Variation of band gap in CdPbS with composition prepared by a precipitation technique

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Cadmium sulphide (CdS) is highly sensitive of light and has high absorption coefficient. 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 sulphide (PbS)(low band gap material). The material of configuration (Cd$_{1-x}$Pb$_x$S) for this study has been prepared by precipitate technique in the methanol with $x = 0.2$, 0.4, 0.6, 0.8. The films of this material were deposited by the vacuum deposition method. Spectroscopic technique has been used for the band gap determination. The variation of band gap with their composition has been reported. It has been found that the band gap decreases with increase in Pb concentration. The nature of the band gap has also been determined in this paper.

Keywords: CdPbS, Precipitation technique, Band gap

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1 Introduction

Cadmium sulphide (CdS) is one of the most studied materials for solar cell application particularly for photo-electrochemical and hetero-junction solar cell$^{1-4}$. The photo-electrochemical cells(pec) devised out of the binary and highly order chalcogenide semiconductors have been the subject of intensive research since they posses the potential as the efficient absorbers in the visible region of the solar spectrum$^5$. 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$^6$.

The preparation of CdS can be carried out by a number of processes, including precipitation technique$^7$. There are so many ways to prepare the ternary compound with CdS (Refs 9,10), here CdPbS has been prepared by the chemical-bath deposition$^8$ method.

2 Experimental Details

The precipitation technique is commonly used to prepare the compound of their various compositions. The reaction vessel contained equal volumes of aqueous one molar solution of thiourea CS(NH$_2$)$_2$ and CdSO$_4$ along with different molar concentrations of Pb(NO$_3$)$_2$ to which ammonium hydroxide NH$_4$OH(2N), was later added to initiate the reaction.

$$x\text{Cd(NH}_3)_2 + (1-x)\text{Pb(NH}_3)_2 + \text{CS(NH}_2)_2 + 2\text{OH}^- \rightarrow \text{Cd}_x\text{Pb}_{1-x}\text{S} + 4\text{NH}_3 + 2\text{H}_2\text{O} + \text{CH}_2\text{N}_2$$

The CdPbS precipitates in the solution. The precipitate is collected by the Whatman filter paper. This dry material is now ready for evaporation. The films of material were deposited on the glass substrates by the vacuum evaporation by VICO Vacuum Coating Unit in a vacuum of $10^{-5}$ torr.

3 Characterization of Samples

The absorption spectra of these films were obtained by using Hitachi Spectrophotometer (U3400 Model). For energy band determination, we used the Tauc Relation$^{11}$.

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

where $h\nu$ is the photoenergy, $\alpha$ the absorption coefficient, $E_g$ the energy band gap, $A$ the constant and $n$ is 1/2 for direct band gap$^{12}$.

To measure the energy band gap from the absorption spectra a graph $(\alpha h\nu)^2$ versus $h\nu$ is plotted. The extrapolation of the straight line to $(\alpha h\nu)^2 = 0$ axis gives the value of the energy band gap.

4 Results and Discussion

Figure 1 shows the absorption spectra of thin Cd$_{1-x}$Pb$_x$S film recorded by Hitachi Spectrophoto-
As CdS is a direct band gap material, therefore graph between \((\alpha h\nu)^2\) and \((h\nu)\) has been drawn using Tauc relation. Figures 2-5 show the plots between \((\alpha h\nu)^2\) and \((h\nu)\) for thin film for different compositions of \(\text{Cd}_{1-x}\text{Pb}_x\text{S}\).

The extrapolation of straight line to \((\alpha h\nu)^2 = 0\) gives the value of band gap for the different values of \(x\). From these graphs (Figs 2-5), the value of energy band gap has been found to vary with the value of \(x\). The nature of the variation of band gap is depicted in Fig. 6.

5 Theory

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

\[
\log(\alpha h\nu) = \log A + n \log(h\nu - E_g)
\]

Thus, to find out the nature of the band gap, we draw a graph between \(\log(h\nu - E_g)\) and \(\log(\alpha h\nu)\) (Fig. 7). Then find out the slope as given in Table 1.
Table 1—Values of $L_n(h\nu-E_g)$ and $L_n(\alpha h\nu)$ for determination of the nature of band gap

<table>
<thead>
<tr>
<th>S.N.</th>
<th>$h\nu$</th>
<th>$h\nu-E_g$</th>
<th>$L_n(h\nu-E_g)$</th>
<th>$L_n(\alpha h\nu)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.098</td>
<td>0.798</td>
<td>-0.225</td>
<td>1.64</td>
</tr>
<tr>
<td>2</td>
<td>2.950</td>
<td>0.650</td>
<td>-0.430</td>
<td>1.53</td>
</tr>
<tr>
<td>3</td>
<td>2.816</td>
<td>0.516</td>
<td>-0.661</td>
<td>1.44</td>
</tr>
<tr>
<td>4</td>
<td>2.693</td>
<td>0.393</td>
<td>-0.933</td>
<td>1.33</td>
</tr>
</tbody>
</table>

\[
n = \frac{Y_2 - Y_1}{X_2 - X_1} = \frac{1.60 - 1.50}{-0.30 - (-0.50)}
\]

\[
n = \frac{0.10}{0.20} = \frac{1}{2}\] (for direct band gap)^12

6 Conclusion

The Cd$_{1-x}$Pb$_x$S has been prepared by the precipitation method. Film of the precipitate was deposited by evaporation method on the glass substrate. We conclude that the concentration of PbS is inversely proportional to the optical band gap. The nature of the band gap for all compositions is a direct band gap.

References