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Current transport mechanism in CdS thin films prepared by vacuum evaporation method at substrate temperatures below room temperature

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ABSTRACT

CdS thin films were deposited by vacuum deposition method at low substrate temperatures instead of the commonly used vacuum deposition at high substrate temperatures ($T_S > 300$ K). The effect of low substrate temperature on the current transport mechanisms in polycrystalline CdS thin films has been studied as a function of temperature over the temperature range 100–300 K. Both thermally assisted tunneling of carriers through and thermionic emission over the grain boundary potential have contributions to the conduction in the range 250–300 K for the sample prepared at 300 K substrate temperature. The dominant conduction mechanism of the samples prepared at 200 K and 100 K is determined as thermionic emission over 200 K and Mott's hopping process below 200 K. The Mott's hopping process is not applicable for the sample prepared at 300 K.

1. Introduction

CdS, a II–VI compound semiconductor, has a direct band gap of 2.42 eV at room temperature. CdS polycrystalline thin films have important technological applications in heterojunction solar cells, photo-detector materials, and gas sensors. The optimization of CdS device characteristics has created a need for a better understanding of its electronic properties. Most of the structural, optical, and electrical properties of CdS films depend on the growth method, the growth parameters, and the post deposition treatment. Various techniques have been used to prepare CdS thin films such as vacuum evaporation [1], chemical bath deposition [2], close spaced sublimation [3], spray pyrolysis [4] and pulsed laser deposition [5]. The vacuum evaporation technique is a well established technique for the preparation of uniform films with good crystallinity [6]. The physical properties of the thin films prepared by vacuum evaporation technique depend on many factors such as film thickness, pressure during evaporation, 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.

The current transport mechanisms in CdS thin films grown by various methods have been investigated in detail [8–12]. In this study CdS thin films were grown using the vacuum evaporation method: vacuum deposition at low substrate temperatures (<300 K) instead of the commonly used high substrate temperatures. Previously our research group investigated the structural and optical properties of II–VI group thin films such as CdSe, ZnTe and CdS prepared by vacuum evaporation technique on the cold substrates (<300 K) [13–15]. In this paper we report on the effects of low substrate temperature (100, 200 and 300 K) on the electrical properties of CdS thin films grown on glass substrates by the vacuum evaporation technique as a function of substrate temperature over the range 100–300 K. The electrical properties of CdS thin films were investigated to establish a correlation between the process parameters and the film properties.

2. Experimental details

CdS thin films were prepared by vacuum evaporation technique in quasi-closed volume on soda-lime glass substrates at controlled temperatures [16]. Prior to growth, glass substrates were cleaned in ethanol and then dried in vacuum. The cross-sectional view of the evaporation apparatus is given in Fig. 1. The source–substrate distance was fixed at 9 cm. Source and substrate temperatures were monitored and controlled separately using thermocouples during evaporation. When a base pressure of 8.0×10^{-4} Pa was reached, the substrate was cooled by pumping liquid nitrogen through the substrate cooler made of copper pipe. A resistive heater was placed between the substrate and cooling block to adjust the substrate temperature during deposition. Evaporation rate of the source material was controlled by keeping the source temperature within the range of 923 K and kept relatively low to avoid substrate heating. CdS powder used as source material was better than 99.995% pure. To prevent the splattering of the source, the source was pressed into discs of 13 mm diameter. CdS thin films

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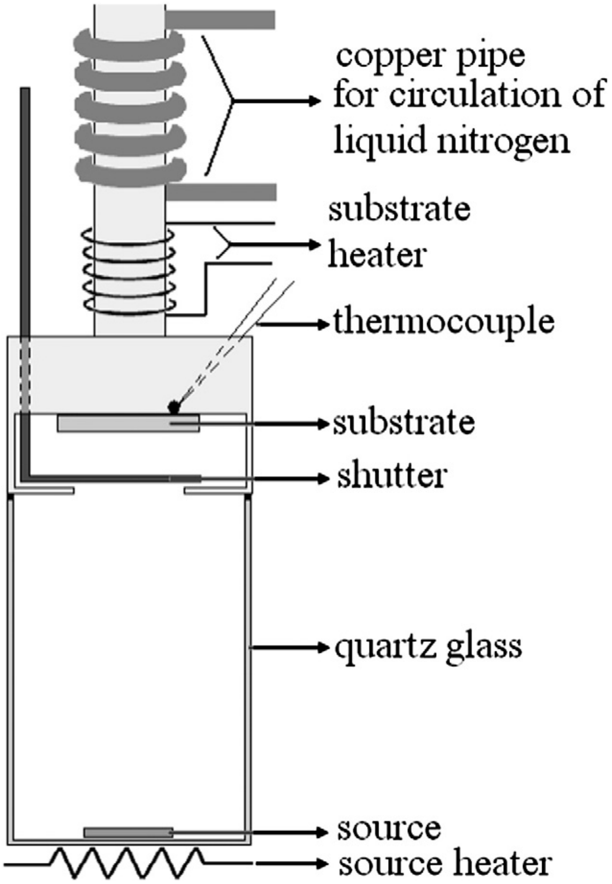

Fig. 1. A cross-sectional view of the thermal evaporation apparatus.

were grown for different substrate temperatures: $T_S = 300$, 200 and 100 K (± 3.0 K). The shutter was continuously kept open.

X-ray diffraction (XRD) data was collected using a Rigaku D/Max-IIIC diffractometer with CuK_α radiation ($\lambda = 1.5418$ Å) over the range of $2\theta = 20°–70°$ at room temperature. Scan speed was 3°/min, and step size was 0.02°. The hot probe method and Hall Effect measurements (in dark) were used to find carrier type and carrier density of the CdS thin films at room temperature. The resistivity of the CdS thin films was measured using the four-point probe method in the dark at room temperature. Transmission measurements were performed to determine the optical properties of the films using a Shimadzu UV-1601 spectrophotometer (spectral range from 400 to 1000 nm). Electrical conductivity was measured in the temperature range 100–300 K using a Leybold–Heraeus HR1 cryostat. The electrical measurements were performed using a Keithley 6221 AC DC current source, a Keithley 2182A Nanovoltmeter, and a Lakeshore 336 temperature controller.

3. Results and discussion

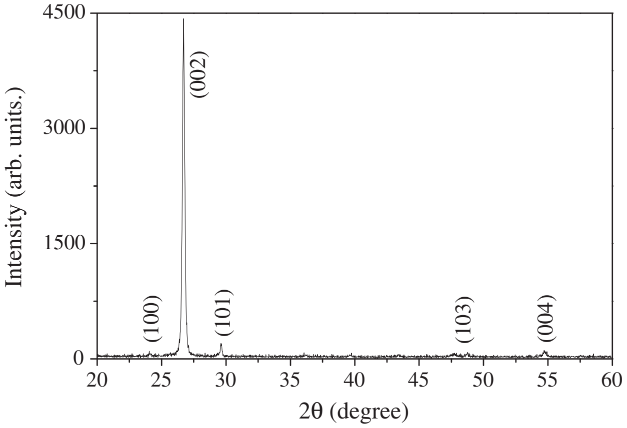

Fig. 2. XRD patterns of the samples prepared at 200 K.

The structural analysis indicates that the CdS thin films are polycrystalline with a hexagonal structure. The patterns of the CdS samples exhibit a dominant (002) preferred orientation. Fig. 2 shows the XRD results of the CdS films deposited at 200 K substrate temperature. The low intensity peaks are attributed to (100), (101), (103) and (004) planes of hexagonal CdS. The grain size of the CdS thin films was calculated according to (002) peak using Scherrer's formula, $D = 0.94\lambda/\beta\cos\theta$, where D is the grain size, β is the full-width at half-maximum (FWHM), θ is the half angle of the diffraction peak and λ is the wavelength of the X-rays. The grain size of the CdS thin films prepared at 300, 200 and 100 K was obtained as 38.2, 34.7 and 34.5 nm (± 0.1 nm), respectively (Table 1). The *c* lattice constants for the CdS thin films determined from the 2θ values of the (002) diffraction peaks were 6.662, 6.680 and 6.711 Å (± 0.005 Å) for the deposition temperature of 300, 200, and 100 K, respectively (Table 1). The sample prepared at 300 K has a smaller *c* lattice constant than the corresponding value of the powder CdS (6.72 Å) indicating that the film is subjected to a tensile stress in the plane parallel to the substrate surface [17].

The semiconductor band gap, E_G, was determined by $\alpha = A(h\nu - E_G)^{1/2}$, which is used for direct-gap materials, where A is a constant. The variation of $(\alpha h\nu)^2$ as a function of the $h\nu$ shows a linear behavior near the band gap. The value of the band gap E_G is given by the intercept of the straight line with the energy axis. The variation of $(\alpha h\nu)^2$ as a function of the $h\nu$ for the CdS films formed at 200 K substrate temperature is shown in Fig. 3. The band gap of the samples is approximately 2.42 eV. The thickness *d* of samples was determined from the interference pattern in the optical transmittance spectrum [18]. The film thicknesses of the CdS thin films prepared at 300, 200 and 100 K were determined as 1.0, 1.5 and 1.6 μm, respectively.

The hot probe method used to find the carrier type of the CdS films verified them as having n-type conductivity. The resistivity (ρ) and carrier concentration (n) of CdS films were determined by the four-point probe technique and Hall Effect measurements at room temperature, respectively (Table 2) [15]. The electron mobility μ was determined from the relation $\mu = |R_H|\sigma$, where R_H is Hall coefficient, σ is conductivity. The resistivity values of the samples were found to be 4.5×10^3, 1.2×10^4 and 7.5×10^3 Ω-cm for the samples prepared at 300, 200, and 100 K, respectively. Several groups have reported that the resistivity of CdS films decreases as the thickness increases [11,19,20]. Since grain boundary scattering is the primary mechanism that is responsible for the observed resistivity behavior, the decrease in resistivity was attributed to the increase in grain size; as the thickness of the CdS films increases the grain size increases and therefore the density of grain boundaries decreases. However in the present work it should be emphasized that the thickness of the film increases with decreasing substrate temperature causing smaller grains instead of expected larger grains hence resistivity rises. The possible reason for the increase in the thickness with decreasing substrate temperature could be the

Table 1
Grain size and lattice parameter of the CdS samples.

T_S (K)	D (nm)	c (Å)
300	38.2	6.662
200	34.7	6.680
100	34.5	6.711