

Optical characterization of Cd(S_xTe_{1-x}) thin films deposited by evaporation

G. Gordillo*, F. Rojas and C. Calderón

Departamento de Física, Universidad Nacional de Colombia, Bogotá

Polycrystalline CdS_xTe_{1-x} thin films, grown on glass substrates by co-evaporation of CdS and CdTe were characterized through spectral transmittance and x-ray diffraction measurements. The film thickness *d* and the optical constants were determined by simple straightforward calculations using the transmission spectrum alone.

From x-ray diffraction measurements and data of the chemical composition obtained from x-ray fluorescence measurements, is shown that thin films of CdS_xTe_{1-x} mixed crystals with any composition can be obtained by this method.

Keywords: CdS_xTe_{1-x}; Thin films; Optical constants; Solar cells

1. Introduction

It is well-known that in CdS/CdTe solar cells, internal diffusion processes as well as important current losses, caused by carrier's capture in interface state, are present [1,2]; that leads to a deterioration of the device performance [3]. Both, Internal diffusion and interface states density can be reduced incorporating a thin layer of the ternary compound Cd(S_xTe_{1-x}) between the CdTe and CdS layers [4,5].

In this work a procedure is described to prepare a ternary compound CdS_xTe_{1-x} by the evaporation method, with chemical compositions varying between X=0 (CdTe) and X=1 (CdS). Additionally, binary compounds (CdS and CdTe), as well as the ternary compound were characterized through transmittance measurements to obtain information on their optical constants that are used to get an optimum design of the solar cells.

2. Experimental

The CdS_xTe_{1-x} thin films were deposited using a system like that showed in Fig.1. A cylindrical graphite source constituted by two coaxial chambers, was used, from which the precursor compounds (CdS and CdTe) are simultaneously evaporated. The species constituting the CdS and CdTe precursors exit from their respective chambers through openings of different cross sections. Both, the evaporation source and the substrate are heated up by radiation coming from graphite resistors and the respective temperatures controlled with a PID controller.

The chemical composition of the CdS_xTe_{1-x} thin films was varied in a wide range through the ratio of the CdS flux to the CdTe flux. This can be done by varying the cross section area of the exit nozzles for CdS and CdTe. The evaporation temperature also affects the chemical

composition of the CdS_xTe_{1-x} thin films, because the CdS and CdTe sublimate at different temperature. In table 1 are listed the main deposition parameters of the CdS_xTe_{1-x} thin films.

3. Results and discussion

3.1 Determination of the optical constants

The thickness and the optical constants of the CdS_xTe_{1-x} thin films were determined using a procedure developed by Swanepoel [6] which basically consist of the following:

- i) Initially the thickness *d* and complex refractive index $n^* = n - ik$ are determined by simple straightforward calculations using the transmission spectrum alone. *k* is the extinction coefficient which can be expressed in terms of the absorption coefficient α ($k = \alpha\lambda/4\pi$). The thicknesses calculated for the samples with chemical compositions corresponding to *x*=0, *x*=0.33, *x*=0.78 and *x*=1 were 2.2 μm , 3.5 μm , 1.8 μm and 1.9 μm respectively.
- ii) Subsequently, the optical gap *E_g* is determined through the relation: $(\alpha hv) = A(hv - E_g)^{1/2}$, which is valid for direct band gap semiconductors, like those studied in this work.

Fig. 2 shows typical transmittance curves of CdS_xTe_{1-x} thin films with different chemical compositions determined from XRF measurements. It is observed a shift of the transmittance curves toward higher values of λ by increasing the Te content, indicating a decrease of *E_g*.

In Fig. 3 are depicted curves of *n* vs λ , α vs λ y $(\alpha hv)^2$ vs *hν*, corresponding to the samples whose transmittances are shown in Fig.2.

The most relevant aspects of the results in Fig.3 are the following: The refractive index of the CdS_xTe_{1-x} thin films increases with the Te content, being the refractive index of the CdTe films significantly greater than that of the CdS films. This behavior seems to be in part caused by an increase of the conductivity of the CdS_xTe_{1-x} films when their Te content increases, taking into account that the refractive index can be expressed by the relation, $n = 4\pi\sigma/c\alpha$ [7] and that Independently of the chemical composition, the CdS_xTe_{1-x} films present similar values of α at λ values close to the cut off wavelength. The values obtained for *n* are comparable with those reported in the literature [8,9]. On the other hand, the values of α calculated in this work are similar to those

* e-mail: ggordill@ciencias.unal.edu.co

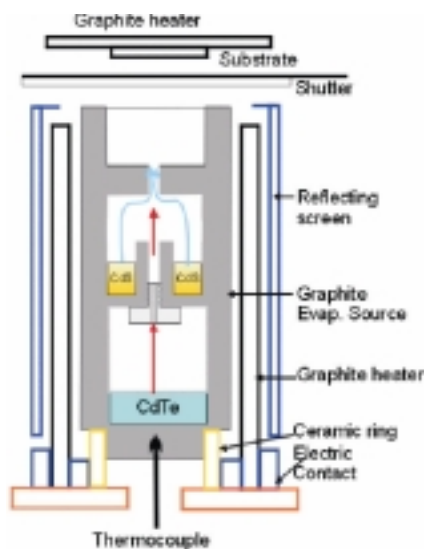


Figure 1. Scheme of the system used for the deposition of CdS_xTe_{1-x} thin films.

reported in ref. 9, for CdS_xTe_{1-x} thin films deposited by the flash evaporation method .

Fig. 4 shows the variation of the optical energy gap E_g of the CdS_xTe_{1-x} thin films as a function of the chemical composition x. The E_g values were obtained from the interception of the straight portion of the (αhv)² vs hv, curves with the hv axis. It is observed that the E_g value increases monotonically between 1.5 eV for x=0 (CdTe) and 2.4 eV for x=1 (CdS). These results are similar to those reported in the literature for CdS_xTe_{1-x} thin films deposited by co-evaporation of CdS and CdTe [10].

3.2 XRD measurements

The structure and lattice parameters of CdS_xTe_{1-x} thin films with different chemical compositions, were determined from XRD measurements using the Cu-K_α line. In Fig. 5 are depicted the corresponding XRD spectra and a curve showing values of the lattice parameter a, calculated as a function of the chemical composition.

At a first attempt to analyze the diffractograms of the samples studied, we found difficulties to get a reliable identification of the reflections observed because,

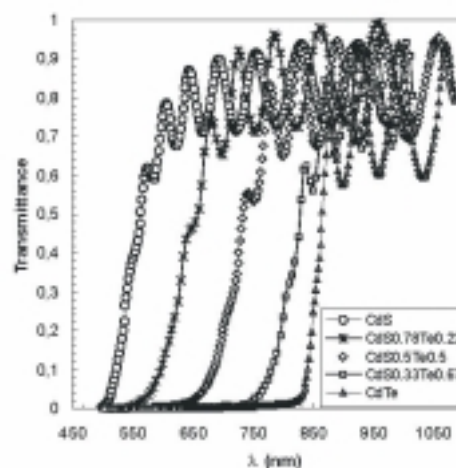


Figure 2: Transmittance curves of CdS_xTe_{1-x} thin films with different chemical compositions.

independently of the chemical composition, all the samples presented the same reflections, shifted a bit from each other. On the other hand, the reflections reported in the PDF data base for this type of compounds with hexagonal structure are quite similar to the reflections associated with the cubic structure.

Comparing the experimental XRD spectra with those calculated theoretically with the help of the Powder Cell simulation program, there were found basis to assume that the CdS_xTe_{1-x} films grew with a mixture of both cubic and hexagonal structure. Even the lattice parameter a, calculated assuming the presence of a mixture of the cubic and hexagonal phases decreases approximately in a linear way when the chemical composition varies from x=0 to x=1, as predicted by the Vegard's law. Since the correlation factor of the linear behavior of the a vs x curves is quite poor (<0.5) we decided to perform XRD measurements to a greater number of samples and calculate again the lattice constant a, as a function of x assuming that at Cd concentrations smaller than 0.5 the samples grow with cubic structure and at chemical compositions corresponding to x≥0.5 the samples grow in the hexagonal phase. In Fig. 5b are depicted the a vs x curves obtained

Table 1. Deposition parameters typically used to deposit CdS (x=1), CdTe (x=0) and CdS_xTe_{1-x} thin films

Parameters	Deposited CdS _x Te _{1-x} thin films				
	CdS (x=1)	CdTe (x=0)	CdS and CdTe		
			x=0.33	x=0.5	x=0.78
Evaporation Temperature (°C)	1000	850	900	900	900
Substrate Temperature (°C)	200	250	250	250	250
CdS - exit nozzle diameter (mm)	1.5		3	3	3
CdTe - exit nozzle diameter (mm)		1	1.4	1.2	0.9
Deposition time (min)	12	12	10	10	10

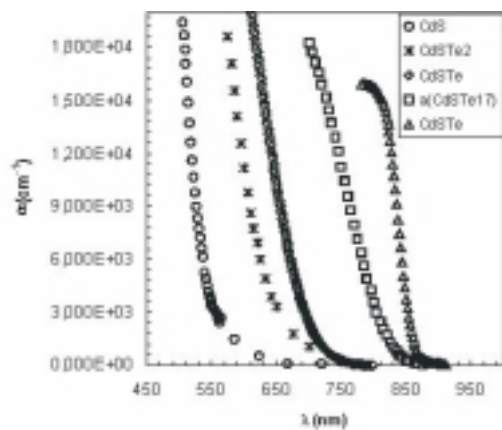
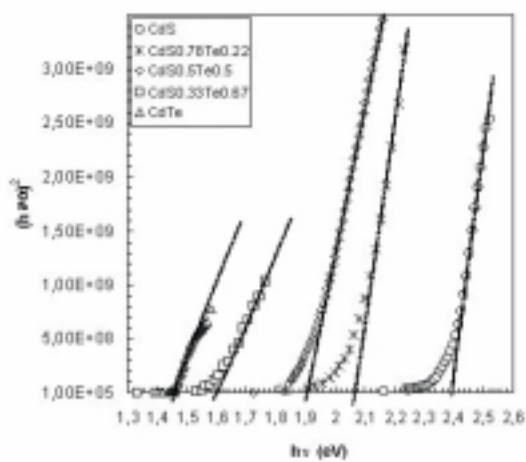
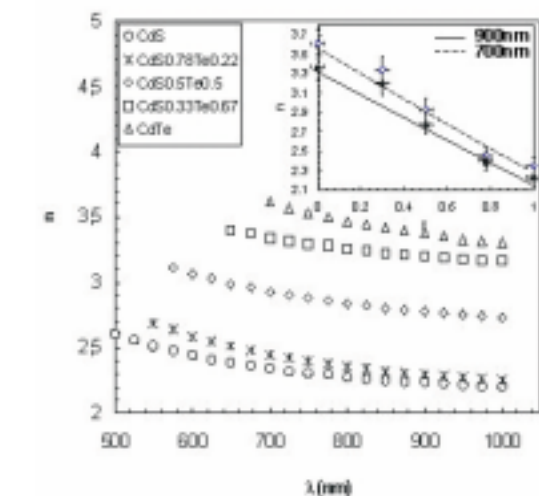


Figure 3. Curves of n vs λ , α vs λ and $(\alpha h\nu)^2$ vs $h\nu$ corresponding to the samples studied in Fig.2. In the inset is observed that the refractive index of the $\text{CdS}_x\text{Te}_{1-x}$ films increases monotonically when the Te-content increases.

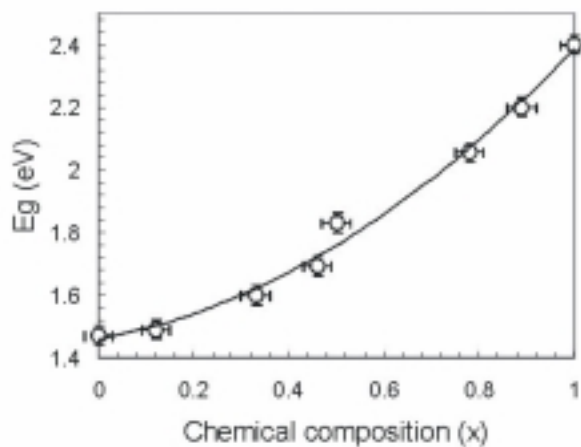


Figure 4. Variation of the optical energy gap E_g and refractive index n (at $\lambda=900\text{ nm}$) of $\text{CdS}_x\text{Te}_{1-x}$ thin films as a function of the chemical composition x .

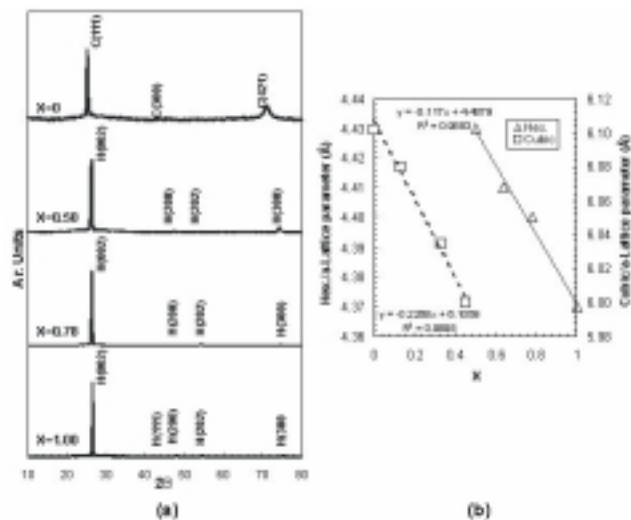


Figure 5. a) XRD spectra for $\text{CdS}_x\text{Te}_{1-x}$ thin films with chemical compositions corresponding to $x=0$, $x=0.5$, $x=0.78$ and $x=1$. b) Calculated a-lattice parameter of $\text{CdS}_x\text{Te}_{1-x}$ thin films as a function of the chemical composition x assuming that at $x < 0.5$ the films grow with cubic structure and at $x \geq 0.5$ with hexagonal structure.

under the last assumption. It can be seen that, in this case, the lattice constant varies linearly with the chemical composition and that the linear behavior of the a vs x curves presents a good correlation factor (0.98). From these results it can be concluded that the $\text{CdS}_x\text{Te}_{1-x}$ films grown by co-evaporation of CdS and CdTe have the tendency to grow in the cubic phase when the Cd content is less than 50% and in the hexagonal phase when the Cd content is greater than 0.5. The existence of the large miscibility gap of the CdS-CdTe system, seems to be associated to the size difference among the VI group elements.

4. Conclusions

Thin films of $\text{CdS}_x\text{Te}_{1-x}$ with compositions varying in a wide range were obtained by co-evaporation of CdS and CdTe on glass substrates at 250 °C. It was found that these types of compounds have the tendency to grow in the cubic-Zincblende phase when the Cd content is less than 50% and in the hexagonal wurtzite phase when the Cd content is greater than 50%.

The optical constants: refractive index n , absorption coefficient α , and optical gap E_g of $\text{CdS}_x\text{Te}_{1-x}$ thin films, were determined by simple straightforward calculations using only the transmission spectrum. Values of α in the range of 10^4cm^{-1} were found for all the samples studied (for $h\nu$ greater than E_g); for the optical gap, values ranging from 1.45 eV to 2.4 eV were found, when the Te content of the $\text{CdS}_x\text{Te}_{1-x}$ films varied between $x=0$ and $x=1$.

The refractive index of the $\text{CdS}_x\text{Te}_{1-x}$ thin films increases by increasing their Te content. This behavior seems to be related with the fact that the CdTe has a higher electrical conductivity than the samples with lower Te content.

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