Spectroscopic Study of Vacuum Evaporated Crystalline Cadmium Zinc Sulphide thin films.

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Abstract: Vacuum evaporated crystalline thin films of $Cd_xZn_{1-x}S$ (X = 0.2 & 0.4) have been prepared in the entire composition range from pure CdS & ZnS evaporated on highly clean glass substrate. Their optical properties, (energy band gap, refractive index & extinction coefficient) have been studied. The energy band gap (E_g) of the films has been calculated from absorption spectra by using Tauc relation. The transmission spectra in the spectral range 300-850 nm has been used to calculate the refractive index (n), extinction coefficient (k) and wavelength (λ) dependence of n and k of the films have been studied. Optical spectroscopies of the films have been done with the help of the Hitachi Spectrophotometer Model U- 3400.

Keywords: Cadmium Sulphide, Zinc Sulphide, Energy band gap, refractive index, and Vacuum evaporated thin film.

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Introduction

The II-VI group compound semiconductors, Cadmium-Zinc Sulphide ($Cd_xZn_{1-x}S$) having a wide band gap is a promising material for use in photovoltaic devices, blue light emitting diodes and laser diodes . [1-4].$Cd_xZn_{1-x}S$ films are of considerable interest for heterojunction solar cells because their use permits a greater open circuit voltage. The properties of polycrystalline $Cd_xZn_{1-x}S$ films produced by various method like vacuum evaporation [5-14] spray pyrolysis [15-17] reactive sputtering [18-19]. chemical bath deposition technique [20-21] and chemical vapour deposition [22] for the purpose of reducing the production cost of heterojunction solar cells have been reported. However the technique of vacuum evaporation, which is reported to be the cheapest and most efficient way to produce CdS-CdZnS heterojunction solar cells [23] has not so for been used for the preparation of $Cd_xZn_{1-x}S$ films. In the present paper we have studied and reported results of optical properties obtained with $Cd_xZn_{1-x}S$ films prepared by vacuum evaporated technique in the entire composition range $0.2 < X < 0.4$.

Experimental Details

Cadmium-Zinc Sulphide powder (99.99% pure) was evaporated at about 650^0C from a narrow mouthed molybdenum boat $Cd_xZn_{1-x}S$ (X = 0.2 & 0.4) films have been prepared by the vacuum evaporated technique. The various compositions of $Cd_xZn_{1-x}S$ were prepared by the ampule sealing method. For this purpose pure cadmium and Zinc were taken in a quartz ampule according to the $Cd_xZn_{1-x}S$ (X = 0.2 & 0.4). The quartz ampules were sealed in the vacuum of the order of 10^{-5} toor and then heated at 750^0C for the period of roughly 12h in a rotating furnace. Quartz ampule was then dropped in ice-cold water and we get the compositions of CdZnS.

For sample preparation of $CdxZn_{1-x}S$ were evaporated at about 650^0C from a deep narrow mouthed molybdenum boat. The evaporated materials were deposited on to highly cleaned glass substrates held at 200^0C in a vacuum of 10^{-5} toor. The substrates were cleaned in aquaregia, washed in distilled water and isopropyl alcohol (IPA). It was separated from CdZnS molybdenum boat by a stainless steel heat shield keeping the substrate at an elevated temperature of about 250^0C helps to eject any sulphur atoms deposited due to thermal decomposition of CdZnS. absorption and transmission spectra of vacuum evaporated CdZnS films were taken at room temperature with the help of Hitachi Spectrophotometer Model U- 3400.In this model all the lenses have been replaced with mirrors. So the image deviation due to chromatic aberration is eliminated in the wavelength range 187-2600nm.The PbS detector is used for the detection of infrared rays. The visible wavelength light source was a long life WL lamp.

The X- ray diffraction pattern of $Cd_xZn_{1-x}S$ films is also reported in the present work by using CuKα radiation with the help of a Philip X- ray diffractometer. The d values are calculated by measuring θ values from the X- ray peaks by using the relationship $2dSin\theta = n\lambda$ (n = 1 in the present study), where the value of λ is 1.54045 for

CuKα. The d values are compared with the standard ASTM data to confirm the structure of $Cd_xZn_{1-x}S$ films.

Results and Discussion

The absorption spectra of $Cd_xZn_{1-x}S$ (X = 0.2 & 0.4) films in the wavelength range 400-650 nm is used to determine the optical band gap (E_g) as shown in fig 1(a). & 1(b). The transmission spectra of the $Cd_xZn_{1-x}S$ thin films in the wavelength range 300-850 nm. Shown in Fig. 2(a) & 2(b) was used to determine the optical constants (refractive index and extinction coefficient).

To measure the energy band gap from absorption spectra the Tauc relation [24] is used.

$$\alpha h\nu = A (h\nu - E_g)^n$$

Where the symbols have their usual meanings.

To measure the energy band gap from absorption spectra a graph of $(\alpha h\nu)^2$ Vs $h\nu$ is plotted. The extra polation of the straight line to $(\alpha h\nu)^2 = 0$ axis gives the value of the energy band gap Fig. 1 (b). From this graph, the value of energy band gap of $Cd_xZn_{1-x}S$ comes out to be 3.25eV & 3.01eV.

The optical constants (refractive index and extinction coefficient) of these films have been determined from transmission spectra by using Manifcier's envelope method. These films showed, in general good transparency (T >75%), exhibiting interference patterns.

The refractive index (n) of the films deposited is given by.

$$n = [N + (N^2 + n_0^2 n_1^2)^{1/2}]^{1/2}$$

n_0 and n_1 are the refractive index of air and substrate(glass) respectively. The number N is given by

$$N = [(n_0^2 + n_1^2)/ 2] + 2\, n_0 n_1 [(T_{max} - T_{min}) / (T_{max} . T_{min})]$$

The calculated values of n & k for $Cd_{0.2}Zn_{0.8}S$ & $Cd_{0.4}Zn_{0.6}S$ films are given in Table Show 1-2.Where T_{max} and T_{min} the upper extreme point and lower extreme point of the envelope at a particular wavelength.

The extinction coefficient k is given by

$$k = (-\lambda/4\pi t) \ln(P)$$

Where t is the thickness of the films deposited

$$P = C_1/ C_2 [1- T_{max/} \; T_{min}] / [1+ T_{max\,/} T_{min}]$$

Where $C_{1} = (n + n_0) (n + n_1)$

and $C_2 = (n - n_0)(n_1 - n)$

Where n is the refractive index of the films at particular wavelength, n_1 is the refractive index of the substrates (glass) and n_0 is the refractive index of the air. It is observed that the refractive index decreases, as the wavelength is increased. However, the extinction coefficient increased with the increased in the wavelength.

The thickness of the film has been measured and it comes out to be 0.175 & 0.78 micron. The plots of n(λ) and k(λ) for the films are shown in Fig (3a) & (3b) respectively and it has been observed that the refractive index (n) decreases, while the extinction coefficient (k) increase with increase in wavelength (λ).

The Structure of CdZnS films is confirmed by X- ray analysis. The X- ray of vacuum $Cd_xZn_{1-x}S$ (X= 0.2, 0.4) films is shown in fig- (4a) all the peaks are Identified except two peaks at 28.1^0 & 46.7^0 which may be in vacuum film. In fig.-(4b) all the peaks are identified except three peaks at $26^{0,}$ 27^0 and 46^0 which may be in $Cd_{0.4}Zn_{0.6}S$ vacuum films.

Conclusion

By this study we conclude that the absorption and transmission spectroscopic techniques are important techniques for measuring the energy band gap (Eg) and optical constants (n,k) of semi conducting thin films. Spectroscopic study of vacuum evaporated crystalline Cadmium Zinc Sulphide thin films. Fig.-(4a) & (4b) is the X- ray diffraction pattern of vacuum $Cd_xZ_{n1-x}S$ films with CuKα radiation. All the peaks are in good agreement with the standard ASTM data for CdZnS film confirms material. The X- ray analysis of CdZnS films confirms the crystalline structure of CdZnS material.These techniques have been verified for various thin films like CdS, ZnS and PbS etc.

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Table.1 Variation of refractive index (n) and extinction (k) for $Cd_{0.2}Zn_{0.8}S$ thin film.

S.no.	λ (nm)	T_{max}(%)	T_{min}(%)	N	n	k
1.	450	68.30	54.00	2.788	2.440	1.198
2.	500	82.50	62.70	2.77	2.435	2.681
3.	550	87.30	65.00	2.770	2.433	3.585
4.	600	89.70	66.70	2.765	2.431	4.032
5.	650	92.10	68.30	2.760	2.429	4.493
6.	700	93.70	70.60	2.672	2.395	4.707
7.	750	96.00	72.20	2.655	2.388	5.238

λ = Wavelength, N = Number, n = refractive index, k = Extinction coefficient

Table.2 Variation of refractive index (n) and extinction (k) for $Cd_{0.4}Zn_{0.6}S$ thin film.

S.no.	λ (nm)	T_{max}(%)	T_{min}(%)	N	n	k
1.	500	70.60	54.80	2.850	2.464	1.289
2.	550	83.30	64.30	2.688	2.398	2.132
3.	600	88.10	67.50	2.664	2.390	2.617
4.	650	90.50	69.00	2.657	2.387	3.015
5.	700	92.90	70.60	2.645	2.383	3.397
6.	750	95.20	72.20	2.629	2.375	3.809
7.	800	97.60	73.80	2.617	2.366	4.224
8.	850	1.000	75.40	2.604	2.317	4.667

λ = Wavelength, N = Number, n = refractive index, k = Extinction coefficient

Figure of Caption

Fig 1(a): Absorption spectra of $Cd_xZn_{1-x}S$ vacuum evaporated thin films.

Fig 1(b): Energy Band gap determination of vacuum evaporated $Cd_{0.2}$ $Zn_{0.8}$ S & $Cd_{0.4}$ $Zn_{0.6}$ S thin films.

Fig 2(a): Transmission spectra of vacuum evaporated $Cd_{0.2}$ $Zn_{0.8}$ S thin film.

Fig 2(b): Transmission spectra of vacuum evaporated $Cd_{0.4}$ $Zn_{0.6}$ S thin film.

Fig 3(a): Variation of refractive index with wavelength of $Cd_{0.2}$ $Zn_{0.8}$ S & $Cd_{0.4}$ $Zn_{0.6}$ S thin films.

Fig 3(b): Variation of extinction coefficient (k) with wavelength (λ) of vacuum evaporated of $Cd_{0.2}$ $Zn_{0.8}$ S & $Cd_{0.4}$ $Zn_{0.6}$ S thin films.

Fig 4 (a): X- Ray diffraction pattern of vacuum evaporated $Cd_{0.2}$ $Zn_{0.8}$ S thin film.

Fig 4 (b): X- Ray diffraction pattern of vacuum evaporated $Cd_{0.4}$ $Zn_{0.6}$S thin film.

Fig 1(a): Absorption spectra of $Cd_xZn_{1-x}S$ vacuum evaporated thin films.

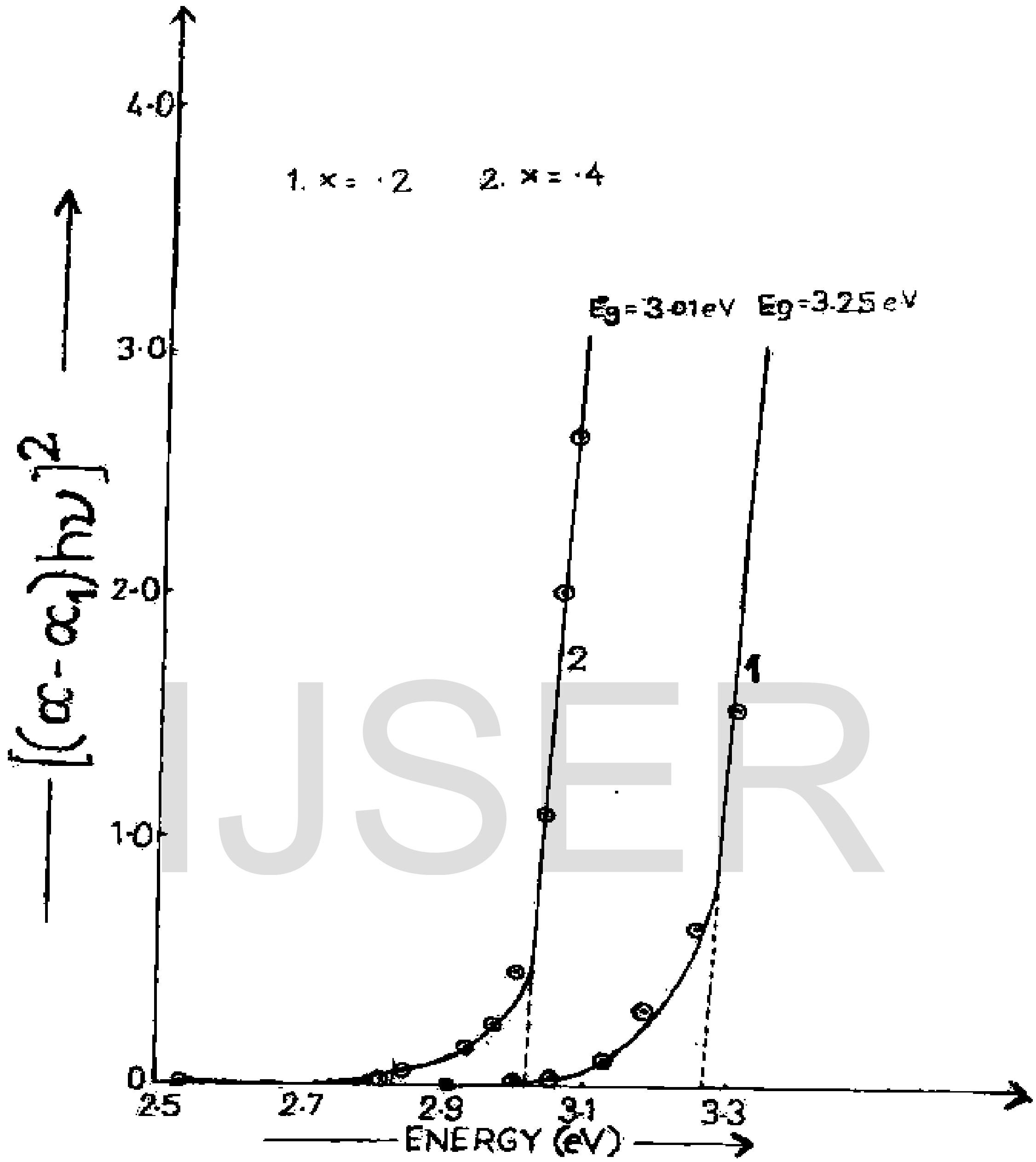

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Fig 1(b): Energy Band gap determination of vacuum evaporated $Cd_{0.2}$ $Zn_{0.8}$ S & $Cd_{0.4}Zn_{0.6}S$ thin films.

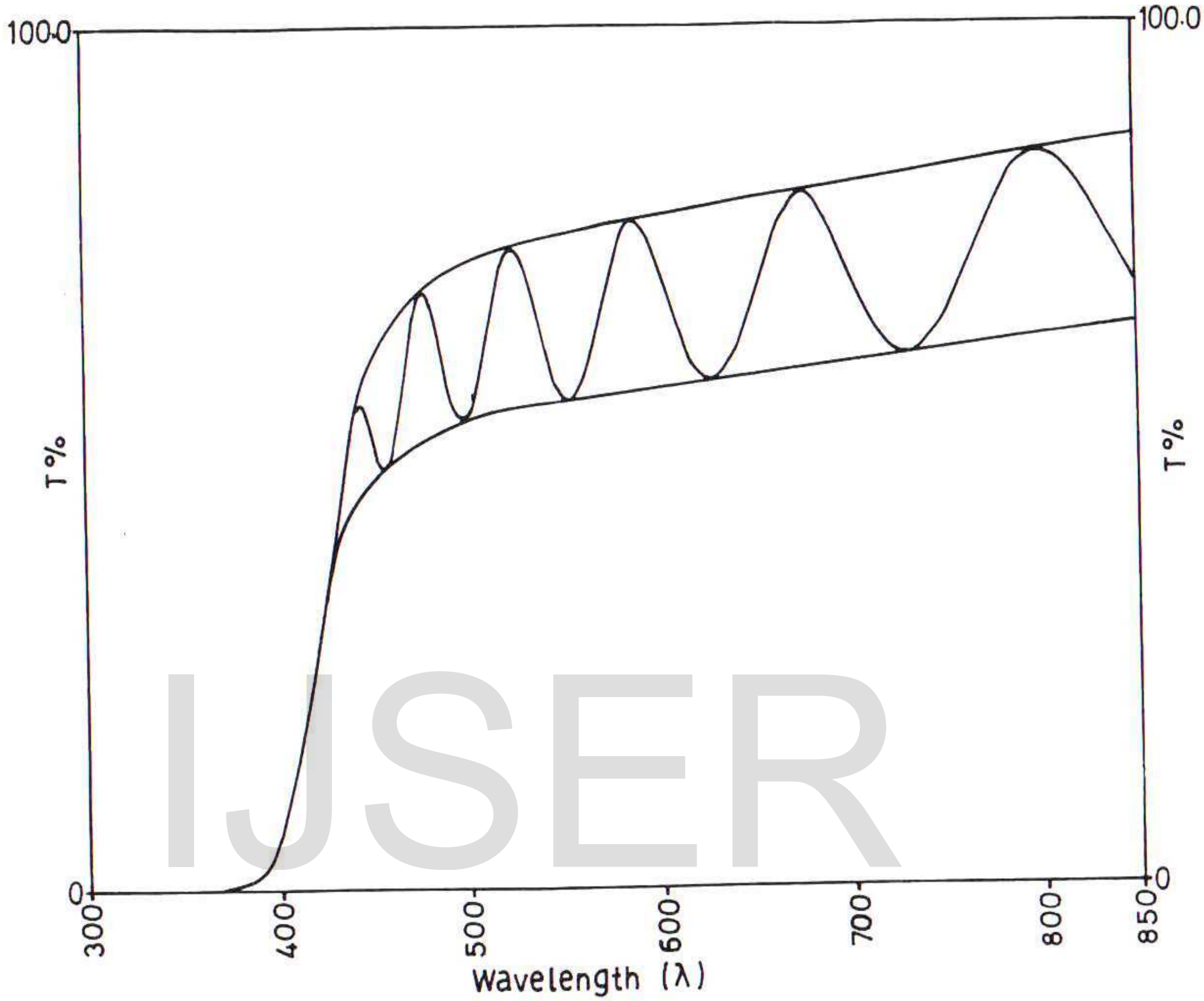

Fig 2(a): Transmission spectra of vacuum evaporated $Cd_{0.2}\,Zn_{0.8}\,S$ thin film.

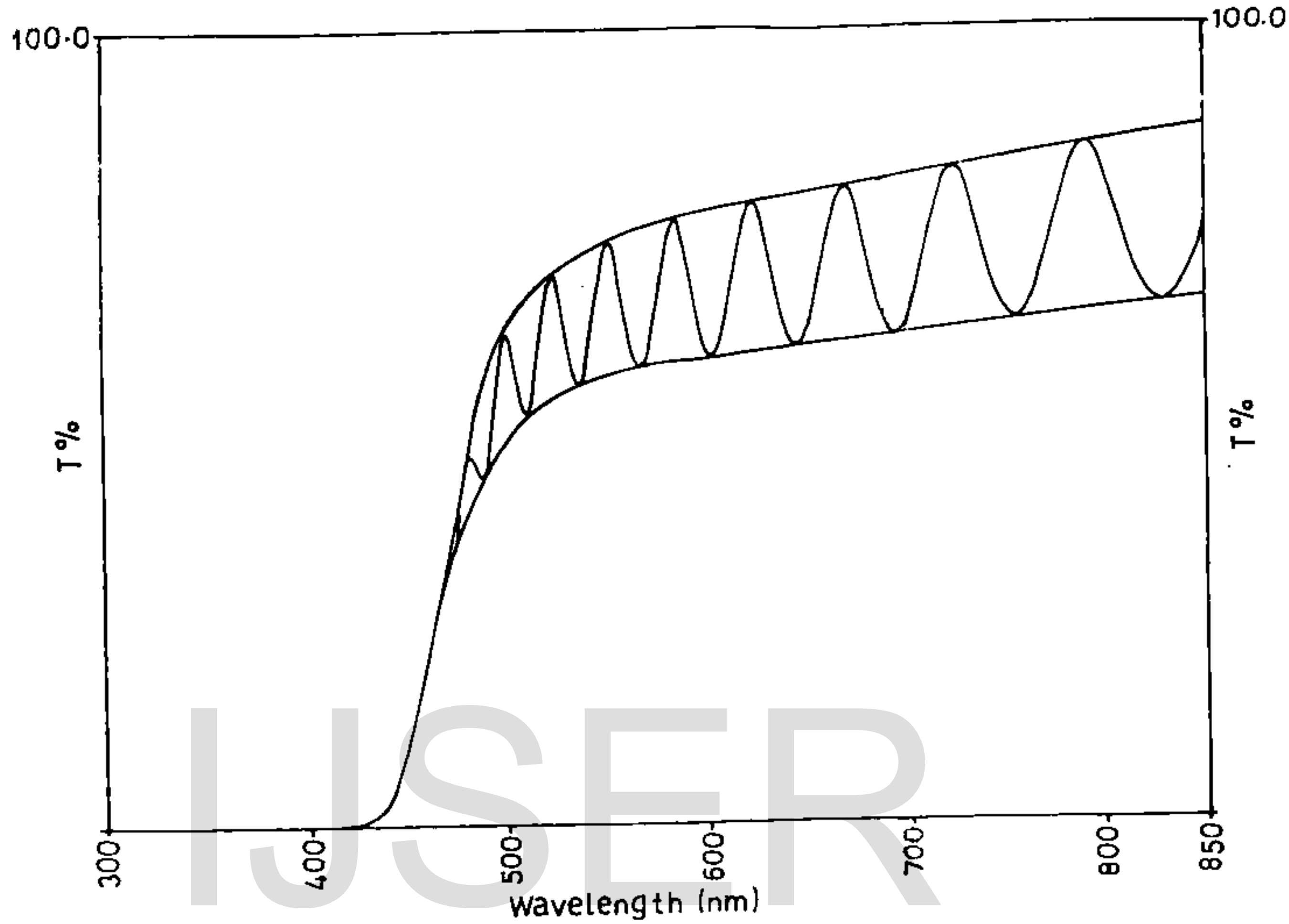

Fig 2(b): Transmission spectra of vacuum evaporated $Cd_{0.4}\,Zn_{0.6}\,S$ thin film.

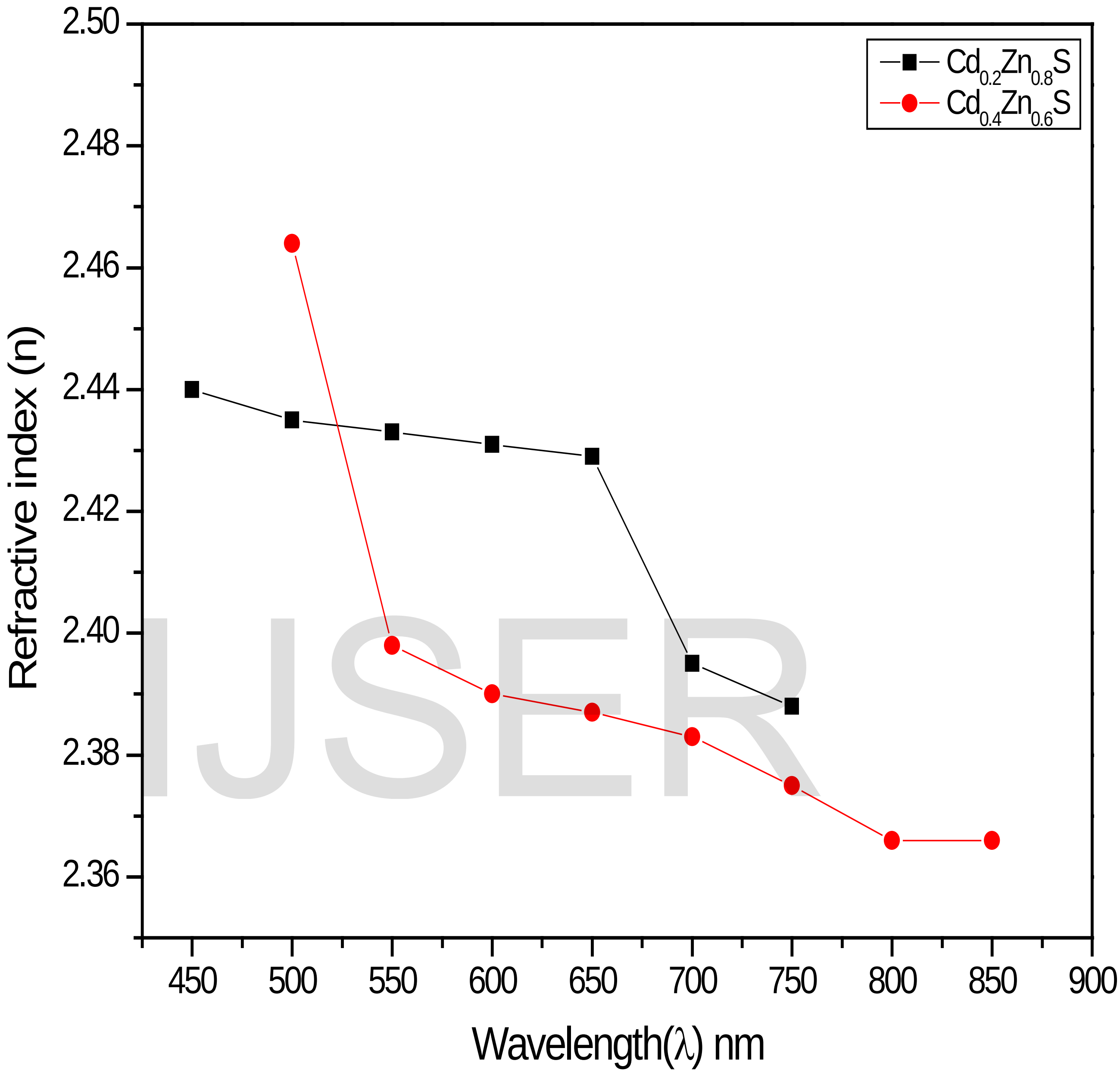

Fig 3(a): Variation of refractive index with wavelength of $Cd_{0.2}$ $Zn_{0.8}$ S & $Cd_{0.4}$ $Zn_{0.6}$ S thin films.

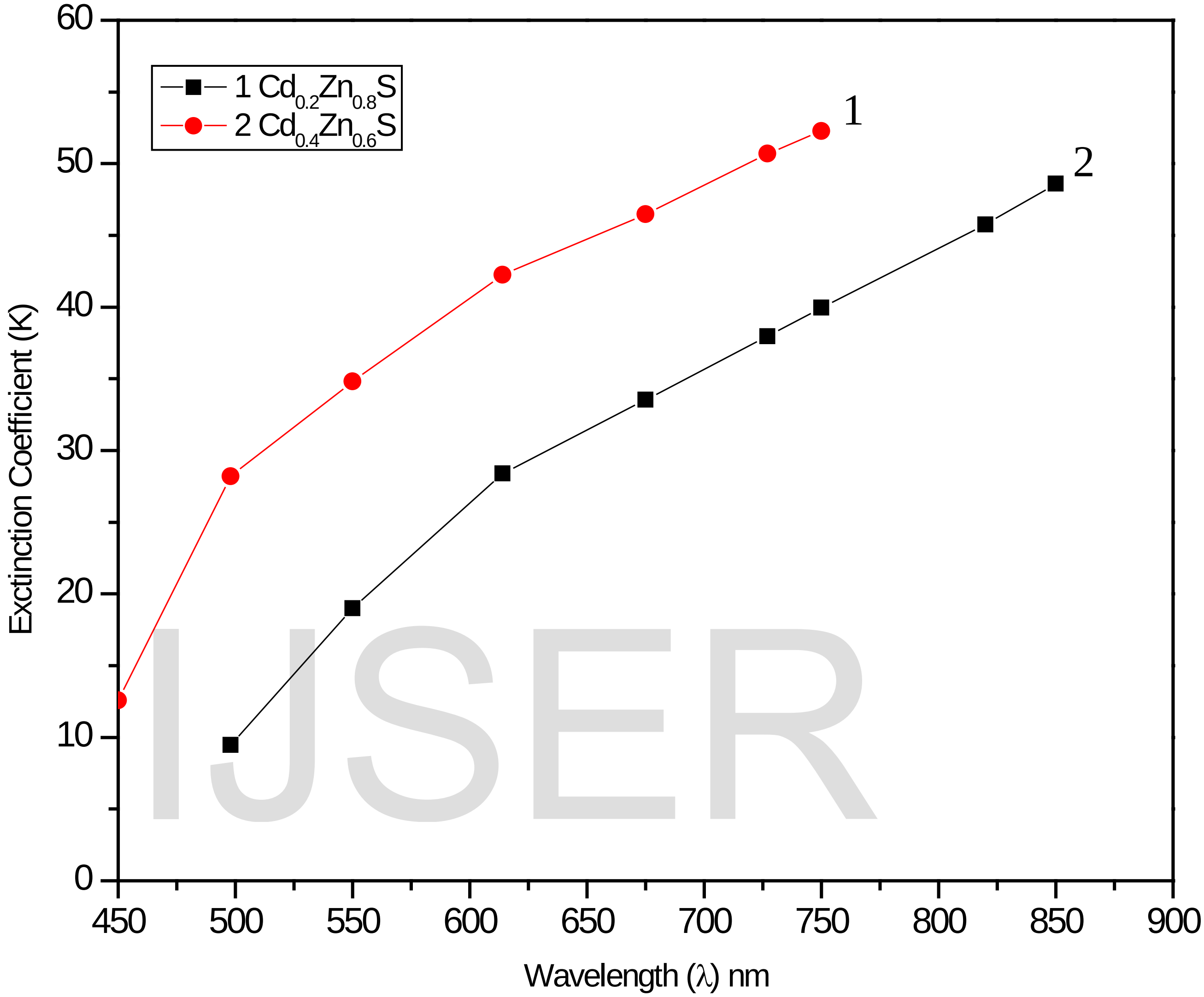

Fig 3(b): Variation of extinction coefficient (k) with wavelength (λ) of vacuum evaporated of $Cd_{0.2}\,Zn_{0.8}\,S$ & $Cd_{0.4}\,Zn_{0.6}\,S$ thin films.

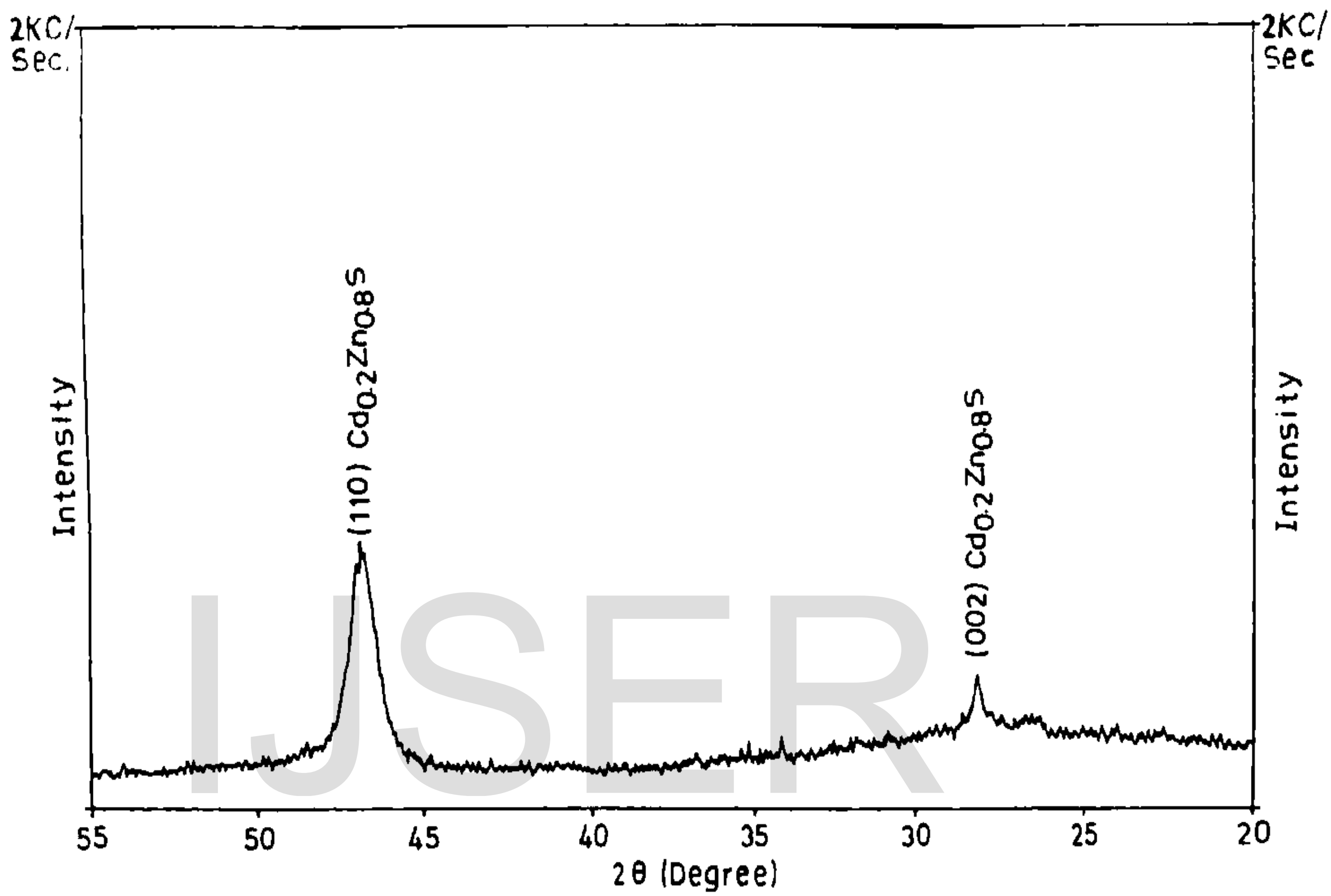

Fig 4 (a): X- Ray diffraction pattern of vacuum evaporated $Cd_{0.2}$ $Zn_{0.8}$ S thin film.

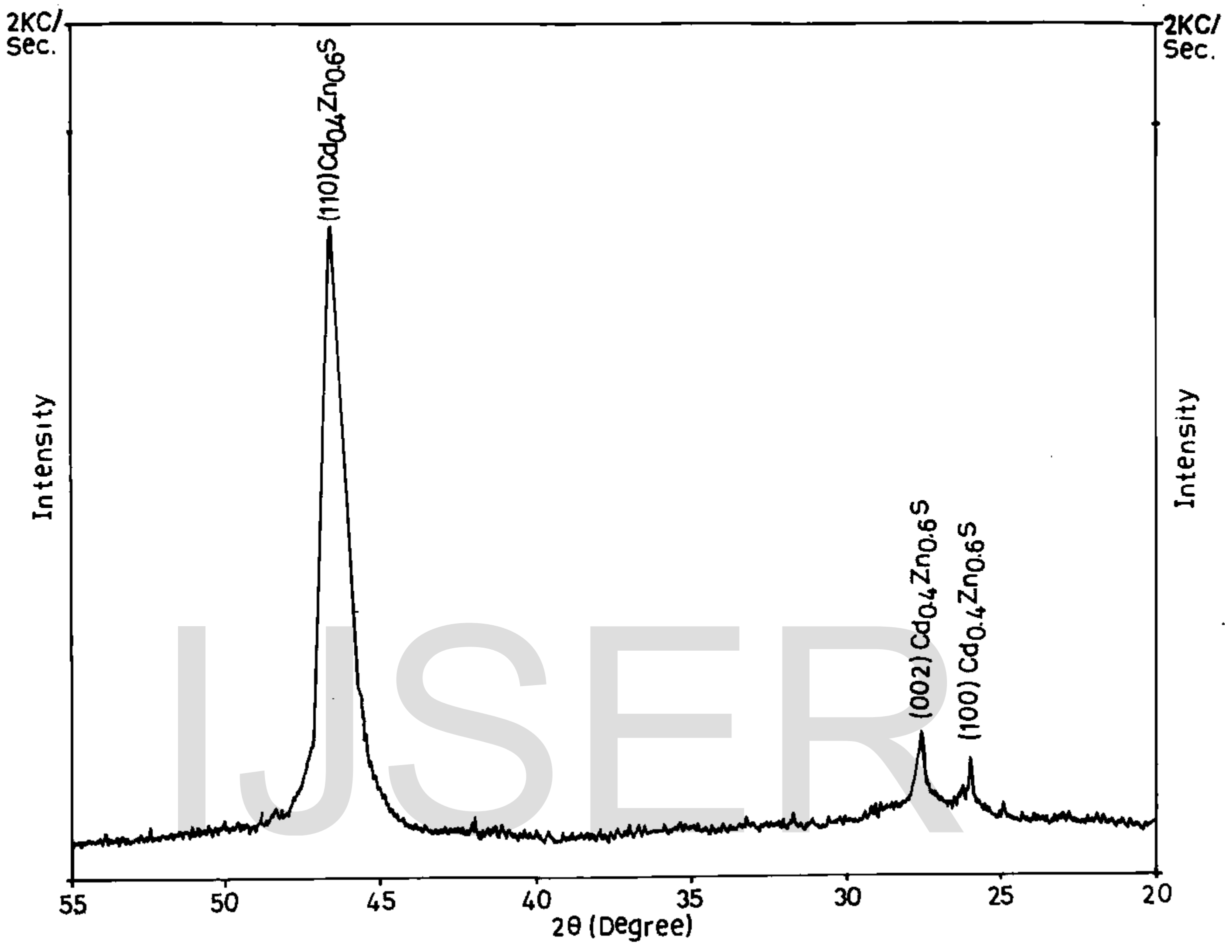

Fig 4 (b): X- Ray diffraction pattern of vacuum evaporated $Cd_{0.4}$ $Zn_{0.6}S$ thin film.