STUDY OF STRUCTURAL AND OPTICAL PROPERTIES OF $Cd_{1-x}Co_xS$ THIN FILMS PREPARED BY THERMAL EVAPORATION METHOD

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Thin films of cobalt doped cadmium sulfide with 50 nm thickness and different cobalt concentrations were deposited on glass substrates by thermal evaporation method. The structure of the films was investigated by X-ray diffractometry (XRD). It was revealed that the films have hexagonal structure with (002) preferred orientation. Transmittance and absorption spectra of the films were measured at wavelength range 250-1100 nm. Then the band gap and refractive index of the films were calculated by using transmittance and absorption spectra. The results indicated reduction of the band gap with increase in cobalt concentration.

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1. Interduction

Among the II–IV semiconductor compounds, cadmium sulfide (with band gap of ~2.42 eV) due to its special physical properties such as photoconductivity in visible and near ultra-violet spectral regions and high optical transparency has been extensively studied [1-3]. Cadmium sulfide thin films have been used in making electronic device, photovoltaic cells and optical detectors too [4-6].

During the last few years, some studies in the field of magnetic materials are focused with the aim of achieving semiconductors that have ferromagnetic properties at room temperature. This was performed by doping of magnetic ions like Mn, Fe, Co or rare earth elements into the host semiconducting lattices. This leads to a new class of materials known as diluted magnetic semiconductors (DMS) which they have ability of applications in spintronic [7]. The cobalt doped CdS has been proposed to be applicable in solar cells, diodes and sensors [8]. Cobalt doping causes exchange interaction creation that affects on structural and optical properties of films. The $Cd_{1-x}Co_xS$ thin films are prepared by several chemical methods such as spray [7], chemical bath [9] and surfactant-assisted [10].

To the best of our knowledge, no report exists based on cobalt doped cadmium sulfide thin films prepared using thermal evaporation. So the $Cd_{1-x}Co_xS$ thin films were deposited by thermal evaporation technique and changes caused by cobalt doping on the structural and optical properties of the films were studied.

2. Experimental

Thin films of pure CdS and Co doped CdS were fabricated by thermal evaporation technique using an Edward coating unite at pressures of less than 7.5×10^{-6} mbar on glass substrates

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at ambient temperature. CdS and Co Powders of 99.99% purity were supplied from Aldrich Company as the source materials. The powders weighted in appropriate amounts (cobalt percentage of x=0, 0.025, 0.05) and were mixed after grinding in mortar perfectly. Then this powder was evaporated from a capped molybdenum boat to deposit the films. The deposition rate was measured and controlled in situ using thickness monitor in control panel of coating machine. The typical growth rate was 20Å/s on average and also thickness of the films was chosen about 50nm.

The crystal structure of the films was determined by x-ray diffraction (XRD) using an x-ray diffractometer (Advance Model D8) with Cuk_{α} radiation (λ=1.5406Å). T he optical transmission spectra of the prepared $Cd_{1-x}Co_xS$ thin films were obtained by Shimadzu UV-Vis spectrophotometer (Model UV-1650 PC) in the spectra range of 250 to 1100 nm. The surface of the films was examined by Field Emission Scanning Electron Microscopy (FESEM).

3. Results and discussion

3. 1 Structural properties

Diffraction spectra of the $Cd_{1-x}Co_xS$ thin films with different concentrations of Co are shown in figure 1. The diffraction pattern of the CdS thin film corresponds to the hexagonal structure with a preferential orientation of (002) planes. Position of the (002) peak extracted from the patterns is listed in table 1for different Co concentration.

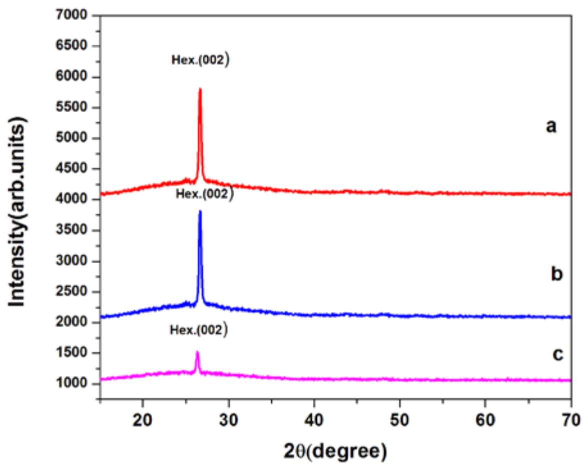

Fig.1: XRD patterns of $Cd_{1-x}Co_xS$ thin films with cobalt concentrations of a) x= 0, b) x= 0.025,and c) x= 0.05.

The (002) peak position is shifted a little towards higher angles with increase of the Co content. This could be due to the CdS lattice modification by the Co doping because of difference in radii of Cd (0.98 Å) and Co (0.74 Å). No diffraction peaks corresponding to Co metal or other impurity phases were observed in diffraction patterns. This may confirms formation of the $Cd_{1-x}Co_xS$ alloys.

Table 1: Position of (002) preferred peak for different cobalt concentration.

Location of (002) peak	Cobalt concentration(x)
$2\theta° = 26.65305$	0
$2\theta° = 26.65308$	0.025
$2\theta° = 26.65341$	0.05

Fig. 2 shows variation of the films lattice parameters as a function of Co concentration. Both lattice parameters, a and c decrease with increase of Co concentration which is evidence of substitution of smaller ion Co^{+2} instead of Cd^{+2}. The calculated lattice parameters, unit cell volume and the average crystalline size extracted from Scherer's equation of the samples are shown in Table 2. The average crystalline size is about 300nm.

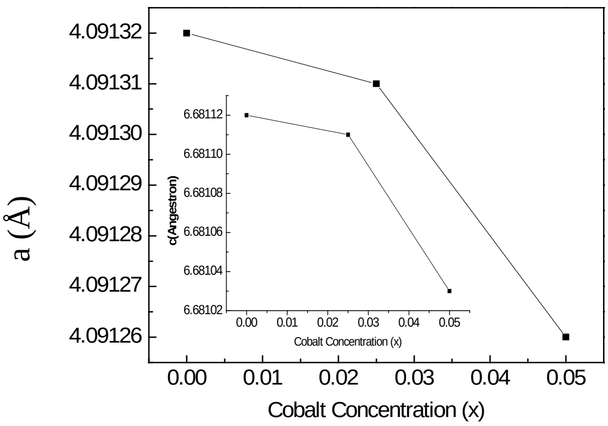

Fig.2: Variation of lattice parameters with cobalt concentration.

The surface morphology of the films was investigated by FESEM and the images are displayed in figure 3. As the figures (a-c) demonstrate, the films surfaces are nearly smooth but the grain size of the CdS film is bigger and the grain sizes reduce with increase of Co concentration [10].

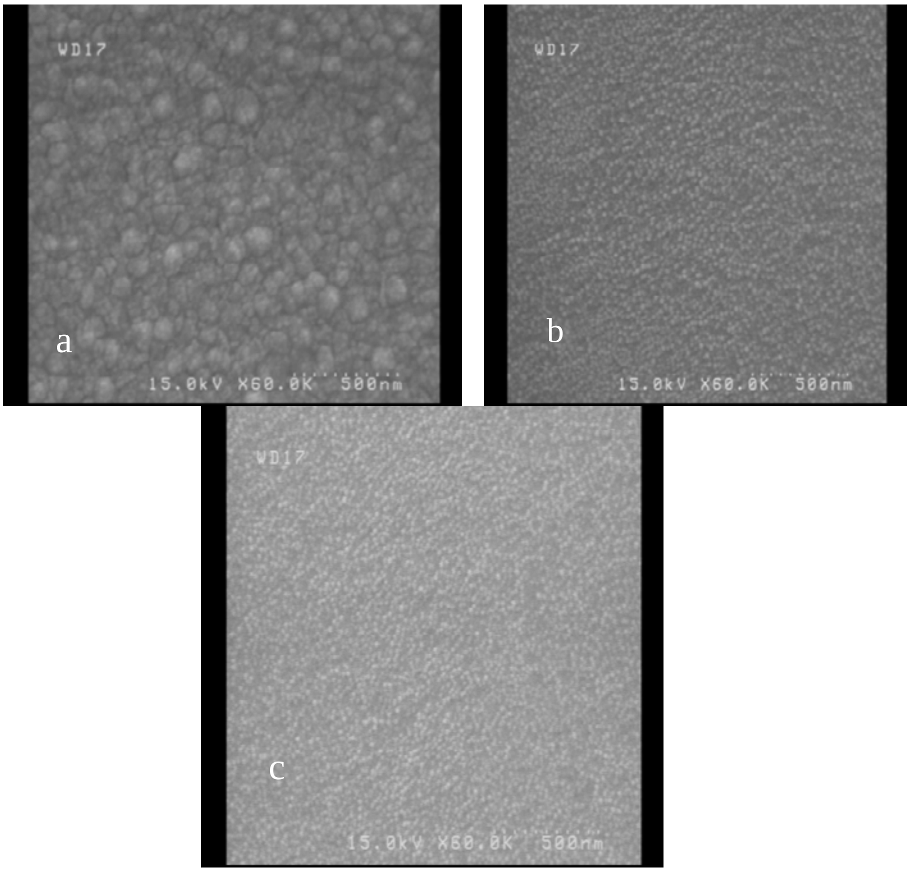

Fig.3: FESEM images of $Cd_{1-x}Co_xS$ thin films with cobalt concentration of a) x= 0 , b) x= 0.025 , c) x= 0.05.

Table 2: Lattice parameters, unit cell volume and the average crystalline size of the $Cd_{1-x}Co_xS$ thin films with cobalt concentration of a) x= 0, b) x= 0.025, c) x= 0.05.

Co concentration (x)	a (˚A)	C (˚A)	Unit cell volume ($˚A^3$)	crystalline size (˚A)
0	4.09132	6.68112	96.852	313.17
0.025	4.09131	6.68111	96.851	309.6
0.05	4.09126	6.68103	96.848	299.78

3-2 Optical properties

Fig. 4 and Fig. 5 show the transmittance and absorbance spectra of the films in the wavelength range 250-1100 nm. The CdS film has higher transmittance compared to the Co doped films. Also decrease in transmittance is observed by increasing Cobalt concentration. The same behavior was observed for $Cd_{1-x}Co_xS$ thin films (x= 0, 0.025, 0.05, 0.075) prepared by spray method [7]. The Co doped films show increase in transmittance in the wavelength higher than 800 nm but the opposite occurs for un-doped CdS film.

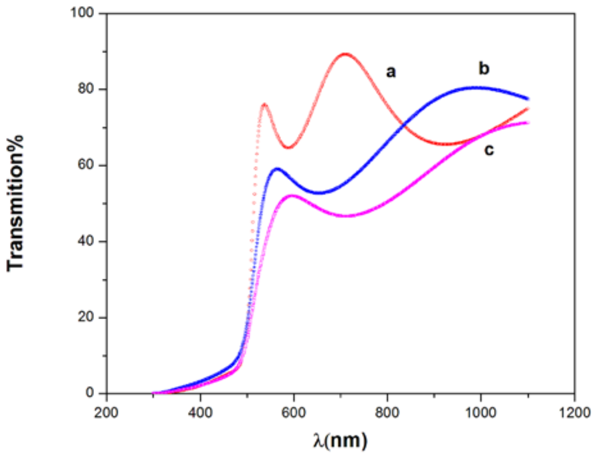

Fig.4. Transmittance spectrum of the $Cd_{1-x}Co_xS$ thin films with Co concentration of a) x= 0 , b) x= 0.025 , c) x= 0.05.

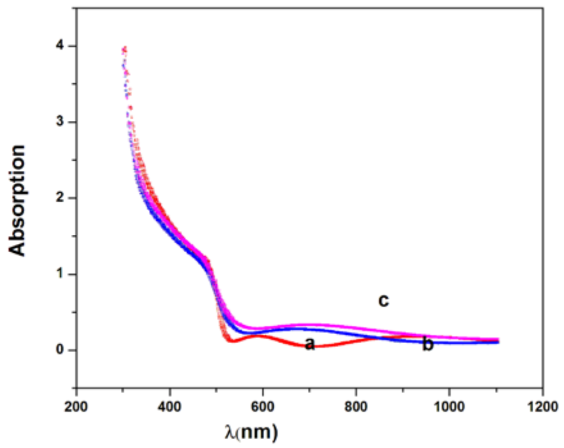

Fig.5: Absorbance spectra of the $Cd_{1-x}Co_xS$ thin films with Co concentration of a) x= 0 , b) x= 0.025 , c) x= 0.05.

From the measured absorbance data, the absorption coefficient α was calculated using Lambert Law [13]:

$$Ln(I_0/I)=2.303A=\alpha d \tag{1}$$

Where I_0 and I are the incident and transmitted light intensity respectively, A is the optical absorbance and d is the film thickness. The band gap energy, E_g, was found using the following relation [14]:

$$\alpha \approx [(h\nu-E_g)^{1/2}]/h\nu \tag{2}$$

Figure 6 shows the plots of $(\alpha h\nu)^2$ versus hν for the films. Extrapolating the linear portion of the curves to the x-axis (α=0) gives the band gaps of the films.

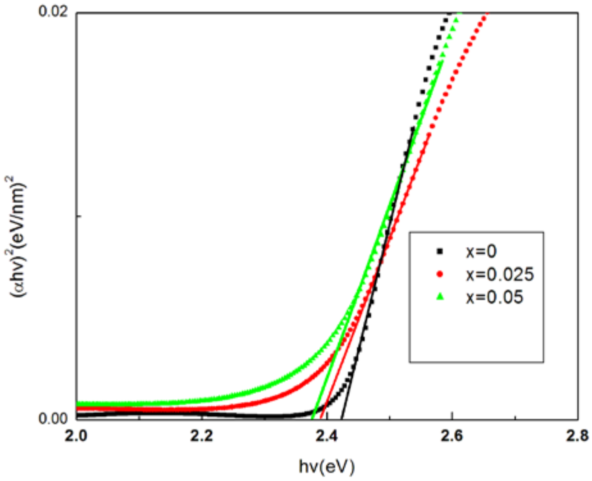

Fig.6: Plot of $(\alpha h\nu)^2$ versus hv for $Cd_{1-x}Co_xS$ thin films with Co concentration of a) x= 0, b) x= 0.025, c) x= 0.05.

Figure 6 shows that the E_g values of the $Cd_{1-x}Co_xS$ thin films decrease with increase in Co concentration, although this reduction is small around 5 meV. This reduction of the band gap is mainly explained by sp–d exchange interactions between the host material s-p band electrons and the localized d electrons of the Co ions [7, 9, and 15].

The refractive indexes of the films were calculated by using PUMA software and they are shown as a function of wavelength in figure 7. As can be seen, the refractive indexes of the films behave similar but increase with Co concentration away from the absorption edge. The refractive index curves of the films were fitted with the following Cauchy equation [16]:

$$n=a+b/\lambda^2 \tag{3}$$

And the extracted Cauchy constants (a and b) form the fitting are tabulated in table 3.

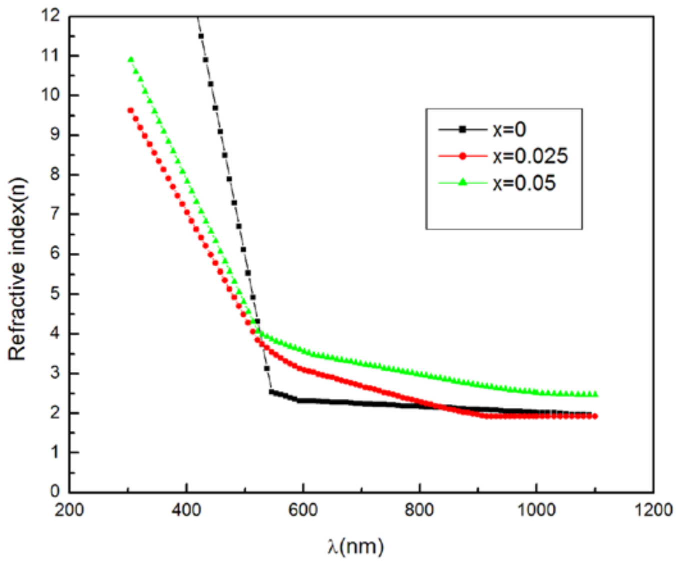

Fig.7: Refractive index versus wavelength for $Cd_{1-x}Co_xS$ thin films with a) x= 0, b) x= 0.025, c) x= 0.05.

Table 3: Cauchy constants of $Cd_{1-x}Co_xS$ thin films with a) x= 0, b) x= 0.025, c) x= 0.05.

X	a	b
0	5.001	1.54×10^4
0.025	3.564	1.94×10^4
0.05	4.186	2.08×10^4

4. Conclusions

Cobalt doped cadmium sulfide thin films were prepared by thermal evaporation method on glass substrate with a thickness of about 50 nm at a pressure of 6×10^{-6} mbar and ambient temperature. X-ray diffraction patterns showed all films have hexagonal structure with (002) preferred orientation. A small shift was observed in (002) peak position by Co doping in CdS which is due to the difference on ionic radii of Cd and Co. The FESEM images of the film surfaces indicated reduction of the grain size by Co doping. Optical studies revealed that the optical band gap of films decreases with increase in Co concentration.

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