

Swift heavy ion induced phase transition in CdTe films deposited by spray pyrolysis in presence of electric field

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ABSTRACT

CdTe polycrystalline thin films possessing hexagonal phase regions are obtained by spray deposition in presence of a high electric field. Thin film samples are irradiated with 100 MeV Ag ions using Pelletron accelerator to study the swift heavy ion induced effects. The ion irradiation results in the transformation of the metastable hexagonal regions in the films to stable cubic phase due to the dense electronic excitations induced by beam irradiation. The phase transformation is seen from the X-ray diffraction patterns. The band gap of the CdTe film changes marginally due to ion irradiation induced phase transformation. The value changes from 1.47 eV for the as deposited sample to 1.44 eV for the sample irradiated at the fluence 1×10^{13} ions/cm². The AFM images show a gradual change in the shape of the particles from rod shape to nearly spherical ones after irradiation.

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1. Introduction

Ion beam induced modification in materials is an active field of continuous research from both scientific and technological viewpoints. The method stands unique because of its capability to deposit very high energy in a localized region thereby attaining spatial selection in modifying the properties of materials. Heavy ions of velocity comparable to or higher than the orbital electron velocity of the lattice atoms (swift heavy ions) dissipate their energy in materials mainly through electronic excitation and ionization. The transient excitations during the energy dissipation can result in a variety of effects in materials leading to the creation of point defects, defect clusters, crystallization, amorphization, phase transformation, etc. within a narrow cylindrical region along the path of the heavy ion beam [1–3]. Few models like, thermal spike, Coulomb explosion and lattice relaxation model have been proposed to explain the transfer of the energy gained by the electronic sub system to the energy responsible for the displacement of

the lattice atoms. According to the thermal spike model, the energy transfer of the heavy ion to the lattice takes place by electron–phonon coupling resulting in a transient high temperature zone within a cylindrical region (thermal spike) along the ion path [4–9]. The Coulomb explosion model is based on the assumption that the intense excitation and ionization occurring along the ion path leads to an unstable zone from which the ions are ejected into non-excited parts of the lattice by Coulomb repulsion, resulting in a mechanical polarization [10–12]. According to the lattice relaxation model, weakening of atomic bonds occurs due to the intense electronic excitation so that a repulsive force starts acting between the atoms leading to their collective rearrangement [13].

In this paper, we report our studies on the effects of swift heavy ion irradiation in CdTe polycrystalline thin films, deposited by spray pyrolysis in presence of an electric field. We observed the stabilization of the metastable hexagonal (wurtzite) phase of CdTe in the films deposited in presence of a high electric field, which is difficult to stabilize using any of the conventional deposition methods [14–16]. The swift heavy ion irradiation results in the transformation of the hexagonal regions in the films to stable cubic phase due to the dense electronic excitations induced by beam

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irradiation. Crystalline to crystalline phase transformations induced by swift heavy ions have been reported in certain single crystals and polycrystalline materials, especially oxides [17–21]. The present study illustrates the possibility of swift heavy ion induced phase transformation in II–VI polycrystalline semiconductor thin films.

2. Experimental details

The spray deposition has been performed inside a specially designed chamber attached to a rotary vacuum pump and a nitrogen gas purging system. For deposition in presence of electric field, a voltage of 1 kV is applied between the spray nozzle and a metal electrode placed 2 mm below it. The precursor solution (0.02 M) for the spray deposition is prepared by dissolving cadmium chloride (CdCl_2) and tellurium dioxide (TeO_2) in a solution containing ammonia and double distilled water in the ratio 1:4. To favour the formation of CdTe on the hot substrate, ~ 7.5 ml. of hydrazine hydrate ($\text{N}_2\text{H}_4\cdot 2\text{H}_2\text{O}$) is added into 250 ml of the spray solution to reduce the valency of tellurium ions from Te^{4+} to Te^{2-} for reacting with the Cd^{2+} ions. The pH of the solution is adjusted at ~ 11.2 using HCl. Nitrogen is used as the carrier gas. The deposition is performed at a substrate temperature of 350°C . The glass substrates are kept at a distance of 17 cm from the spray nozzle [22]. CdTe polycrystalline thin films of thickness ~ 300 nm are prepared in presence and the absence of an electric field to establish the role of the field.

The ion irradiation of the samples is performed using the 15 UD Pelletron accelerator at the Inter University Accelerator Centre, New Delhi. The irradiation is carried out at room temperature in an experimental chamber having a vacuum of 10^{-6} torr. The beam current is maintained around 1 particle nano ampere (pna) during irradiation and the beam is scanned with the help of an electromagnetic scanner to ensure uniformity of irradiation over an area $10\text{ mm} \times 10\text{ mm}$ of the sample. The TRIM simulation indicates the range of the incident ion in the material as about $10\ \mu\text{m}$ and therefore the ions get buried in the substrate only and not in the film. We used the irradiation fluences 1×10^{12} and 1×10^{13} ions/ cm^2 for the study.

The as deposited and the irradiated samples are characterized using X-ray diffraction, optical absorption and atomic force microscopy. A Bruker (AXS D8 Advance) glancing angle X-ray diffractometer with CuK_α radiation having wavelength $1.5406\ \text{\AA}$ is used for structural characterization. The optical absorption of the samples is done using a Hitachi UV-Vis spectrophotometer. The surface topography of the samples is recorded using a Digital Instruments Multimode IIIa atomic force microscope. A Taylor-Hobson Talystep is used for film thickness measurements.

3. Results and discussion

Fig. 1(a) shows the X-ray diffractogram of the CdTe thin film sample deposited in presence of an electric field. To establish the role of electric field, samples have also been deposited without the presence of the field and the corresponding diffraction pattern is given in Fig. 1(b). From the powder diffraction data, it is known that the diffraction pattern of CdTe with cubic symmetry presents some major peaks that overlap with the peaks of CdTe in the hexagonal phase (Fig. 2(a) and (b)). For example, the high intensity peak around $2\theta = 23.70$ may be assigned to both the cubic (1 1 1) peak and the hexagonal (0 0 2) peak since their diffraction angles differ only slightly. But, for the films deposited in presence of an electric field, the occurrence of a peak at $2\theta = 22.33$ corresponding to the hexagonal (1 0 0) alignment and the intensity ratio of the peaks at $2\theta = 23.70$ and $2\theta = 39.23$, which is equal to 1.08 in

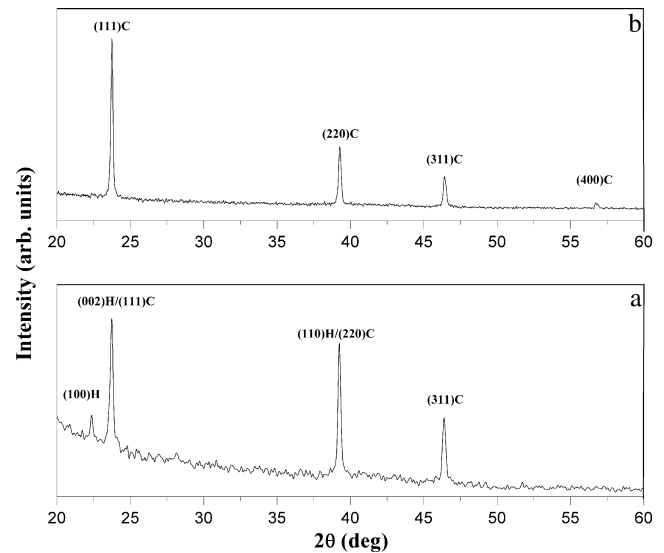


Fig. 1. X-ray diffractogram of CdTe film deposited (a) with electric field (b) without electric field.

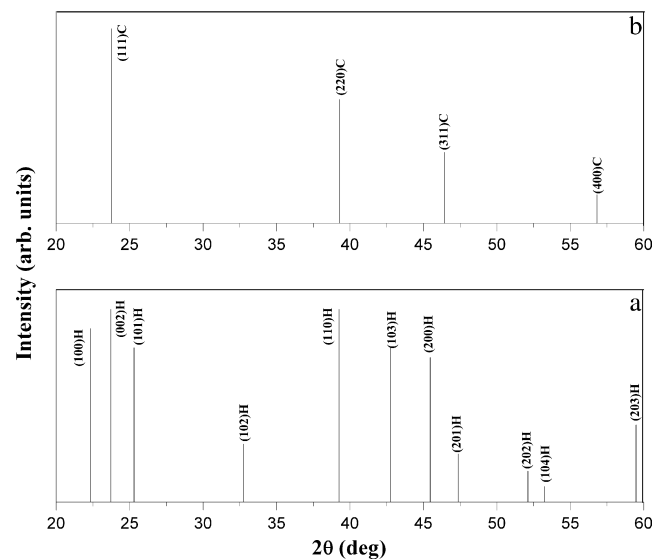


Fig. 2. Powder diffraction data of: (a) hexagonal and (b) cubic CdTe.

the present case, confirm the presence of hexagonal phase in the film. According to the powder diffraction data, for the hexagonal structure, the intensity ratio of the peaks at 23.70 and 39.23 is 1, which is pretty close our result. But, at the same time, the presence of a peak at $2\theta = 46.4$ exhibits the presence of cubic regions also in the film. We therefore conclude that the CdTe films deposited in presence of an electric field is a polycrystalline mixture of phases with the predominance of the hexagonal phase. The peaks at $2\theta = 23.70$ and $2\theta = 39.23$ can therefore be associated with the (0 0 2) H and (1 1 0) H orientations, respectively [14,23]. It is to be realized that the presence of a high electric field during the spray can lead to perturbations in the ABCABCABC... cubic stacking sequence, which leads to stabilization of the hexagonal phase. The X-ray diffractogram of the CdTe film grown without electric field (Fig. 1(b)) shows only the peaks corresponding to cubic zinc blende arrangement, establishing the role of the field [24].

Fig. 3(a) and (b) show the X-ray diffractogram of the CdTe thin film samples, deposited in presence of an electric field after irradiation at fluences 1×10^{12} ions/ cm^2 and 1×10^{13} ions/ cm^2 ,

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