



Optical properties of nanocrystalline CdTe thin films

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ABSTRACT

CdTe thin films were prepared by vacuum evaporation on glass substrates. The XRD diffractogram revealed a zinc blend structure with a strong reflection from the (1 1 1) plane. The diameter of the nanocrystallites was estimated by using the XRD pattern and the Scherrer formula and found to be 23 nm. The transmittance and absorbance measurements were recorded in the wavelength range 600–1100 nm. The first derivative of the absorbance was used to estimate the effective bandgap energies of the nanocrystallites and the hyperbolic band model was used to estimate their radii. The photoluminescence (PL) signal was weak but contains a set of strong sharp lines. These sharp lines are interpreted in terms of the discrete transitions between the valence and conduction bands of the quantum dots. Also the hyperbolic band model was used to estimate the radii of the nanocrystallites depending on the PL spectra.

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1. Introduction

Nanocrystalline semiconductors possess a number of novel physicochemical properties such as quantum size effects, size-dependent chemical reactivity, optical non-linearity, efficient photoelectron emission and melting point reduction providing for unique applications of these materials [1]. It was indeed shown several years ago that the growth of a highly lattice mismatched semiconductor layer onto a substrate could lead to the spontaneous formation of semiconductor clusters with sizes in the quantum range [2]. Misfit stresses occur in crystalline films due to the geometric mismatch at interface boundaries between crystalline lattices of films and substrate. Therefore a stress is also developed in the film due to the lattice misfit. However, the stress has two components: thermal stress arising from the difference of expansion coefficient of the film and substrate and internal stress due to the accumulation effect of the crystallographic flaws that are built into the film during deposition [3].

These nanoparticles have the crystalline structure of their bulk counter parts and hence are characterized by the fully occupied valence band and empty conduction band separated by the energy gap. However, the charge carriers in these bands e.g., the electrons in the conduction band and holes in the valence band experience an overall confining potential due to the finite size of these particles. As a result there will be size-dependent discrete states in the conduction and valence bands resulting in the

effective enhancement of the bandgap; the so-called quantum size effect. It has been argued that in these semiconductor nanoparticles the hyperbolic band model gives a better fit to the observed quantum size effect as compared to the effective mass approximation [4].

The study of optical properties of nanocrystals has become the topic of both theoretical and experimental interest. Most studied nanocrystalline semiconductors belong to the II–VI group as they are relatively easy to synthesize and generally prepared as particulates or in thin film form. In this work CdTe nanocrystallites were produced by vacuum evaporation on glass substrates at ambient temperature. X-ray diffraction (XRD), scanning electron microscope imaging (SEM), transmittance, absorbance and photoluminescence (PL) measurements have been used to study the properties of the CdTe nanocrystallites.

2. Experimental part

Thin films of CdTe were deposited by vacuum evaporation on glass substrates of dimensions ($6 \times 2.6 \times 0.1 \text{ cm}^3$) at ambient temperature in a high vacuum system ($\sim 10^{-5} \text{ mbar}$) provided with a Turbo pump. The evaporation rate which was about 10 Å/s was measured with a cooled quartz crystal monitor. The distance between the source and the substrate was about 30 cm.

The transmittance of the films was measured by using a double beam Shimadzu UV 1601 (PC) spectrophotometer with respect to a piece of glass of the same kind of the substrates in the wavelength range 600–1100 nm. X-ray measurements were made with a Philips PW1840 Compact X-ray diffractometer system with Cu K_α ($\lambda = 1.5405 \text{ Å}$). The measurements were recorded at a

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diffraction angle 2θ from 30° to 82° . The SEM images were taken by a LEITZ-AMR 1000 A scanning electron microscope. The PL spectra were recorded at $T=23$ K by a system which consists of an Air Product He cryostat DISPLEX DE-202 capable of cooling down to 10 K, where the Ar ion laser of wavelength 488 nm was used as an excitation source. The laser power was 10 mW and the diameter of the laser beam on the sample was about 2 mm. The PL signal was collected by a multi-channel optical spectrometer (an Avantes Fiberoptic Spectrometer AVS-S2000) which hosts two gratings. The first grating has a range: 640–1280 nm and the second grating has a range: 190–860 nm. The spectrometer resolution (FWHM) ranges from 0.3–10 nm depending on the recorded region and the grating.

3. Results and discussion

Fig. 1 shows the XRD diffractogram of a vacuum-evaporated CdTe thin film of thickness about $1\mu\text{m}$. The material is polycrystalline in the zinc blend phase with the (1 1 1) as the preferential orientation. The grain size was calculated from the Scherrer formula (Eq. (1)) for the three reflections in the diffractogram C(1 1 1), C(2 2 0) and C(3 1 1) and the results are inserted in Table 1. Scherrer's formula is known as

$$d = \frac{\lambda}{D \cos \theta} \quad (1)$$

where d is the grain size (diameter of the nanocrystallites), λ is the X-ray wavelength used, D is the angular line width of the half-maximum intensity and θ is the Bragg angle. As the table shows the films are nanocrystalline in nature and the diameter of the nanocrystallites is restricted in the range 7.8–23 nm. But since the amplitude of the (1 1 1) peak is much larger than those of the C(2 2 0) and C(3 1 1) peaks, the average crystallite size is

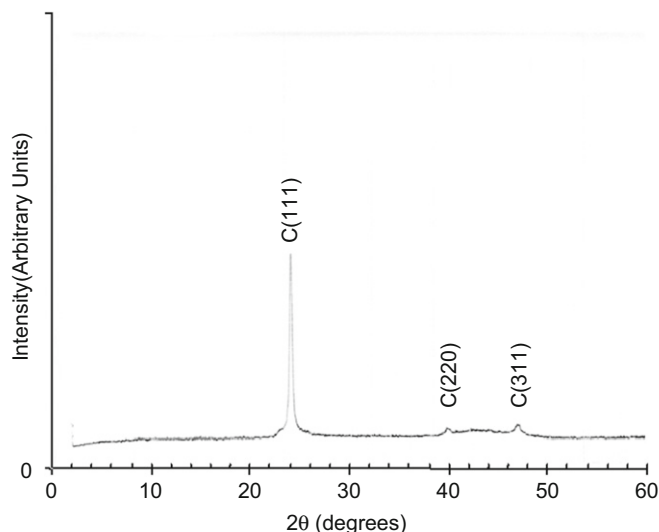


Fig. 1. X-ray diffractogram of vacuum-evaporated CdTe thin films.

Table 1

The grain size of the nanoparticles estimated from the XRD diffractogram and Scherrer formula.

Peak	d (nm)
C(1 1 1)	23
C(2 2 0)	7.8
C(3 1 1)	9.6

considered as that obtained from the C(1 1 1) peak that is 23 nm. This value is close to that obtained by Sotelo-Lerma et al. [5].

Fig. 2 displays the SEM image for one of the as-deposited vacuum evaporated CdTe thin films. The film appears to be regular with a very small density of large aggregates scattered on the surface. One reason of the smallness of the grain size was the low substrate temperature (ambient temperature), since according to Chu et al [6] the average grain size in the film depends on the substrate temperature and the thickness of the film. A second reason is the misfit stresses which develop in the film due to the geometric mismatch at interface boundaries between the film and the substrate which results in the formation of quantum dots.

The transmittance measurements were used to produce the first derivative of the absorbance which is plotted against the wavelength and shown in Fig. 3. The minima of the first derivative were displayed in Table 2 and used to find the optical bandgap energies. As we see there is a wide range of bandgap energies that is; 1.48–2.04 eV. The increase in the bandgap energy could be explained as follows; the nanoparticles have the crystalline structure of their bulk counter parts and hence are characterized by the fully occupied valence band and an empty conduction band separated by the energy gap (E_g). However, the charge carriers in these bands experience an overall confining

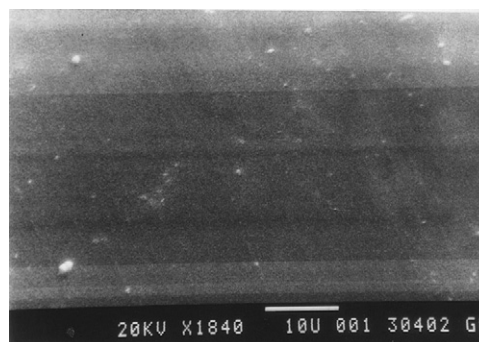


Fig. 2. SEM image of the as-deposited vacuum evaporated CdTe thin films of thickness about $1\mu\text{m}$.

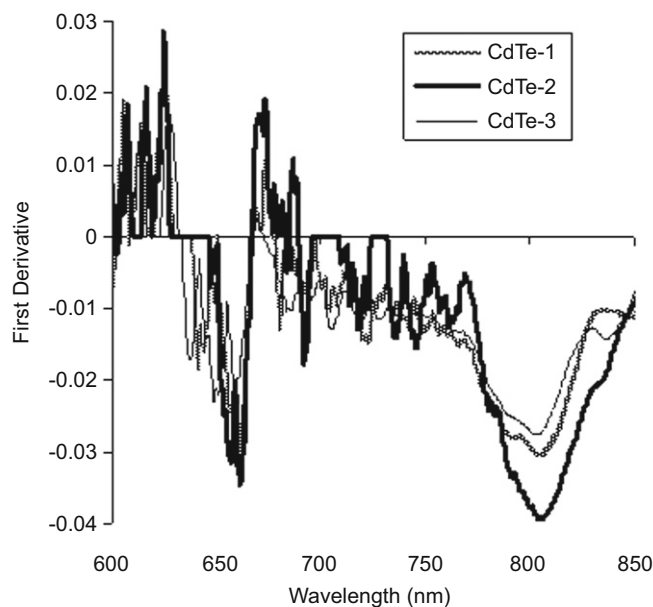


Fig. 3. The first derivative of the absorbance curves. Note: CdTe-1, CdTe-2 and CdTe-3 are the names of the samples.

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