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STRUCTURAL AND OPTICAL PROPERTIES OF CdTe THIN FILMS SYNTHESIZED BY LASER ABLATION ON SODA LIME GLASS SUBSTRATE

N. MAHMOOD*, M.N. KHAN[1], J. BASHIR[1], BUSHRA ILYAS and S.M.J. AKHTAR

Optics Laboratories, P.O. Box 1021, Nilore, Islamabad, Pakistan

[1]Physics Division, Directorate of Science, PINSTECH, P.O. Nilore, Islamabad, Pakistan

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Cadmium Telluride thin films with thicknesses 46 nm were deposited on soda lime glass substrates at room temperature by pulsed laser ablation technique. These films were then annealed in air at different temperatures. X-ray diffraction measurements showed that the as grown films are amorphous transforming to crystalline structure with annealing. Crystalline films with good quality were obtained when annealed at 200 - 300 ^{o}C. The results are in confirmation to the optical and atomic force microscopic studies on these films. The crystalline films possess cubic zinc blende structure. The growth occurred preferentially in the (111) direction. Annealing at higher temperatures >300 ^{o}C revealed that, the films reacts with glass substrate resulting in the deterioration of films crystallinity. The crystalline film showed a transmission of more than 80%. The optical parameters determined by the ellipsometry measurements showed values in close proximity to the bulk CdTe demonstrating its potential for photovoltaic device application.

Keywords: *Photovoltaic, X-ray diffraction, CdTe thin films, Optical parameters*

1. Introduction

Cadmium Telluride (CdTe) is II-VI semi-conducting material with immense technological applications. CdTe has long been considered as potential candidate for the development of photovoltaic cells because of its direct band gap, high absorption coefficient and its doping ability for both n- and p-type carriers. CdTe thin films have gained the renewed interest due to its important applications in technology of thin films devices such as photovoltaic cells, photo detectors and field effect transistors [1-2]. Previously different techniques had been employed to produce thin films of this material for its effective utilization in device fabrication but were not feasible by synthesis at high cost. The low temperature synthesis of this material on different substrates had been carried out during the last few years [3-4]. Deposition parameters such as deposition rate, substrate temperature, source temperature and post deposition heat treatments influencing the thermophysical properties of this material had also been described earlier [5]. Earlier syntheses of CdTe films include techniques like vacuum deposition [6-7], electrodeposition [8], molecular beam epitaxy [9-10], metal organic chemical vapor deposition (MOCVD) [11-12], closed space sublimation [13-14] and recent screen printing techniques [15-16]. These techniques have an advantage over one another's but none of these proved to be cost effective. The effective and low cost synthesis of this material with enhanced structural and optical properties for utilization in commercial device fabrication has been a demand for a long time. In this paper we report for the first time room temperature synthesis of nanocrystalline CdTe thin films using pulsed laser ablation technique on low cost soda lime glass substrate. The structural and optical properties of these films have been studied using tools such as X-ray diffraction, optical as well as atomic force microscopy and ellipsomety measurements. The results presented are being compared with earlier published data.

2. Experiment

CdTe thin films were synthesized by laser ablation on soda lime glass substrates at room temperature in a system designed and constructed

* Corresponding author : nasir@pinstech.org.pk

in our laboratory. Nd: YAG Laser (Quantel) was used to ablate the CdTe target inside the vacuum chamber maintained at 4.0 x 10^{-6} mbar. The pulsed laser wavelength was 1064 nm, average pulse energy 400 mJ/pulse, power density 2.67x10^9 W/cm^2, fluence 26.67 J/cm^2, pulse duration 10 ns, laser beam diameter 10 mm and 10 Hz repetition rate. The Schematic of the laser ablation setup is shown in Fig. 1.

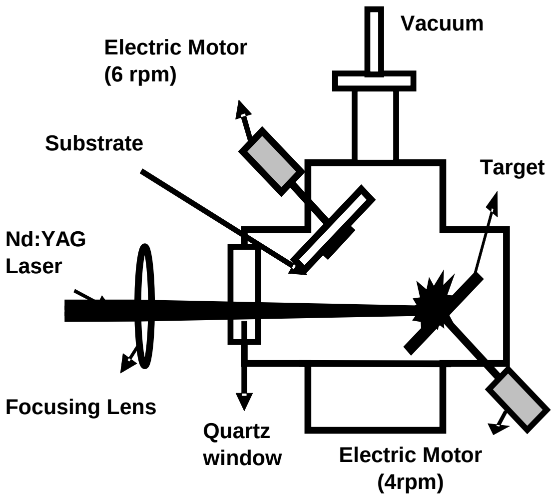

Figure 1. Schematic diagram for the laser ablation system.

The laser pulses were focused on the rotating target (CdTe disc) through a quartz lens with a focal length of 30 cm. CdTe target was a pre-sintered powder of CdTe pressed at pressure of 6 tons in a circular disc form with diameter 15 mm and thickness of 5 mm. The incidence angle to the ablation target was 45°. The focused spot size on the target was about 1.5 mm^2. The distance between substrate and target was kept at 4 cm. No reactive gas was introduced in the chamber during deposition. For uniform deposition the target and substrate holder were rotating with 4 rpm and 6 rpm respectively. The deposition time was around 20 minutes. After deposition, annealing of these thin films was carried out in air at different temperatures of 200- 500 °C in a step of 100 °C for 2 hrs. The structures of these films were characterized by X-ray diffraction. The surface morphology was characterized through metallurgical optical microscope Olympus BX51 as well as atomic force microscope (E -AFM system). Transmission (%T) of these CdTe films was measured in the 350 ~ 2500 nm range using Perkin Elmer FTIR spectrum 2000. Absorption co-efficient (α), optical band gap (E_g) was calculated from this data. The optical parameters of the film such as refractive indices (n), extinction-co-efficient (k), real dielectric constant (ε_1) and imaginary dielectric constant (ε_2) were derived from the measured ellipsometric data in the range 400 ~750 nm by Ellipsometer (SE-850, SENTECH).

3. Results and Discussion

Fig. 2 shows X-ray diffraction (XRD) patterns of the as grown and that of annealed films. It revealed that the as grown thin film has amorphous structure showing a broad band in the X-ray diffraction pattern. This broad band transforms to crystalline structure with annealing temperature. The well defined sharp and strong reflection centering at an angle 2θ = 23.82° with annealing is an indication of grain growth which occurred along the (111) preferential plane of cubic structure. Annealing at higher temperatures >300 °C, no improvement in the grain size has been observed rather the peak shape deteriorated, showing double edges as well as re-broadening as can be seen in XRD pattern of the annealed sample at 500 °C. This phenomenon can be attributed to chemical reaction occurring between the CdTe films and substrate material at higher temperatures. The lattice constants determined for the crystalline films considering cubic symmetry are a = 6.464 Å. This value is well in agreement to ASTM value of a_o = 6.481Å reported earlier for CdTe thin films [17].

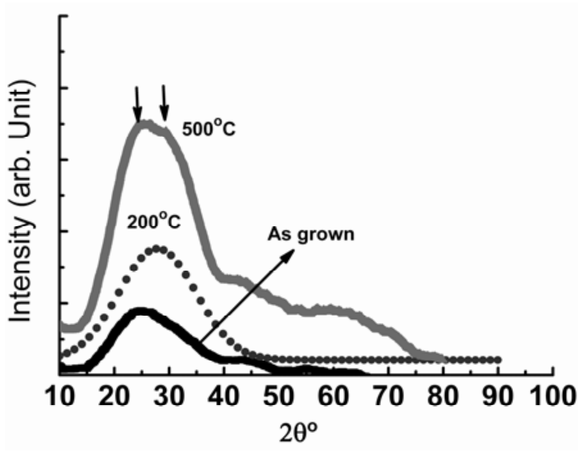

Figure 2. XRD patterns of the deposited thin films.

Surface morphology of the thin films examined by optical and atomic force microscopy is shown in Fig. 3(a-b). The as grown film shows the dispersed Cd and Te amorphous phases with inherent

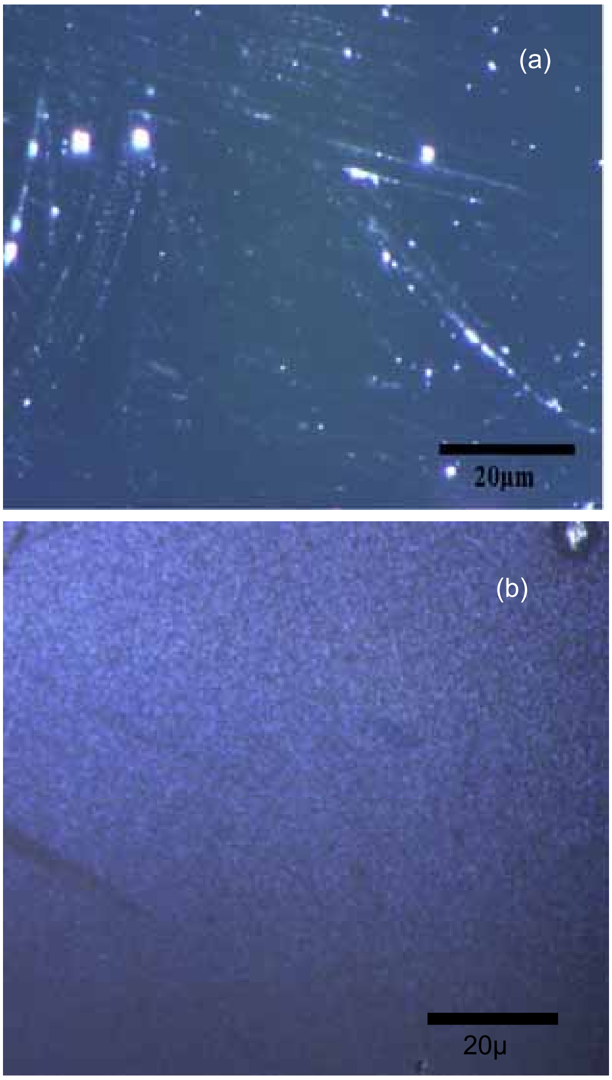

Figure 3. Optical micrograph on same magnification for (a) as grown (b) film annealed at 200 ^{o}C.

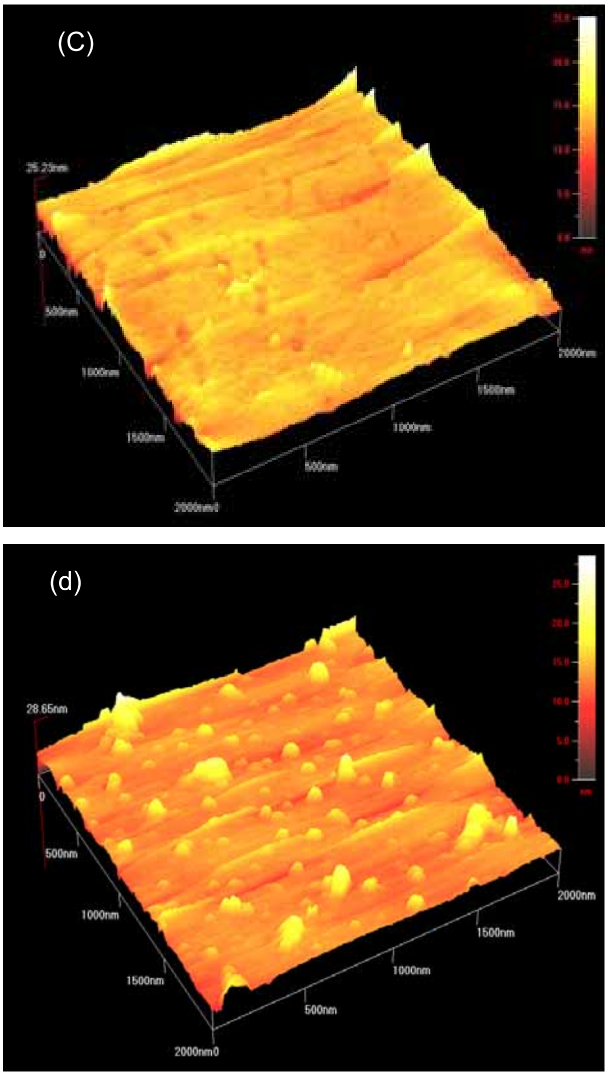

Figure 3. AFM images (c) As grown (d) film annealed at 200^{o}C

scratches and other defects visible on the substrate surface Fig. 3 (a).The film annealed at 200 ^{o}C on same magnification clearly shows the crystalline structure with grains uniformly distributed on the substrate surface Fig. 3 (b). The atomic force microscope images showed the layered growth for the as grown film Fig. 3 (c) while the annealed film at 200 ^{o}C shows the crystalline structure with smooth surfaces (Fig.3d). The energy supplied by annealing process was enough to promote the reaction between dispersed Cd and Te layers. The results are in good comparison to the one reported earlier [18]. In laser ablation the growth process is initiated by the nucleation of islands within all possible orientations on substrate surface and then adhesion of the deposited material while keeping the substrate at a certain constant temperature. We carried out the growth at room temperature. There post heat treatment in air is playing the dominant role in the growth process, converting Cd and Te free phases to interdiffuse and drive the growth to occur in the (111) direction. This preferential (111) growth had already been observed for CdTe thin films grown by other techniques and reported to be independent of substrate material and temperature, but in certain cases it happened only for high substrate temperatures, usually above 500^{o}C [19]. The production of highly oriented films at such low temperature is a greater advantage of the laser ablation technique, which has not been reported so far.

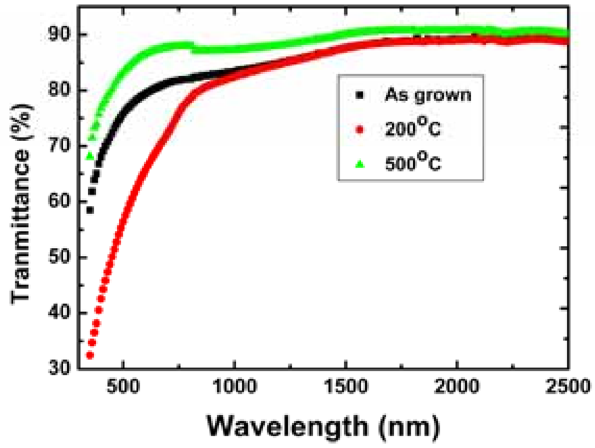

Figure 4. Transmittance versus wavelength for the as grown as well as films annealed at different temperatures.

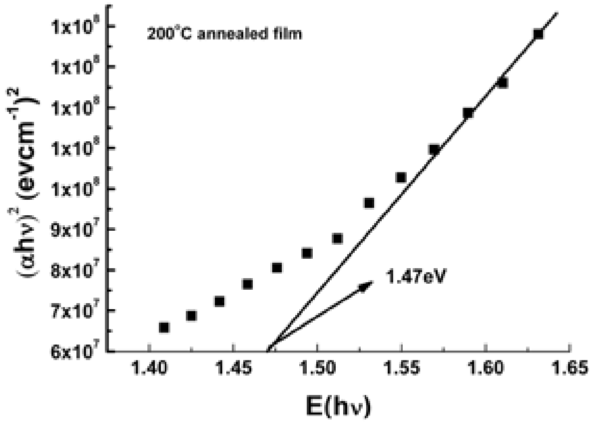

Figure 5. The variation of $(\alpha h\nu)^2$ with energy (hν) for the film annealed at 200°C.

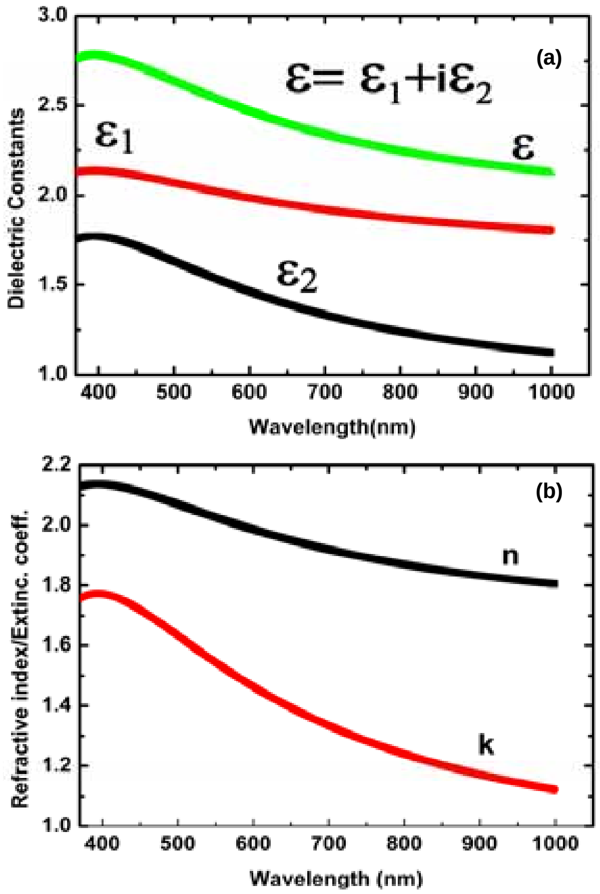

Figure 6. Optical parameters derived from the ellipsometric spectroscopy data.

Transmittance versus wavelength measurements for the as-deposited and CdTe thin films annealed at different temperatures are shown in Fig. 4. The experimentally measured transmittance increases with increasing photon energy. The transmittance values in the visible region are low but more than 80 % has been obtained for these films. The XRD data along with microstructure analyses by optical and AFM have unveiled that CdTe crystallization starts around 200°C. The films annealed at temperature of 200°C showed the characteristic absorption edge at 830 nm, when compared with the as grown and that to the film annealed at higher temperatures at 500°C, which lacks such absorption edges.

From the data shown in Fig. 4, we determined the absorption coefficient, α, as a function of wavelength. The variation of $(\alpha h\nu)^2$ with energy, $h\nu$, is shown in Fig. 5, for the film annealed at 200 °C. The band gap energy is obtained by intercepting the linear portion of the absorption curves to the energy axis. The band gap value 1.47 eV obtained is independent of the annealing temperature and coincides with those reported earlier in the literature for bulk CdTe [20-22].

The optical parameters were derived from the ellipsometry measurements carried out at room temperature on the film annealed at 200 °C. The derived optical parameters such as complex dielectric function $\varepsilon(\omega)$ and its real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts are shown in Fig. 6(a), while the refractive index (n) and extinction coefficient (k) data in the wavelength range 400-750 nm are shown in Fig. 6 (b). The film thickness and derived optical parameters shown in Figs 6 were obtained by bulk calculation of the spectroscopic ellipsometry data using Cauchy model. The film thickness comes out to be 46 nm. Cauchy equation describes the dispersion of film refractive index as a slowly varying function of wavelength, λ, with an exponential absorption tail. It also reflects the actual film property which strongly depends on the film deposition process. The imaginary part $\varepsilon_2(\omega)$ of the dielectric constant of the film depends on the absorption coefficient α and is related to valence to conduction band transitions having a close relation to its band structure. Both the refractive index and extinction coefficients shown in Fig 6 are oscillatory in nature. Earlier it has been reported that in the case of glass substrate, the CdTe films have refractive index which is smaller than that of the monocrystalline CdTe attributed to the polycrystalline structure of the film [4, 23]. It was also found that refractive index of CdTe film on the monocrystalline Si substrate in the visible spectrum is 2.1, which is appreciably smaller than average value 2.5 of CdTe films grown on the CdHgTe substrate [24]. This refractive index decrease in our case can also be explained by the varied structure of the film containing single grids of basic CdTe materials with porous ones.

4. Conclusions

Cadmium Telluride thin films of nm thicknesses were successfully deposited on well cleaned soda lime glass substrates by pulsed laser deposition technique under a pressure of 4×10^{-6} mbar at room temperature. By analysis of the X-ray diffraction patterns it is found that the as deposited CdTe film exhibits amorphous structure gradually changing to crystalline one when annealed at temperature > 200 ^oC. The peaks at $2\theta = 23.82^o$ indicates that the annealed CdTe film possesses zinc-blende cubic structure with a preferential growth along the (111) plane. The measured lattice parameter is a = 6.464 Å is close to ASTM value of a_o = 6.481Å well in agreement to the ealier published data [17]. XRD, optical and atomic force analyses showed that CdTe crystallization occurs between 200-300 ^oC. The crystalline film showed comparable optical properties to the bulk CdTe materials showing its tendency for photovoltaic applications.

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