

INFLUENCE OF Fe DOPING CONCENTRATION ON STRUCTURAL PROPERTIES OF CdS BASED THIN FILMS PREPARED ON SILICON SUBSTRATES BY ELECTRON BEAM EVAPORATION

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We studied the structural, elemental composition and micro structural properties of CdS nanocrystalline thin films doped with transition metal Fe, grown by electron beam evaporation on silicon substrates (Si) at room temperature. In this work we have doped different Fe concentration in the range of 5% to 15 %. Fe doping does not lead to the formation of any secondary phase, either in the form of metallic clusters or impurity complexes. The X-ray diffraction (XRD), energy dispersive spectroscopy (EDS) and atomic force microscopy (AFM) have been used to characterize the Fe doped CdS thin films. XRD analysis shows that Fe doping has a significant effect on crystalline quality and grain size in the films, the average grain size varies from 23 nm to 58 nm, by increasing Fe doping concentration and conformed the nanocrystalline nature of the films. The results obtained from EDS studies did not deviate much from the composition of starting precursor alloys, which indicated that the composition was nearly stoichiometric. From the investigation of surface morphology using AFM, nanocrystalline nature of the films was observed. The films exhibited smooth fine grainy surface at higher Fe doping concentrations.

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1. Introduction

Magnetic semiconductors are semiconductor materials that exhibit both ferromagnetism or a similar response and useful semiconductor properties. If implemented in devices, these materials could provide a new type of control of conduction. Whereas traditional electronics are based on control of charge carriers (n- or p-type), practical magnetic semiconductors would also allow control of quantum spin state (up or down). This would theoretically provide near-total spin polarization which is an important property for spintronics applications, e.g. spin transistors. While many traditional magnetic materials, such as magnetite, are also semiconductors. Materials scientists generally predict that magnetic semiconductors will only find widespread use if they are similar to well-developed semiconductor materials. To that end, dilute magnetic semiconductors have recently been a major focus of magnetic semiconductor research. These are based on traditional semiconductors, but are doped with transition metals instead of, or in addition to, electronically active elements. During the last few years, there has been much interest in dilute magnetic semiconductors (DMSs) due to their potential applications in spintronic devices, which can manipulate both charge and spin degrees of freedom simultaneously in single material. CdS-based DMS is also a good candidate for such applications as magneto-optical devices (magnetic

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field sensors, isolators and magneto-optical switches), field-emission displays, solar cells and gas sensors. DMSs are II–VI, IV–VI, or III–V compounds in which fraction of non-magnetic cations has been substituted by magnetic transition metal or rare-earth metal ions [1] - [19].

CdS is an important II-IV binary semiconductor with energy gap of 2.42 eV at room temperature (RT) and with many excellent physical and chemical properties. It is well-known that Fe-doping can lead to remarkable change in the properties of DMS. Fe is a good ferromagnetic material with low coercivity and high Curie temperature. Substitutional Fe²⁺ possesses both spin and orbital moment ($S = 2$, $L = 2$). Therefore, Fe based CdS can lead to a number of possibilities for fabrication of magneto-optic device and magnetic sensors [20] - [21].

In the present work, the micro structural properties of the Fe doped CdS nanocrystalline thin films with different Fe concentrations deposited on silicon substrate (Si) by electron beam evaporation were investigated. The structure and composition of the films were characterized by the X-ray diffraction (XRD) and the energy dispersive spectroscopy (EDS). We have also investigated the nanocrystalline nature of the films from the surface morphology using atomic force microscopy (AFM).

2. Experimental

The series of Fe doped CdS polycrystalline alloys ($\text{Cd}_{1-x}\text{Fe}_x\text{S}$) with different content of Fe ($x = 0.05, 0.1, \text{ and } 0.15$) was synthesized by solid state reaction method. Stoichiometric amounts of high purity (99.999 %) analytical grade CdS and FeS powders (Sigma-Aldrich co., USA) were mixed by grinding for about 7 hr. The mixed powders were pressed into a disk-shape pellet. Electron beam evaporation technique was utilized for growing Fe doped CdS thin films ($\text{Cd}_{1-x}\text{Fe}_x\text{S}$) with various Fe-concentrations ($x = 0.05, 0.1, \text{ and } 0.15$) using high vacuum coating unit type. The growth chamber exhibits a base pressure of 8.0×10^{-6} mbar and a working pressure of 6.0×10^{-4} mbar. The substrate to source distance was kept at 50 mm. The films were deposited on ultrasonically cleaned silicon substrates maintained at room temperature. The electron beam intensity and energy were fixed at 20 mA and 5 KeV. During deposition of the films, the substrate holder was rotated to improve the uniformity of the films.

Crystal structure of as-deposited films was studied by X-ray diffraction (XRD). The data were collected by-step-scan modes in $\theta - 2\theta$ range between 20° and 80° with step-size of 0.02° and step time of 0.6 s. The X-ray diffractometer was operated at 40 KV and 30 mA with $\text{CuK}\alpha_1$ radiation of wavelength 1.5406 Å. The elemental composition of the films was analyzed by using energy dispersive X-ray spectrometer (EDXS) unit interfaced with a scanning electron microscope, SEM, operating at an accelerating voltage of 30 KV which was used to study the morphology of the films. The grain size and root mean square (RMS) surface roughness of the films were obtained by atomic force microscopy.

3. Results and discussions

3.1. XRD results

XRD patterns of the as deposited $\text{Cd}_{1-x}\text{Fe}_x\text{S}$ thin films with different Fe concentration ($0.05 \leq x \leq 0.15$) at room temperature are shown in Fig. 1. When reviewed along the diffraction patterns of the films, we found, for $x=0.05$, a dominant peak around $2\theta \sim 26.56^\circ$ with weak peaks at $\sim 26.58^\circ$, and 26.62° . These diffraction peaks correspond to the planes (002), (101), and (101) respectively, which were indexed on the basis of hexagonal CdS type structure (JCPDS No.41-1049). Other additional diffraction peaks were not detected, indicating that Fe ions might have entered into the CdS lattice.

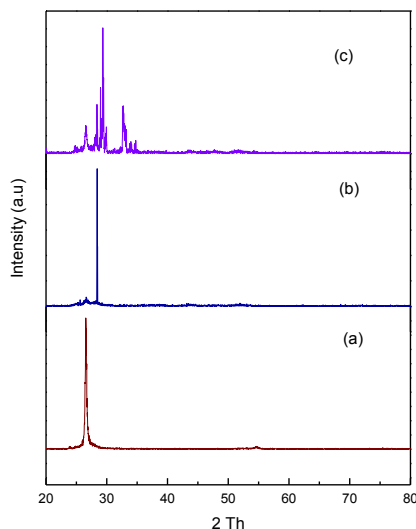


Fig.1. X-ray diffraction patterns of the $Cd_{1-x}Fe_xS$ nanocrystalline films.
(a) $x = 0.05$, (b) $x = 0.1$, (c) $x = 0.15$

The XRD patterns exhibited strong preferred crystallographic orientations along (002) plane. We observe a slight systematic shift of the main peak (002) towards higher values of diffraction angle 2θ by increasing Fe concentration. It suggests that the decrease in the lattice parameters due to the fact that substitution of larger ionic radius of Cd^{2+} (0.97\AA) by smaller ionic radius of Fe^{2+} (0.76\AA) requires a local contraction of the lattice to accommodate the Fe^{2+} ion. The shifting of the peak position also confirms that the Fe is replaced in Cd atom positions and did not form any chemical reaction with sulphur to form new compounds. The lattice parameters a and c of the hexagonal unit cell of $Cd_{1-x}Fe_xS$ thin films ($0.05 < x < 0.15$) were calculated from the most intense XRD peak positions by supposing two reflections of different indices ($h_1=0, k_1=0, l_1=2$) and ($h_1=1, k_1=0, l_1=1$).

The average grain size (crystallite size), values are calculated from the full width at half maximum (FWHM) intensity of the XRD peaks using Scherrer's relation [22]

$$D_{hkl} = \frac{k\lambda}{\beta \cos \theta} \quad (1)$$

Where k is a shape factor usually ~ 0.9 , λ the wavelength of the X-ray diffraction used (1.5406\AA), β the full width at half maximum (FWHM) of the peak which has maximum intensity and θ the Bragg angle. The average grain size is in the range 60 nm to 23 nm, conforming the nanocrystalline nature of $Cd_{1-x}Fe_xS$ films.

3.2 EDS results

The results obtained did not deviate much from the composition of starting precursor alloys. Fig. 2 shows the EDS results. The ratio of Cd: Fe: S is observed to be about 44.58 at %: 4.79 at % : 50.43 at % for films with $x = 0.1$ which indicated that the composition was nearly stoichiometric.

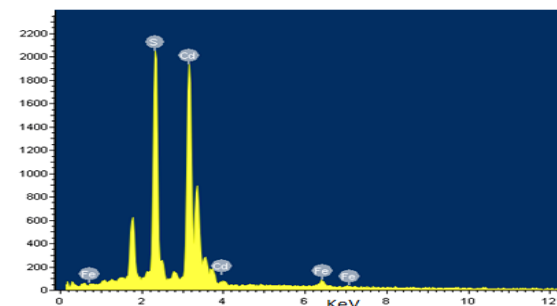


Fig.2. EDS Spectrum

3.3 AFM results

From the AFM results, the films exhibit smooth free grainy surface. AFM allows us to get quantitative information on microstructure properties of the sample surface and to plot topographies representing the surface relief. Therefore RMS surface roughness and average surface grain size were calculated from AFM micrographs.

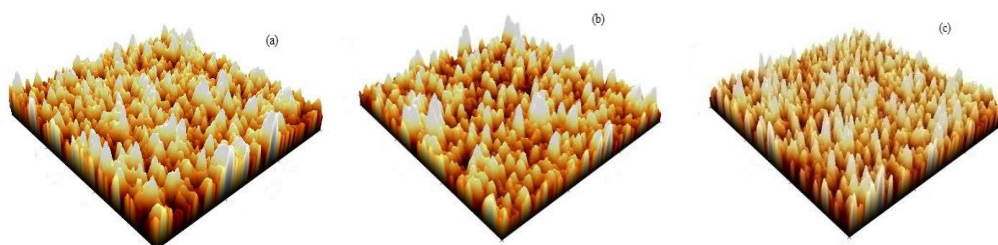


Fig.3. 3D AFM images of $Cd_{1-x}Fe_xS$ nano crystalline films (a) $x = 0.05$, (b) $x = 0.1$, (c) $x = 0.15$

Fig. 3 shows typical 3D AFM monographs of the $Cd_{1-x}Fe_xS$ films with concentrations $x = 0.05$, $x = 0.1$, $x = 0.15$. The surface relief clearly shows roughness and granular crystalline nature is evident from the figures.

The average surface grain size varies from 57 nm to 22 nm as the Fe content increases from 0.05 to 0.2. The grain size evaluated from AFM is comparable with those obtained from XRD studies. The RMS surface roughness decreased with increasing Fe content from $x = 0.05$ to $x = 0.2$.

4. Conclusions

In summary, Fe doped CdS nanocrystalline films were grown by electron beam evaporation method. XRD studies showed a single phase with a hexagonal structure. Fe doping has a significant effect on crystalline quality and grain size of the films. Grain size decreases as Fe concentration increases. These Fe doped CdS based films seem to be good candidates for the future spintronic applications.

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