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Influence of post-deposition heat treatment on optical properties derived from UV–vis of cadmium telluride (CdTe) thin films deposited on amorphous substrate

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ABSTRACT

In this work, we report on post-deposition heat treatment (annealing)-induced change in optical properties derived from UV–vis study of CdTe thin films prepared on amorphous glass substrate by electron beam evaporation technique. Annealing effect gives rise to the enhancement in crystalline nature (zinc blende structure) of CdTe films with (1 1 1) preferred orientation. The average transmittance was increased with the annealing temperature and the slight shift in transmission threshold towards higher wavelength region revealed the systematic reduction in optical energy band gap. The existence of shallow level just below the conduction band, within the band gap was identified in the range of 0.23 and 0.14 eV for the films annealed at 200 and 450 °C, respectively. The optical quality of deposited films was confirmed by the photoluminescence study. In addition, the scanning electron microscopic measurement supports the result of X-ray diffraction study. The Swanepoel, Hervé-Vandamme, and Wemple–DiDomenico models have been employed to evaluate the various optical parameters of CdTe films. These results are correlated well with other physical properties and discussed with the possible concepts underlying the phenomena.

1. Introduction

A variety of binary semiconductors especially from II–VI group have been studied extensively due to their potential use in photoconductive devices and solar cells [1]. Cadmium telluride (CdTe) is an important II–VI semiconducting material potentially used for the fabrication of opto-electronic devices, photovoltaic cells, laser windows, gamma ray detector, and p-n diodes owing to its optimum band gap and high absorption coefficient [2]. CdTe semiconductor exists in either zinc blende (cubic) or wurtzite (hexagonal) structure. Further, CdTe can exhibit both n-type and p-type conductivity, which makes it useful for both homojunction and heterojunction configurations.

It should be noted that the CdTe films have some specific structural and sub-structural peculiarities, namely: the coexistence of two polymorphous modifications of material, high concentration of twins, stacking faults, defects, dislocation, and high level of micro-deformation [3]. Besides, the extended and point defects in CdTe are the electrically active states. Therefore, they have strong effect on the optical and photoelectric properties of thin films and thus considerably determine solar cells efficiency [4]. Moreover, the photovoltaic device performance of CdTe films basically depends on their structural, optical, surface morphological, compositional, and electrical properties. It is important that the improvement of material's properties requires a closer inspection of growth conditions and also the above said properties of thin films. At present, the modification of structural and optical properties of CdTe films under different conditions is a matter of intense research. These include post-deposition heating (annealing), ultraviolet irradiation, direct current injection, and irradiation by a beam of ions or electrons. Among them, the post-deposition heat treatment is the effective and simplest way to tune the above-mentioned physical properties of CdTe films.

Till now, various techniques have been employed to deposit CdTe films, viz. thermal evaporation [5], closed space sublimation [6], liquid-phase deposition [7], pulsed laser deposition [8], pulsed laser evaporation [9], molecular beam epitaxy [10], chemical vapour deposition [11], and electrodeposition [12]. It is worthwhile to mention here that the electron beam evaporation (EBE) technique, one of the physical vapour deposition methods, has been

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considered largely for the preparation of device quality thin films owing to the maximum possibility of direct transfer of energy to the source. Though the production cost of films by EBE technique is high (than the chemical methods), they impart some feasible devised-based qualities to the films, which are the key factors deciding the performance of the films for their suitability in developing special devices. To date, very few reports are available on CdTe thin films prepared by electron beam evaporation technique [13]. For instance, Murali *et al.* [13] studied the effect of substrate temperature on the electrical properties of CdTe films deposited by electron beam evaporation technique. In our earlier work, we have reported the change in physical properties of electron beam-evaporated CdTe films prepared at room temperature (RT) by the effect of Cu addition [14]. However, no attempt has been made to study the detailed optical parameters (such as optical constants, dielectric constants, dispersion energy parameters, etc.) of electron beam-evaporated CdTe films by the effect of post-deposition heat treatment. Therefore, a lot more needs to be done to understand the effects of annealing on the detailed optical properties of thin CdTe films. These studies will be extremely useful to design a better absorber layer for solar cell applications. In this work, we report on post-deposition heat treatment-induced change in the structural, optical, luminescence, surface morphological, and compositional properties of electron beam-evaporated CdTe thin films.

2. Experimental details

2.1. Deposition of thin films

Thin films of CdTe were deposited on 7059 corning glass substrates (Sigma-Aldrich; 75 mm length × 25 mm width × 1 mm thickness) by electron beam evaporation (EBE) technique (HIND-HIVAC vacuum coating unit model 12A4D with electron beam power supply model EBG-PS-3K) under a chamber pressure of 2×10^{-5} mbar at room temperature (RT). Substrate cleaning plays a vital role in the deposition of thin films especially by EBE technique. Prior to the deposition, the glass substrates were kept in hot chromic acid for 1 h to remove organic impurities from the substrate surface, followed by a thorough cleaning with deionized water. Further, the glass substrates were ultrasonically cleaned with 2-propanol, acetone, and deionized water, 15 min each and finally dried in hot air oven. Cadmium telluride powder (Sigma-Aldrich; 99.99% purity) was made into pellet of 10 mm diameter with 4 mm thickness. The pelletized CdTe ingots were placed in graphite crucible (12 mm outer diameter × 10 mm inner diameter × 6 mm depth) and kept on water-cooled copper hearth of the electron gun, inside the vacuum chamber. The distance between the substrate and the target material was kept fixed at 12 cm. The chamber was evacuated to a high vacuum of the order of 2×10^{-5} mbar using rotary and diffusion pumps and the chamber pressure was measured by pirani and penning gauges. In the electron gun, the electrons extracted from a dc-heated cathode of tungsten filament, by the application of electric field, pass through an anode, and deflected through an angle of about 180° by the magnetic field and reach the target material. The surface of CdTe pellet on the graphite crucible was scanned by the resultant and deflected electron beam with an accelerating voltage of 5 kV and a power density of about 1.5 kW cm^{-2}. The ablated material was evaporated and the vapour phase condensed and deposited as thin film on the substrate. The homogeneous distribution of evaporated CdTe particles on the substrate was attained by continuously rotating the substrate during deposition. The deposition time was 10 min and the deposition rate was 0.1 μm/min. The thickness of deposited film was in the range of ∼1 (±0.03) μm, measured by surface profilometer (Mitutoyo, SJ-301). Later on, the as-deposited films were annealed in air (post heat treatment) (T_{annea}) at 200, 300, 400, and 450 °C for 10 min.

2.2. Characterization techniques

The structural property of annealed CdTe thin film was analysed by X-ray diffraction (XRD; X' pert Pro PANalytical) study using Cu Kα radiation (λ = 0.154 nm) over a 2θ scan range of 10–80°. The optical properties of films were studied by UV–vis–NIR spectrophotometer (JASCO) in the wavelength range of 300–2500 nm. The deuterium (25 W) and tungsten halogen (20 W) lamps were used as the light source, and the spot size of measurement was 5 mm. In the double beam UV–vis–NIR optical measurement, the optical contribution from the glass substrate was compensated by introducing it as a reference in the measurement. Hence, the contribution from the substrate was nullified and the final optical spectrum is only due to the deposited film. Therefore, all the optical spectra are normalized with respect to the substrate. The photoluminescence (PL) property of film was studied using luminescence spectrophotometer (cary eclipse VARIAN). Xenon flash lamp (15 W) and photomultiplier tube were used as the source of excitation and detector, respectively. The films were excited at the wavelength of 600 nm and the measurement area was 6 mm^2. Surface morphology of the film was studied using scanning electron microscopy (SEM; TESCAN VEGA 3) and atomic force microscopy (AFM; Nanoscope-E). The SEM measurement was carried out with an accelerating voltage of 30 kV and the current levels of 30–120 pA. The tungsten was used as the electron source in SEM. Whereas, the AFM measurement was done in air environment with the scan rates of 5–10 Hz. The silicon nitride (Bruker Instruments, USA) contact mode tip was used for the AFM study. The compositional study was done by energy dispersive X-ray analysis (EDAX; BRUKER GMBH) with an excitation accelerating voltage of 1.2 kV and the excitation current of 600 pA.

3. Results and discussion

3.1. Structural property

Generally, vapour-deposited CdTe thin films exist in (111) orientation and the as-deposited CdTe thin films at RT show columnar grains with submicron size. However in some cases, randomly oriented films can also be obtained [15]. In our earlier case, the RT-deposited CdTe films are amorphous in nature [14]. Fig. 1a shows the XRD patterns of CdTe films annealed at 200, 300, 400, and 450 °C. The onset of crystallinity was observed for the film annealed at 200 °C, which is evident from the inset of Fig. 1a. When the annealing temperature was increased to 300 °C, the film possesses polycrystalline nature, pronounced with zinc blende structure, which agrees well with the standard JCPDS data (card Nos. 65-0880 and 65-1046). Highly ordered XRD peaks observed at 2θ = 23.72, 39.26, and 46.28° correspond to (1 1 1), (2 2 0), and (3 1 1) planes, respectively. The annealing temperature (up to 400 °C) induced increase in XRD peak intensity was observed. This may be due to the increase in surface mobility of adatoms on the substrate surface because of enough thermal energy at higher annealing temperature. Other aspect is that the grain size of the films increases with increasing annealing temperature. At higher annealing temperature, the atomic, ionic, or molecular species of CdTe formed on the substrate surface acquire a large thermal energy and hence a large mobility. Therefore, a large number of nucleus are formed which coalesce to form a continuous film with large grains on the substrate at higher temperature [16]. However, when the annealing temperature was increased further to 450 °C, there is a decrease in intensity of the peaks. At higher annealing temperature, there is a possibility for the dissociation and desorption of adatoms that