# EFFECT OF Pb INCORPORATION ON ENERGY BAND GAP OF CdS THIN FILMS.

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The thin films of $Cd_{1-x}Pb_xS$ ($0 \le x \le 1$) have been deposited onto clean glass substrates by economical bath deposition technique. The deposition parameters were optimized to obtain good quality thin films. The absorption spectra of these films have been recorded using spectrophotometer. The energy band gap ($E_g$) and absorption coefficient ($\alpha$) has been determined using these spectra. It is found that the band gap decreases with increase in Pb concentration. It is observed that energy band gap is varied from 2.47 eV (CdS) to 0.49 eV (PbS) as composition parameter 'x' increased from 0 to 1. The nature of the band gap has also determined in this paper.

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## 1. Introduction

Cadmium sulphide (CdS) which belongs to II-VI compound materials, is one of the most promising semiconducting candidate because of its wide range of applications in various optoelectronic, pizo-electronic and semiconducting devices [1-2]. Thin films of CdS are of considerable interest for their efficient use in the fabrication of solar cells [3]. Because of its optical properties, CdS is used in CdTe devices as an optical window [4]. CdS is highly sensitive to light and has high absorption coefficient. The only disadvantage with CdS is its wide band gap (2.4 eV). The band gap of CdS has been tailored by mixing it with lead ions. As the CdS and PbS are highly sensitive to light and in view of their practical application, a study of their mixed thin films structure as electrochemical converters is of technical importance [5].

The CdS films have been prepared by a variety of methods such as chemical bath deposition [6], spray pyrolysis [7], vacuum deposition [8], molecular beam epitaxy [9] and solution growth [10]. Among these techniques chemical bath deposition technique is favored because of its relatively simple, inexpensive and scalable technique for the deposition of high quality and large area films.

In this work it is proposed to report the results indicating that by proper choice of lead concentration with CdS concentration one can change the various optical properties of these thin film layers for opto-electronic, photovoltaic and photoconductive applications.

## 2. Experimental

The chemicals used, such as cadmium sulphate, lead sulphate, thiourea, liquor ammonia and sodium hydroxide were of analytical grade. The glass substrates were cleaned using chromic acid, followed by rinsing in the alcohol and double distilled water.

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For deposition of $Cd_{1-x}Pb_xS$ (0≤ x ≤ 1) thin films, equimolar solutions of cadmium sulphate, lead sulphate and thiourea were mixed in stoichiometric proportion to obtain 'x' value form 0 to 1. Triethanolamine was used as a complexing agent and pH of the reaction mixture was adjusted to about 10.5 ± 0.1 with the help of sodium hydroxide. Thoroughly cleaned optically plane glass substrates were mounted on a specially designed substrate holder and were rotated with a constant speed in the reaction mixture to achieve uniform and continuous stirring of the reaction solution. To obtain good quality thin film samples, the time and temperature of the deposition and speed of the substrate rotation were optimized. These parameters were selected as 60 min, 80 $^0$C and 65 rpm respectively.

The film thickness of the 'as-deposited' samples was measured by gravimetric weight difference method. The optical absorption spectra were recorded at room temperature using UV-VIS-IR spectrophotometer (Carry-5000 Japan) in the wavelength range 350-3300 nm. The absorption coefficient, energy band gap and mode of transition were determined from these studies.

## 3. Results and discussion

### 3.1. Thickness measurement

Film thickness is important parameter in the study of film properties. The film thickness was measured by a weight difference method using the relation

$$t = \frac{m}{\rho A} \qquad (1)$$

where m is the mass of the film deposited onto the substrate, A is the area of the deposited film and ρ the density of the bulk material. The film thickness was found to vary from 810 nm to 1378 nm as composition parameter 'x' increased from 0 to 1, as shown in Fig. 1. The film thickness is listed in Table 1.

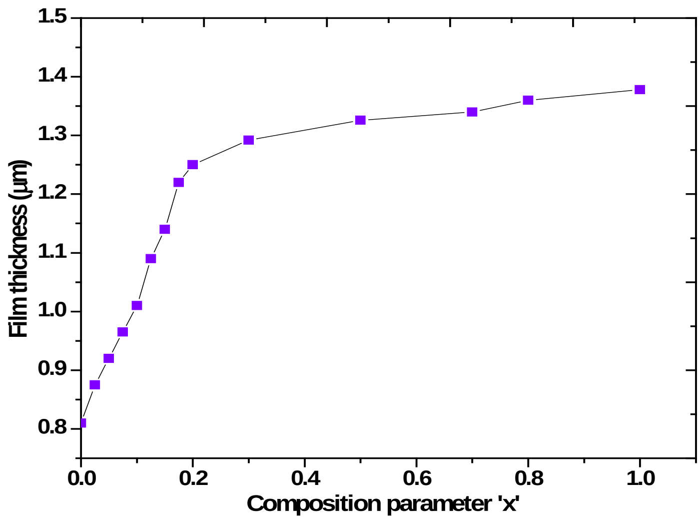


*Fig. 1. Variation of film thickness with composition parameter 'x'.*

### 3.2. Optical studies

The material properties that are of interest for these films are the optical properties within the range of UV-VIS-IR which strongly depend on the refractive index, dielectric constant and the energy band gap of the film and depends very much on the nature of the film [11]. The study of the solid-state properties of the film would give one an idea of these characteristics which arises as a result of the interaction between photon energies and the structure of the thin film or between the energy configuration and other optical constants like refractive index and extinction coefficient [12].

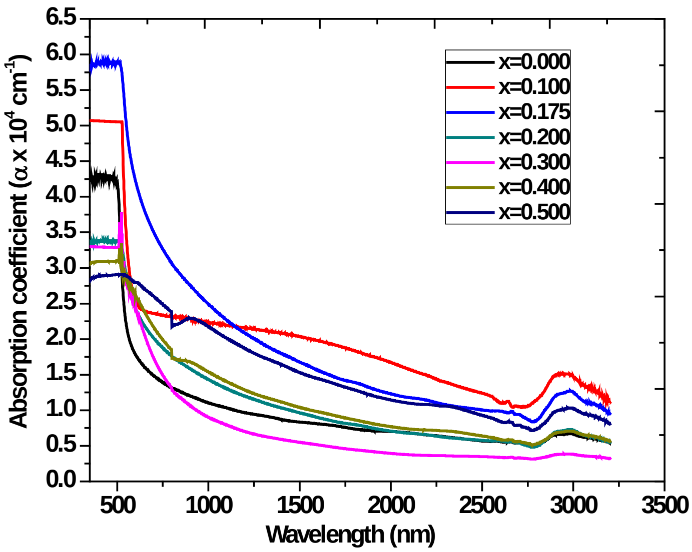


*Fig.2. Variation of absorption coefficient versus wavelength of $Cd_{1-x}Pb_xS$ thin films.*

The optical absorption spectra of these film samples have been studied to evaluate the absorption coefficient (α), energy band gap ($E_g$) and nature of transition involved. Fig. 2 shows the wavelength dependence of the absorption coefficient for a few typical compositions. It is observed that the optical absorption coefficient is high for all the film samples ($\alpha = 10^4$ $cm^{-1}$). The theory of optical absorption gives the relation between the absorption coefficient (α) and the photon energy (hν) as [13]

$$\alpha h\upsilon = A(h\upsilon - E_g)^n \qquad (2)$$

where is the absorption coefficient (α), hν is the photon energy, $E_g$ is the optical band gap and A is the constant which is related to the effective masses associated with the valance band and the conduction band. The n assumes values of 1/2, 2, 3/2 and 3 for allowed direct, allowed indirect, forbidden direct and forbidden indirect transitions, respectively. For allowed direct type of transitions

$$\alpha h\upsilon = A(h\upsilon - E_g)^{1/2} \qquad (3)$$

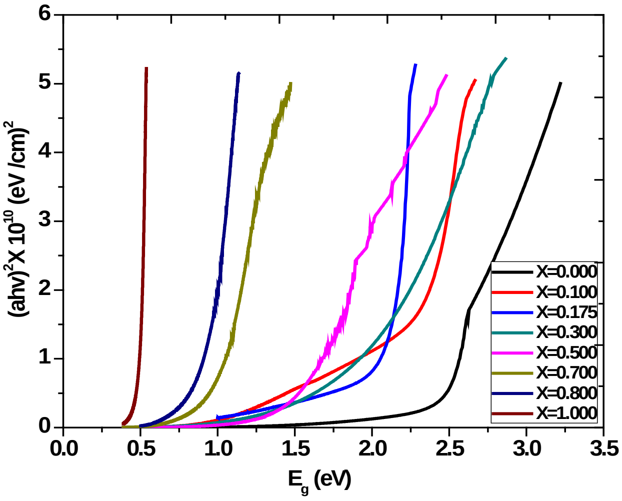


*Fig.3 Plot of $(\alpha h\nu)^2$ versus hν for $Cd_{1-x}Pb_xS$ ($0 \leq x \leq 1$) thin films.*

The plot of $(\alpha h\nu)^2$ versus hν is a straight line whose intercept on energy axis at α = 0 gives the band gap energy ($E_g$) of the $Cd_{1-x}Pb_xS$ ($0 \leq x \leq 1$) thin films. The plot of $(\alpha h\nu)^2$ versus hν were plotted and are shown in Fig. 3. The band gap energies were estimated by extrapolating straight line portion of the plots to the energy axis. The optical band gap of pure CdS is found to be 2.47 eV and decreases continuously down to 0.49 eV for PbS as the composition parameter 'x' increased from 0 to 1. The other compositions have in between $E_g$ values. The band gap energy values are given in Table 1. It is observed that variation of $E_g$ with film composition is not linear, shown in Fig. 4, such type of non-linearity has been reported for CdZnS [14-15]. Such type of behavior may be attributed to the slight variation in film composition than bulk composition and thickness. The broad and fine tunable band gap properties of ternary compounds $Cd_{1-x}Pb_xS$ ($0 \leq x \leq 1$) thin films are suitable for many scientific studies and technological applications such as gas sensors, transparent electrodes, solar cells, piezoelectric and opto-electronic devices.

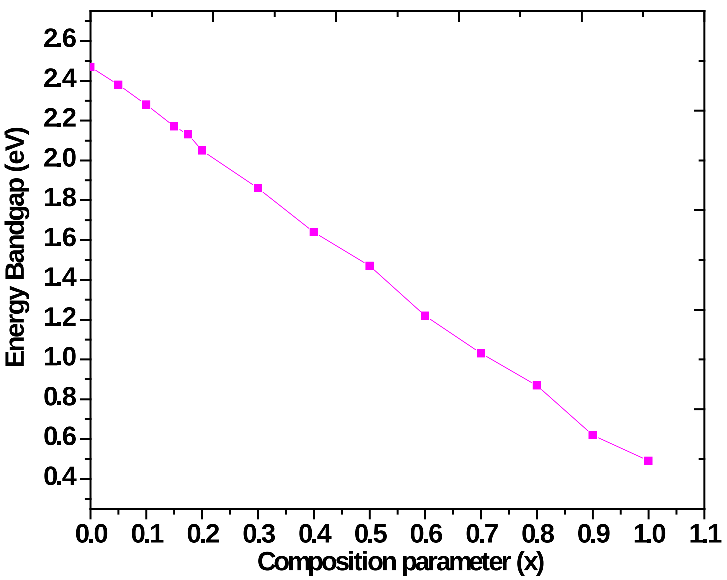


*Fig.4 Variation of energy band gap versus composition parameter 'x'.*

The modes of optical transitions in these film samples have been determined as suggested by Pal et.al. [16]. Eq. 3 can be rearranged as

$$\ln(\alpha h\upsilon) = \ln(A) + 0.5\ln(h\upsilon - E_g) \tag{3}$$

The plot of ln(αhv) versus ln $(hv-E_g)$ is a straight line whose slope gives the power factor n. Fig. 5 indicates the results of above analysis for typical samples and the calculated values of n for all the compositions are listed in Table 1. The obtained values of n suggest that the fundamental absorption edge in the films is formed by the direct allowed transition.

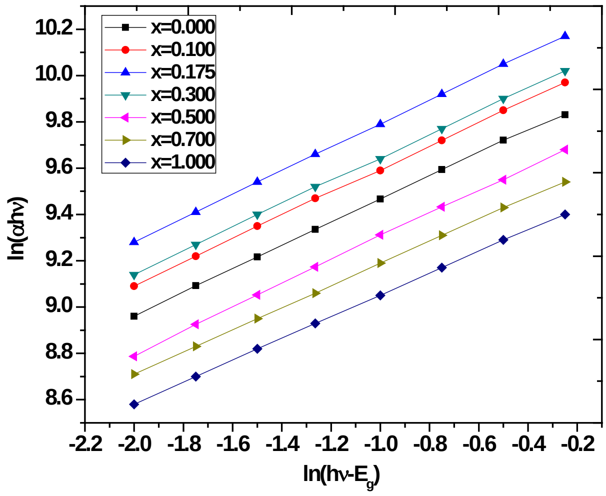


*Fig. 5. Variation of ln (αhv) versus ln $(hv\text{-}E_g)$ for $Cd_{1-x}Pb_xS$ $(0 \le x \le 1)$ thin films.*

## 4. Conclusions

The ternary $Cd_{1-x}Pb_xS$ $(0 \le x \le 1)$ thin films have been deposited by simple chemical bath deposition technique. The optical studies revealed that film exhibit direct band gap which strongly dependent on composition parameter ‘x’. The optical band gap is tailored from 2.47 eV (CdS) to 0.49 eV (PbS) which is required for solar cell and opto-electronic device applications. The absorption spectra of these composites showed high coefficient of absorption with direct allowed type of optical transitions. From optical studies the band gap was found to decrease with Pb incorporation in CdS film.

*Table 1. Some of the characteristic properties of $Cd_{1-x}Pb_xS$ ($0 \le x \le 1$) thin film structures.*

| Composition Parameter (x) | Thickness (nm) | Energy band gap ($E_g$) | Power factor (n) |
|---|---|---|---|
| 0.000 | 810 | 2.47 | 0.51 |
| 0.100 | 1010 | 2.28 | 0.52 |
| 0.175 | 1220 | 2.13 | 0.51 |
| 0.200 | 1250 | 2.04 | 0.53 |
| 0.300 | 1292 | 1.86 | 0.52 |
| 0.400 | 1301 | 1.64 | 0.46 |
| 0.500 | 1308 | 1.47 | 0.57 |
| 0.600 | 1315 | 1.22 | 0.48 |
| 0.700 | 1322 | 1.01 | 0.55 |
| 0.800 | 1360 | 0.85 | 0.58 |
| 0.900 | 1367 | 0.62 | 0.47 |
| 1.000 | 1378 | 0.49 | 0.53 |

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