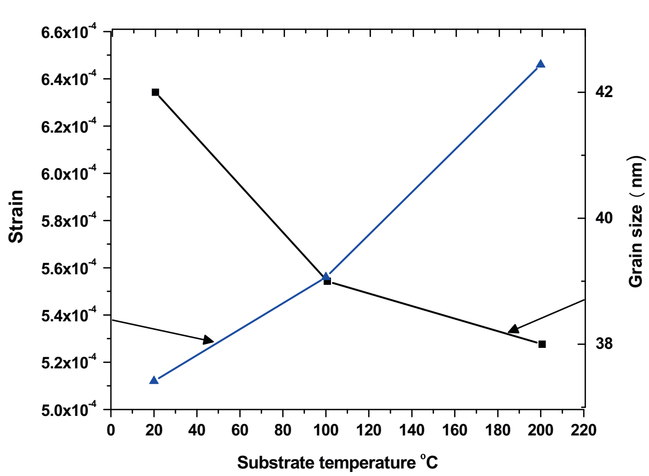

Fig. 5. Grain size and stress as a function of substrate temperature.

the presence of the peaks 101 and 103 indicates that the phase is hexagonal CdS [7–9]. It is observed that the XRD pattern of all CdS films shows a most preferred orientation along the (002) plane. The intensities of the (002) diffraction peak in the XRD patterns of films as a function at substrate temperature are shown in Fig. 4 It is clear that from this figure that the intensity decreases with an increase of the substrate temperature.

Table 1 shows that observed d-spacing and the respective prominent peaks correspond to reflection from the (002), (101), (103) and (004) plans, which coincide well with the JCPDS data. The lattice parameters, a and c of the unit cell were calculated by using the classical relations [10]. The lattice constant has been evaluated from the highest angle reflection data (002). The obtained lattice parameter values are given in Table 1 the JCPD card values are also given for comparison. It was found that the observed values are in good agreement with the standard data. The average size of the crystallites (D) is calculated using the Scherer's formula [11].

$$D = 0.9\lambda/\beta\cos(\theta) \quad (2)$$

where λ is the wavelength of the X-ray used, β is the full-width at half-maximum (FWHM) of the peak which has maximum intensity, and (θ) is the Bragg's angle. The variation of the grain size with substrate temperature is shown in Fig. 6. It is clear from this figure that the grain size decreased with increasing substrate temperature. The dislocation density (δ), defined as the length of dislocation lines per unit volume, has been estimated using the equation [12].

$$\delta = 1/D^2 \quad (3)$$

where (δ) is the measure of the amount of defect in a crystal. Therefore, the small values of (δ) obtained in the present study confirmed the good crystallinity of the CdS films. The number of crystallites per unit area (N) and the strain (ε) of the films were determined with the use of the following formula [13].

$$N = t/D^3 \quad (4)$$

$$\varepsilon = \beta\ \cos(\theta)/4 \quad (5)$$

The dependence of the strain of CdS thin films on substrate temperature is shown in Fig. 5. It can be seen that when the substrate temperature increases the strain decreases and this decrease in strain indicates a decrease in the concentration of lattice imperfection as the substrate temperature increases. To quantitatively investigate the degree of preferred orientation, the texture coefficient $TC(hkl)$ was calculated using the following Eq. [14]

$$TC(hkl) = \frac{I(hkl)}{I_o(hkl)} \frac{\sum I_o(hkl)}{\sum I(hkl)} \tag{6}$$

where I is the measure of intensity, I the JCPS standard intensity. Sample with a randomly oriented crystallite presents $TC(hkl) = 1$ while the larger the values, greater than (1), the larger the abundance of crystallites orientation. The texture coefficient was calculated for the reflection plan (002). The variation of texture coefficient of CdS films with the substrate temperature is shown in Fig. 6. It is can be seen that the highest TC for (002) plans of all films reveal that the films have very good crystallinity.

Table 2 shows the calculated values of crystallite size (D), dislocation density (δ), number of crystallites per unit area (N), Strain (ε), $TC(hkl)$ and (t) the thickness of the CdS films deposited on glass substrates at different substrates temperature.

Fig. 7 shows a selected area electron diffraction pattern of CdS film deposited at the substrate temperature 200 °C. The pattern shows different circular rings, which indicates that the film is polycrystalline in nature. Dominant diffraction patterns are indexed (002), (101), (103) plans of hexagonal CdS. The interplanar distances (d) for different ($h\ k\ l$) plans were calculated using the relation.

$$d = L\lambda_e / R \tag{7}$$

where L is the camera constant, R the radius of the diffracted ring and λ_e the electron wavelength

$$\lambda_e = (150/V)^{1/2} \tag{8}$$

where (V) is the voltage. The calculated values of (d) are shown in Table 1 which is in good agreement with that of XRD data.

3.3. Surface morphology

The surface morphology of the evaporated CdS films was analyzed by transmission electron microscopy (TEM).The TEM image of the films deposited at substrate temperatures 100 and 200 °C are shown in Fig. 8. The TEM image shows a uniform surface with well-defined grain boundaries. No Cluster formation is observed and the grain appears homogenous and uniform. The grain size values of the CdS films are found to be in the range of (0.042–0.36 μm). These values are comparable with that estimated from the XRD result Table 2.

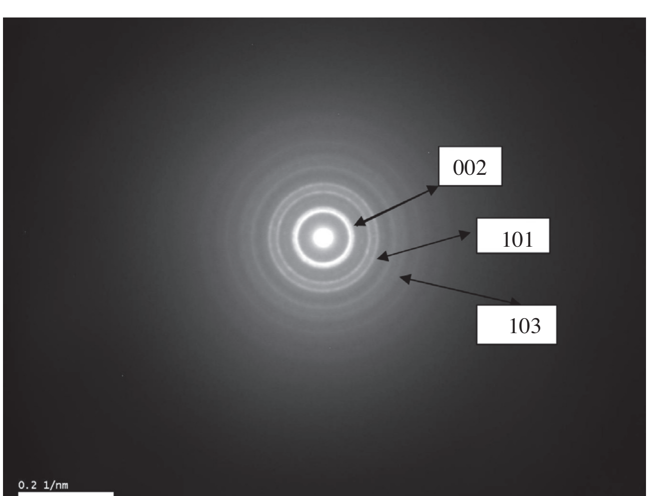

Fig. 7. The diffraction rings in a selected area electron diffraction pattern of CdS thin film deposed at substrate temperature 200 °C.

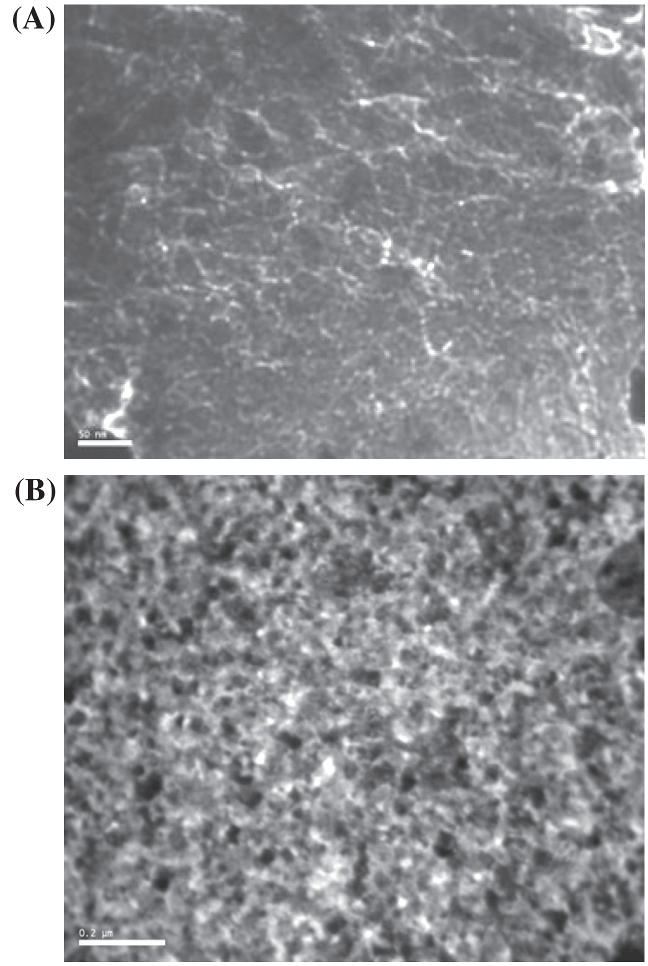

Fig. 8. Transmission electron microscope image of CdS films prepared at substrate temperature (A) 100 °C (B) 200 °C.

3.4. Optical properties-3

Optical properties of CdS films grown by thermal evaporation at different substrate temperatures were measured at room temper-

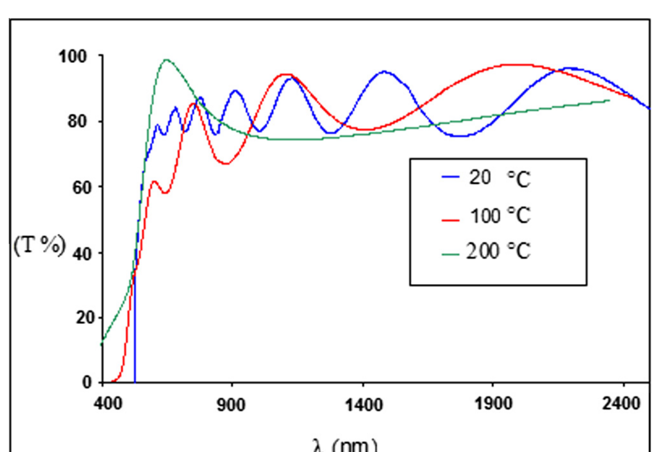

Fig. 9. Transmittance spectra of CdS thin films at different substrate temperatures.

ature in the wavelength range (400–2500 nm). Fig. 9 shows the optical transmission spectrum (T) of the CdS films, the spectrum shows interference pattern with a sudden fall of transmittance near the band edge which is an indication of good crystallinity in CdS films. As can be seen from this figure the obtained CdS thin films are characterized with high transmission, greater than 80% for wavelength values greater than 500 nm. The absorption coefficients (α) of the films are determined from the formula [15].

$$\alpha = \ln(1/T)/t \tag{9}$$

CdS is a direct band gap material and for a direct allowed transition, the absorption coefficient (α) is related to b and gap (Eg) by the relation [16].

$$\alpha = \mathrm{A}(hv - E_g)^{1/2}/hv \tag{10}$$

where A is the constant and h is the plank's constant.

The optical band gap can be obtained by extrapolating the linear portion of the plot $(\alpha h\upsilon)^2$ versus hυ at α = 0 as shown in Fig. 10. The optical band gap for the films is in the range (2.3–2.43 eV). These values are in good agreement with the reported ones [8]. It is clear that the energy gap decreases as the substrate temperature increases. Such behavior has also been observed by [17]. The observed straight-line behavior in the high absorption region for CdS thin films, shown in fig. 9, indicates that the films have a direct band gap. This wide band gap and the high optical transparency in the visible range observed for the deposited CdS films make them possible widow layers in solar cells.

3.5. Electrical properties

The variation of dc electrical conductivity (σ) of CdS thin films as a function of substrate temperature is shown in Fig. 11. The conductivity of the films increases, from 3.2 to 22 $(\Omega\,\mathrm{cm})^{-1}$, with a decrease of substrate temperature. This increase might be due to the decrease of residual defects and the increase of crystallite size in the films (observed from Fig. 5). In general, the conductivity of the films increases with increase of either grain size and/or films thickness up to a certain limit [18]. However in the present work the thickness of the films increases with decreasing substrate temperature causing large grains (observed in Table 2). Hence conductivity increases with decreasing substrate temperature.

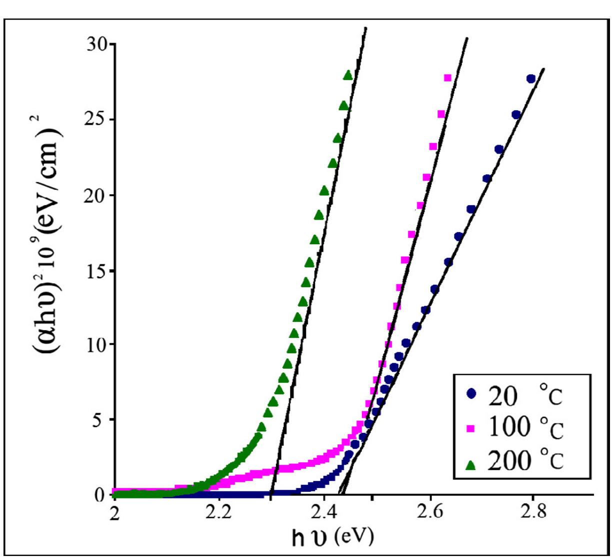

Fig. 10. Plot of $(\alpha h\upsilon)^2$ vs. $h\upsilon$ of CdS films at different substrate temperatures.

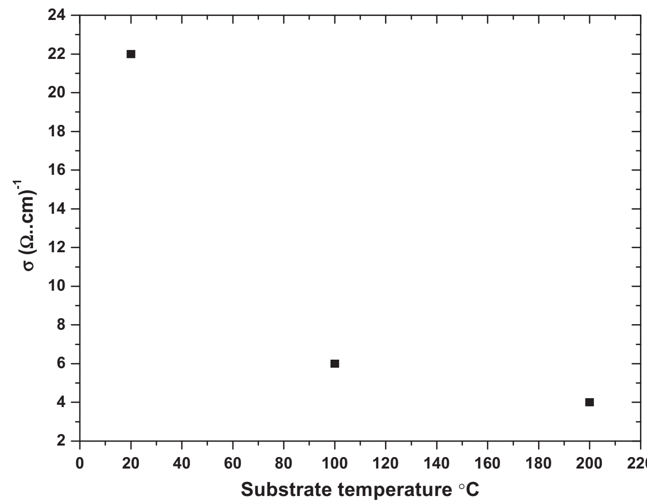

Fig. 11. Effect of substrate temperature on electrical conductivity of CdS films.

4. Conclusions

Good quality, adherent and uniform CdS thin films were grown by the thermal evaporation technique onto glass substrates at different substrate temperatures. X-ray diffraction patterns and (SEM) of these films indicated that they have hexagonal structures oriented along the (002) plane. The lattice parameter has been determined and their values are compared with the JCSDS Chart. The crystallite size was measured by (TEM) and by X-ray. The average grain size of films was found to be 0.04 μm which was found to be decreased with the increase of the substrate temperatures. All the films exhibit high transmittance (75–85%). The optical band gap values decreased with the increase in substrate temperature. DC electrical conductivity measurements provide a value of σ in the range 3.2–22 $(\Omega\,\mathrm{cm})^{-1}$.

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