JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS Vol. 10, No. 3, March 2008, p. 665 - 667

# On the optical properties of CdS thin films

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Cadmium sulfide thin films (d = 0.12 – 1.25 μm) were deposited onto glass substrates by the quasi-closed volume technique under vacuum. The investigations shown that the films are polycrystalline and have a hexagonal (wurtzite) structure. Reflection, transmission and absorption spectra were studied in spectral range 300 – 1400 nm. Energy bandgap calculated from absorption spectra (assuming that allowed direct band-to-band transitions are predominant) ranged between 2.30 and 2.60 eV. The effect of the heat treatment (consisting of several heating/cooling cycles within a temperature range ΔT = 300 – 500 K) on the optical properties has been studied. The heat treated samples are characterized by higher values of transmission coefficient. This fact is probably due to the increase of crystallite size (the decrease of intercrystallite boundaries).

(Received September 25, 2007; accepted March 12, 2008)

*Keywords*: Cadmium sulfide, Thin films, TEM, Optical properties

## 1. Introduction

Cadmium sulfide (CdS) thin films have been intensively studied due to their interesting characteristics (wide band gap, direct band-to-band optical transition, high transmittance in visible domain, etc. [1-6]), which make this compound suitable for many important applications (economical heterojonction, solar cell, sensitive photodetectors, electron-beam pumped lasers, displays, etc [1-3,7,8]). CdS is easily prepared as thin films on to various substrates by different techniques such as spray pyrolysis, vacuum evaporation, sputtering molecular beam epitaxy, etc. [3,5,8-11]. It has been found that the structural, electronic transport and optical properties of CdS thin films are strongly determined by preparation method and deposition condition [3-4,9,11].

In this paper we present a study on the microstructural and optical characteristics of CdS thin film deposited by quasi-closed volume technique under vacuum [12,13]. Versatility of this method facilitates a rigorous control of the deposition parameters (the substrate temperature, deposition rates, temperature of evaporation source, etc.) [12,13]. The dependence of optical properties of CdS thin films on the deposition condition and post-deposition heat treatment is investigated.

## 2. Experimental

CdS thin films have been deposited onto glass substrates by thermal evaporation under vacuum of high purity (99,999%) CdS polycrystalline powders. The quasi-closed volume technique was used [12,13].

The deposition equipment permitted to prepare thin films in different and strictly controlled condition: substrate temperature, $T_s$, ranged between 300 K and 575 K; source temperature was, $T_{ev}$= 1000 K- 1150 K; source substrate distance was, D=8 cm; deposition rate, was $r_d$=15Å/s.

The film thickness was determined by using multiple-beam Fizeau fringe method [14] and for studied samples varied between 0.12 μm and 1.25 μm.

Cristalline structure and microstructure of CdS thin films were characterized by using X-ray diffraction (XRD) technique and transmission electron microscopy including electron difraction (ED) and high-resolution electron microscopy (HRTEM).

TEM investigation were performed with a Philips CM12O (λ=0.037Å) equipment operated at 100 kV.

The surface morphology was studied by atomic force microscopy (AFM).

Transmission and reflection spectra in the spectral range 300-1400nm, were recorded using a PMQ.II (C.Zeiss) type spectrophotometer and a ETA-STC spectrometer.

The absorption coefficient $\alpha$, was determined from the expression [15,16]

$$\alpha = \frac{1}{d} ln \frac{(1-R_T)^2}{T_\lambda}, \qquad (1)$$

where $d$ is film thickness and $R_T$ and $T_\lambda$ denote the reflection and transmission coefficient, respectiveley at a determined wawelenght λ.

## 3. Results and discussion

Electron diffraction patterns shown that all the films are polycrystalline and have a wurtzite (hexagonal) structure and do not show any other phases.

A typical ED pattern is presented in Fig. 1. The electron diffraction rings corresponding to the reflection from various sets of planes, which are indicated in the respective pattern, can be clearly observed. These planes correspond to wurtzite structure of CdS.

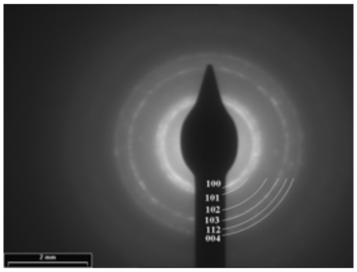

*Fig. 1. Electron diffraction pattern for as deposited CdS film (d = 0.47 μm).*

The lattice parameters of the hexagonal structure calculated from interplanare distances indicated in ED patterns were: $a$ = 0.412 nm, $c$ = 0.668 nm. These values are in a good agreement with standard values of crystalline structure of CdS [12,17].

In order to obtain films with stabile structure, after preparation CdS films were subjected to a heat treatment. This consisited of several succesive heating/cooling cycles (with a temperature rate of 5K/min) within a temperature range 300-550 K (ED pattern Fig. 2). After heat treatment the temperature dependence of the electrical conductivity becomes reversible [17,18].

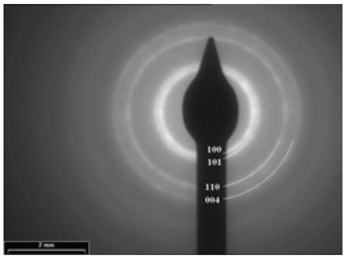

*Fig. 2. Electron diffraction pattern for heat-treated CdS film (d = 0.47 μm).*

After heat treatment, the orientation of the film crystallites is maintained. In addition, the film crystalline structure is improved and the orientation degree of crystallites increases.

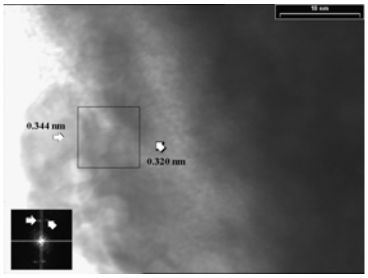

*Fig. 3. HRTEM image for as deposited CdS film (d=0.47μm).*

High-resolution TEM images with Fourier transform were used for identifying and determining interplanar spacing in the domains with adjacent crystallites (Figs 3 and 4). Interference fringes in the HRTEM images correspond to (002) and (101) planes and have the following values: $d_{002}$=0.340 nm and $d_{101}$=0.313 nm respectively.

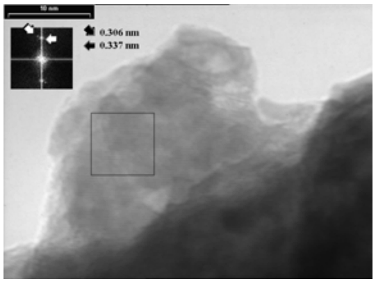

*Fig. 4. HRTEM image for heat-treated CdS film (d=0.47μm).*

Bright-Field TEM images shown that the films are homogenous (Figs.5 and 6).

*Fig. 5. BFTEM image for as deposited CdS film (d=0.47μm).*

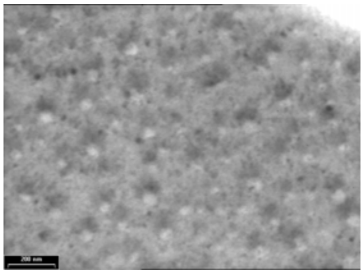

*Fig. 6. BFTEM image for heat-treated CdS film (d=0.47μm).*

The heat treatment leads to an increase of crystallite size. In this way, for a film with thickness $d$ = 0.47 μm the average crystallite size increases from 5.17 nm to 27.5 nm (Fig. 7).

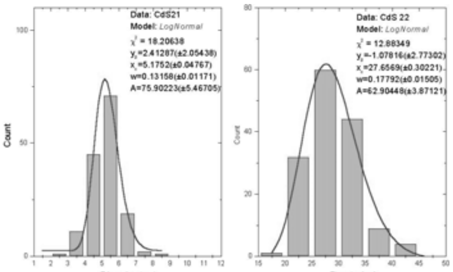

*Fig. 7. Grain size for a CdS film (d=0.47μm) before (left) and after (right) the heat treatment.*

These structural characteristics of CdS thin films are confirmed by XRD technique [17,18].

By studying the optical properties (especially transmission and absorption spectra for photon energies placed in the vicinity of fundamental absorption edge) of CdS thin films, many useful informations can be obtained about the characteristics of optical transmission, vaue of bandgap, impurity energy levels etc. [15,16,20].

A typical transmission spectrum is presented in Fig. 8 for a CdS thin film. It can be observed that, in the wavelength range 500 – 1200 nm the films have a good transparency (T>80%). After the heat treatment transmission coefficient is increasing. We consider that this behaviour is due to the increase of the crystallite size and decrease of intercrystallite boundaries. [7,12].

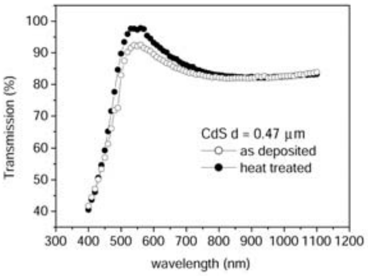

*Fig. 8. Transmission spectra for a CdS film (d=0.47µm) before and after the heat treatment.*

It is known that CdS is a direct semiconductor compound [2,3,15,16]. Consequently the dependence of the absorption coefficient on the photon energy for allowed direct band-to-band transitions (neglecting exciton effect) is described by expression [7,15,19,20]

$$\alpha h\nu = A_d \left(h\nu - E_{g0}\right)^{1/2}, \qquad (2)$$

where $h\nu$ is incident photon energy, $E_{g0}$ denotes the optical bandgap and $A_d$ represents a characteristic parameter (independent of photon energy for respective transitions).

Fig 9 shows the photon energy dependence of $(\alpha h\nu)^2$ for as-deposited and respectively heat-treated film. The plot of $(\alpha h\nu)^2$ as a function of hν is found to have a linear part and extrapolation of the straight line part to $(\alpha h\nu)^2 = 0$ gives $E_{g0}$. For studied films the values of $E_{g0}$ ranged between 2.30 and 2.60 eV. These values are in good agreement with those reported for CdS single crystals [1-3,20].

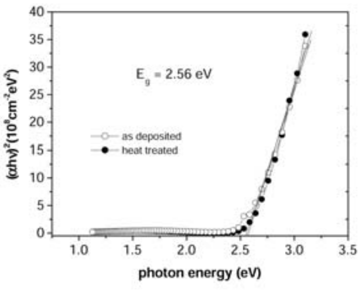

*Fig. 9. Bandgap energy calculation for a CdS film (d=0.47µm).*

## 4. Conclusions

CdS thin films are polycrystalline and have a hexagonal structure. The heat treated samples are characterized by higher values of transmission coefficient. This fact is probably due to the increase of crystallite size (the decrease of intercrystallite boundaries). The values of the optical bandgap energy, calculated from the absorption spectra, ranged between 2.30 eV and 2.60 eV.

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