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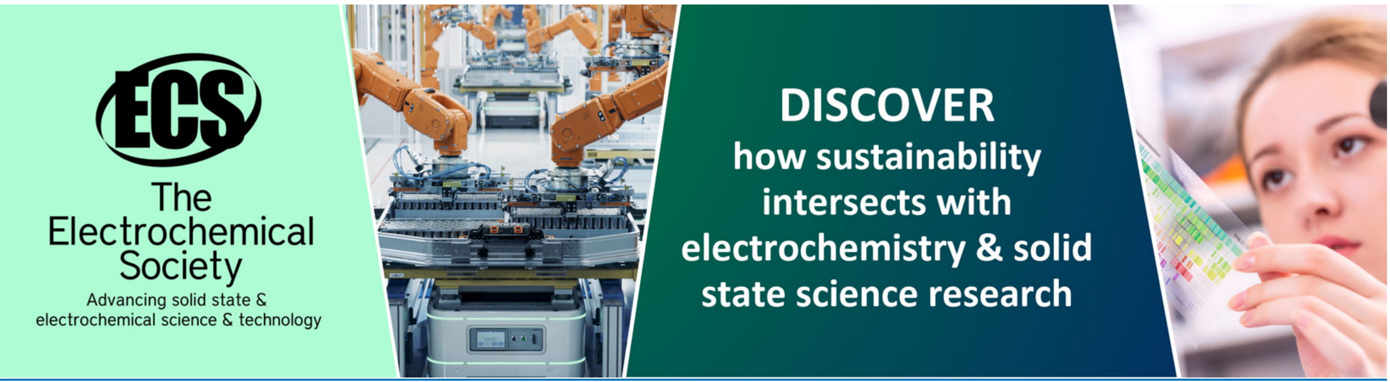

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Exploration of optical behavior of $Cd_{1-x}Ni_xTe$ thin films by spectroscopic ellipsometry

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Abstract

We report on the tunability over the optical behavior of e-beam evaporated nanocrystalline thin films of $Cd_{1-x}Ni_xTe$ ($0 \leqslant x \leqslant 0.15$). X-ray diffraction analysis reveals the polycrystalline nature of the film having zinc blend structure with a preferred growth direction along (111) plane parallel to the substrate. X-ray diffraction results also indicate that the grain size of the films decreases from 27.13 nm to 16.23 nm with an increase in Ni concentration from 0 to 15 at%. The compositional analysis of the film was carried out by energy dispersive x-ray analysis (EDX) which confirms the successful inclusion of Ni in CdTe matrix. Spectroscopic ellipsometery (SE) results demonstrate that the band gap of the grown films increases from 1.48 eV to 1.86 eV while refractive index (n) and extinction coefficient (k) decrease with the increasing Ni concentration. The increase in band gap energy of $Cd_{1-x}Ni_xTe$ films as a function of Ni concentration was confirmed by spectrophotometric analysis.

Keywords: e-beam evaporation, $Cd_{1-x}Ni_xTe$ nanocrystalline films, ellipsometry, band gap energy

Introduction

Among various chalcogenides, cadmium telluride (CdTe), is recognized as an extremely versatile material having narrow band gap ($E_g = 1.5$ eV) with a very high absorption coefficient ($\alpha > 104\,\mathrm{cm}^{-1}$) [1]. It is the only binary II–VI compound which shows both n-type and p-type behavior and hence can be exploited for various technological applications such as solar cells, infrared detectors, field effect transistor, gamma ray detectors and photoconductors [2–9].

Recent studies have shown that the dopant elements could significantly change the mechanical, electrical as well as optical properties of CdTe [10–13]. Generally, lithium, phosphorous and arsenic are reported to achieve the hole concentration around $10^{17}\,cm^{-3}$, whereas aluminum, iodine and indium are reported as donor elements for CdTe to achieve electron concentration as high as $10^{18}\,cm^{-3}$ [14–16].

Introducing transition metals such as Zn, Cr, Co, Ti or Ni in CdTe, still maintains the zinc blend structure while having slight structural distortions along with readjustment of electronic configurations [17–21]. Such changes in structure as well as electronic configuration result in some unusual changes in magnetic, optical and electrical properties which may be exploited for novel device applications. During the last two decades, extensive research has been carried out on transition metal doped CdTe, however, only structural, electrical and magnetic properties remained under consideration while optical behavior of transition metal doped CdTe still demands detailed investigation [22].

Here, we report the study of optical properties $Cd_{1-x}Ni_xTe$ thin films deposited on glass substrate at room temperature via electron beam evaporation technique while varying Ni concentration. The films were characterized by x-ray diffraction (XRD), energy dispersive x-ray spectroscopy (EDX), spectrophotometer and spectroscopic ellipsometer. We have followed the Ni concentration effect on the grain size, band gap, refractive index and extinction coefficient of CdTe thin films.

Experimental procedure

Cadmium telluride (99.99%) and nickel (99.999%) powder were used for the deposition of $Cd_{1-x}Ni_xTe$ thin films with different Ni compositions ranging from $x = 0$ to 15 at.%. Electron beam evaporation technique was used for the deposition of the thin films on soda lime glass substrates. First of all, CdTe and Ni powder were blended mechanically by pestle and mortar for 1.5 h to achieve homogeneously mixed source material for evaporation. A mechanical press was used for the fabrication of pellets while using a dye having 10 mm diameter and load of 7 tons for pressing.

Glass substrates were cleaned ultrasonically in acetone bath for 25 min and then with iso-propanol for 15 min, the substrates were then dried by using a hot air gun. The vacuum of the evaporation chamber was 10^{-6} mbar for the deposition of the thin films. All $Cd_{1-x}Ni_xTe$ thin films were prepared under the same growth parameters.

An x-ray diffractometer (Bruker D-8) having Cu-k_α source ($\lambda = 1.54186$ Å) was used for structural analysis of the prepared thin films. Ni filter was used to suppress K_β radiations. Operating voltage and current of x-ray source were kept at 40 kV and 40 mA, respectively. The XRD scans were performed at $\theta/2\theta$ geometry in angular range of 10 to 90° at a scan rate of $2°\,min^{-1}$ and step size of 0.025°.

A spectroscopic ellipsometer (J. A. Woollam Co.) with double grating monochromator and a lamp of wavelength ranging from 370 to 1670 nm was used to determine the band gap, optical constants and film thickness. The experimental data was fitted by using WASE software. Angle of incident arm with the horizontal was kept at 70° for each sample. Dual source spectrophotometer (Hitachi U- 4001) was utilized in the wavelength region of 300 to 2500 nm to obtain the transmission spectra of the deposited films.

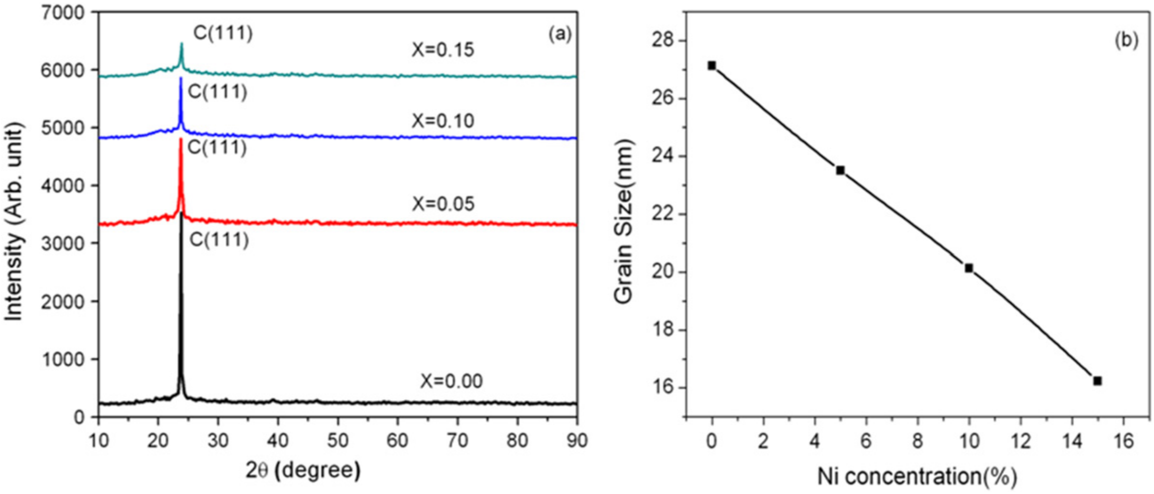

Figure 1. (a) XRD spectra of $Cd_{1-x}Ni_xTe$ at various Ni compositions (b) grain size variation as a function Ni composition.

Results and discussion

XRD analysis of $Cd_{1-x}Ni_xTe$ with varying Ni concentration ranging from $x = 0$ to 15 at.% is shown in figure 1(a). The presence of sharp and well defined peaks confirmed the zinc blend structure with polycrystalline nature and the preferred growth orientation along (111) plane of the films. No evidence of Ni precipitates and other secondary phases was found in the XRD spectra which verified that CdTe maintains its zinc blend structure with the addition of Ni up to 15 at.%.

The grain size was calculated by using Scherrer formula.

$$D = \frac{0.9\lambda}{\beta^{*}\cos\theta} \tag{1}$$

where λ is equal to 1.5405 Å (Cu-K_α) and θ is Bragg's angle. It was found that the grain size decreases from 27.13 nm to 16.23 nm with increasing Ni content, as shown in figure 1(b).

Figure 2 shows EDX spectra of the deposited films and the results of EDX analysis are summarized in table 1. The results confirmed that the composition of the films almost follows the composition of the source material. Moreover, from EDX results it was observed that Ni content increased at the expense of cadmium suggesting the possible substitutional replacement of Cd with Ni.

Optical constants and film thickness were determined by using spectroscopic ellipsometer. The ellipsometric parameters such as psi (ψ) and delta (Δ) were measured (figure 3) as a function of wavelength ranging from 370 to 1670 nm at an incident angle of 70° which are assigned as experimental data. The effective medium approximation (EMA) model was used for curve fitting to determine the optical constants and film thickness. The thicknesses obtained from the best fitted data are summarized in table 2, whereas the composition of Ni in the prepared samples obtained from ellipsometric analysis is shown in table 1.

The refractive index and extinction coefficient of the films as a function of wavelength are illustrated in figures 4(a) and (b). It was observed that the refractive index (n) and extinction coefficient (k) decrease with increasing Ni concentration in $Cd_{1-x}Ni_xTe$ thin films as shown in

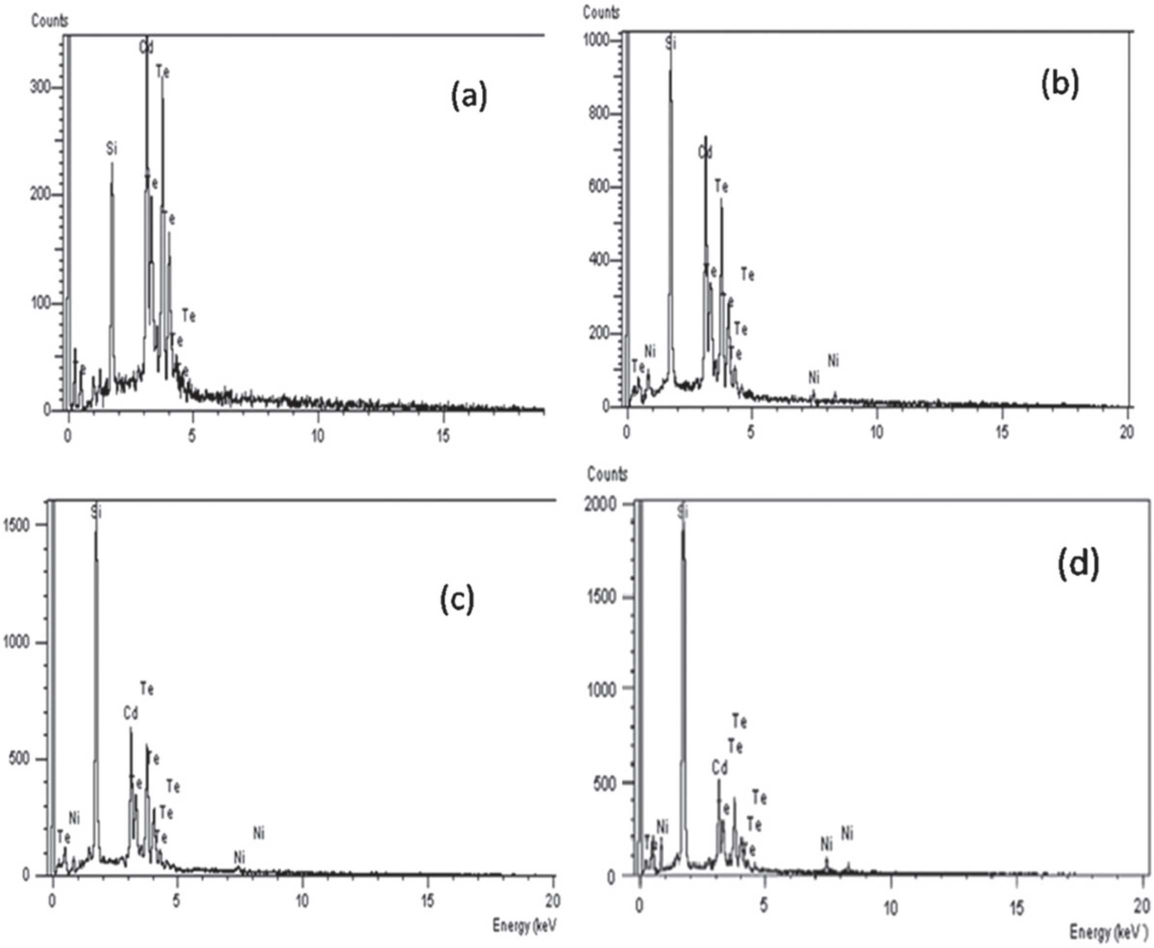

Figure 2. EDX spectra of $Cd_{1-x}Ni_xTe$ thin films with (a) $x = 0\%$, (b) $x = 5\%$, (c) $x = 10\%$ and (d) $x = 15\%$.

Table 1. Detail of compositional results.

Alloy	Precursor composition (%)		EDAX composition (%)		Ellipsometric composition (%)	
$Cd_{1-x}Ni_xTe$	CdTe	Ni	Cd	Te	Ni	Ni
$x = 0.00$	100	0	48.11	51.89	0.00	0
$x = 0.05$	95	5	45.21	50.27	4.83	5.2
$x = 0.10$	90	10	40.81	50.76	9.06	9.5
$x = 0.15$	85	15	35.19	51.30	12.97	13

figures 5(a) and (b). The decreasing trend of n and k with increasing Ni concentration may be attributed to decrease in grain size. The absorption coefficient was calculated by using equation (2).

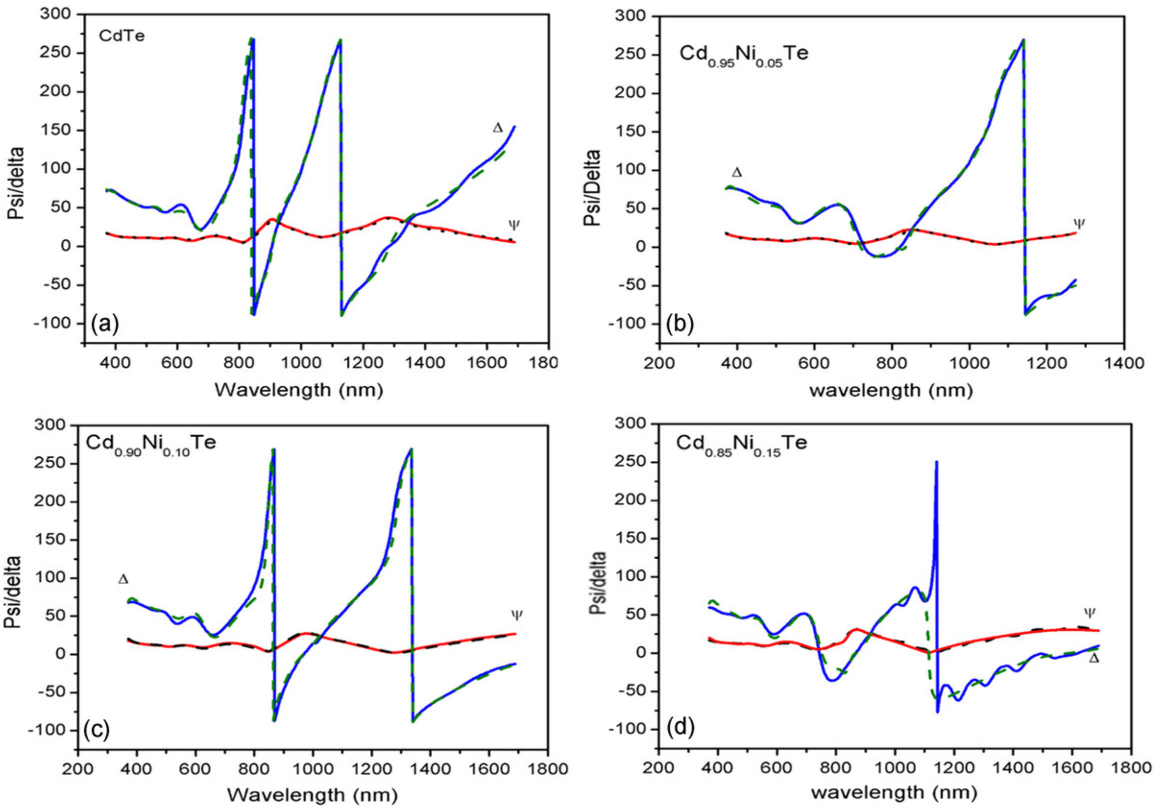

Figure 3. psi (ψ) and delta (Δ) as a function of wavelength.

Table 2. Thickness of the films.

Sr. No.	$Cd_{1-x}Ni_xTe$	Film Thickness (nm)
1	CdTe	492
2	$Cd_{0.95}Ni_{0.05}Te$	392
3	$Cd_{0.90}Ni_{0.1}Te$	362
4	$Cd_{0.85}Ni_{0.15}Te$	316

$$\alpha = \frac{4\pi k}{\lambda}, \tag{2}$$

where k is the extinction coefficient calculated from ellipsometry data. Tauc relation for direct band gap materials was used to estimate the band gap of the deposited films. It was observed (figure 6(b)) that the band gap of the nanocrystalline thin films blue shifted from 1.48 to 1.86 eV as the Ni concentration varied from 0 to 15%.

In order to confirm the ellipsometry results, band gap was also calculated from the optical transmission spectra (shown in figure 7) of nanocrystalline $Cd_{1-x}Ni_xTe$ thin films in the spectral region 300–2500 nm obtained by suing a UV–vis–NIR spectrophotometer.

The relation given below was used to calculate the absorption coefficient of the deposited films.

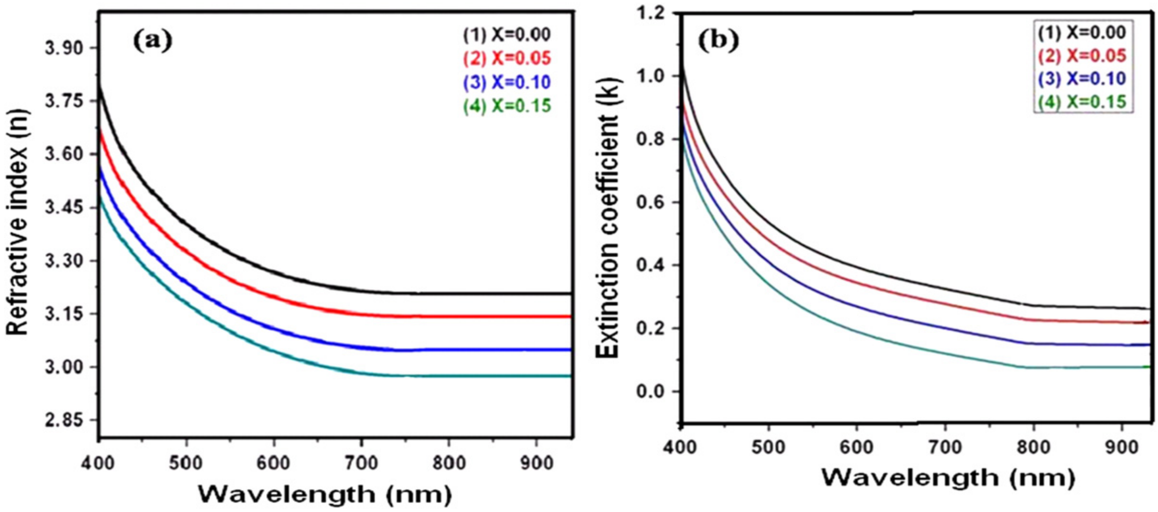

Figure 4. (a) and (b) shows the deviation of the (n, k) values as a function of wavelength. Respectively.

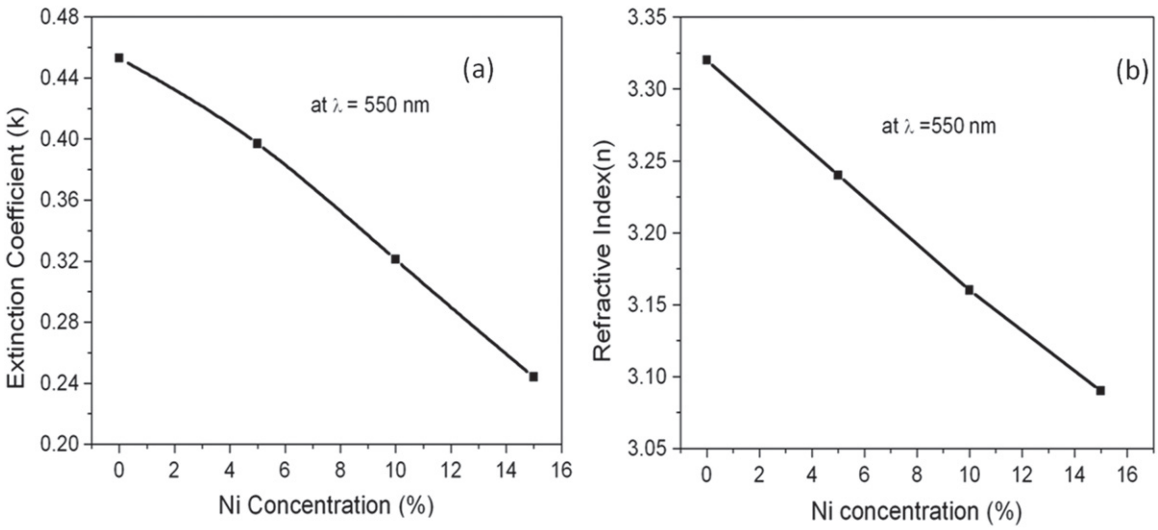

Figure 5. (a) and (b) shows the change in n and k values as a function of Ni concentration, respectively.

$$\alpha = \frac{-\ln T}{t}\, nm^{-1}. \tag{3}$$

Where T is the normalized transmittance value at a particular wavelength and t is the thickness of the film. Then $(\alpha h\nu)^2$ was plotted against $h\nu$ for each composition and the linear portion of the curves was extrapolated up to $(\alpha h\nu)^2 = 0$ axis which gives the value of band gap energy. The variation of band gap with composition was again found to be linear varying 1.52 to 1.84 eV as the Ni content increases from 0 to 15 at.% as shown in figures 8(a) and (b), which almost agrees with the results obtained from ellipsometry data.

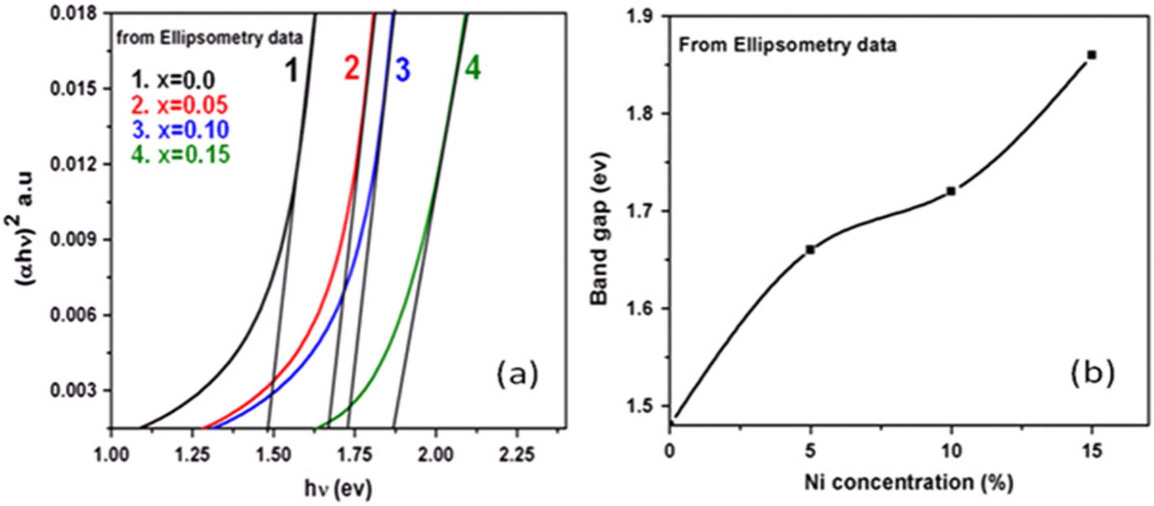

Figure 6. (a) Band gap (E_g) as a function of photon energy (b) E_g variation with Ni concentration.

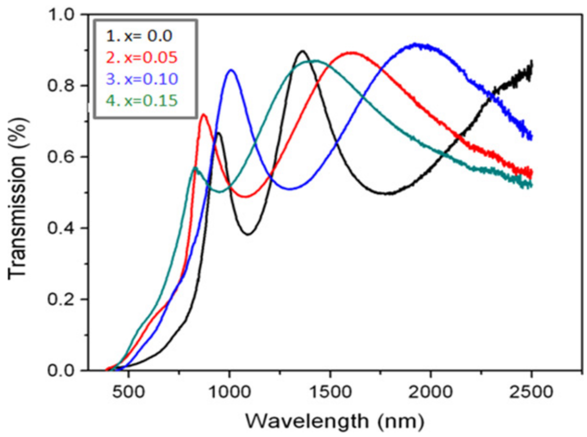

Figure 7. Transmission spectra of $Cd_{1-x}Ni_xTe$ thin films.

Conclusion

In summary, the electron beam evaporated $Cd_{1-x}Ni_xTe$ nanocrystalline thin films were deposited on glass substrate at room temperature. XRD study revealed the zinc blend structure and polycrystalline nature of the films, whereas the grain size decreased from 27.13 nm to 16.23 nm as the Ni concentration increased from 0 to 15 at.%. EDX results confirmed the presence Ni at the expense of Cd in CdTe. It was observed that the optical constants (n, k) decrease with the increasing Ni concentration while the band gap of the deposited films increases with Ni content.

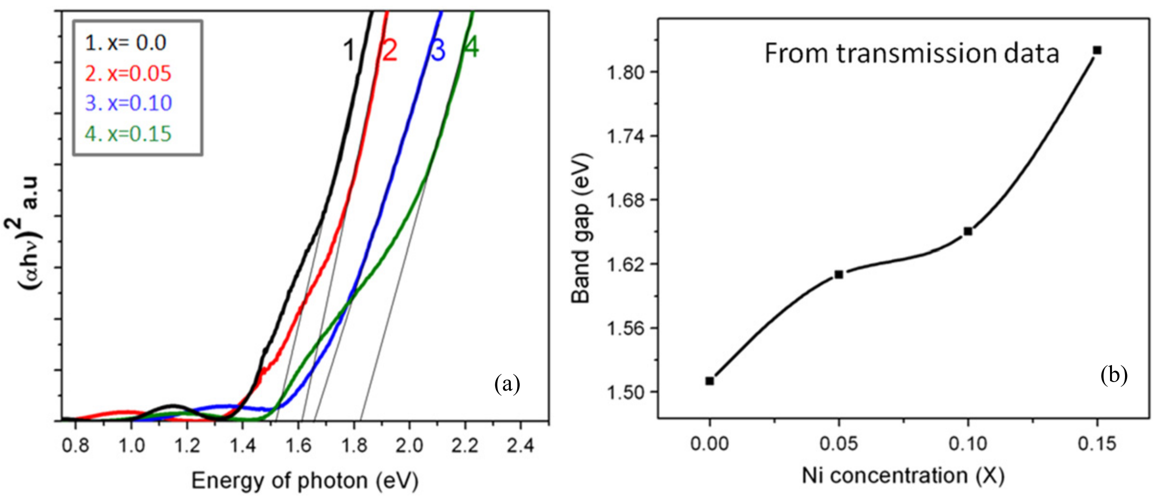

Figure 8. (a) Band gap calculation from transmission data. (b) Variation of E_g with Ni concentration.

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