Effect of Doping Pb on the Structural and Optical Properties of Nanostructured CdS films

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Abstract

Pure and Pb doped CdS films were prepared by chemical bath deposition method onto glass substrates at room temperature. The structural and optical properties of the prepared films were characterized using XRD and UV-VIS spectroscopy. X-ray diffraction patterns revealed polycrystalline nature of the films. The particle size of the crystallites was determined from the XRD patterns using Scherrer formula and was found to be 27.31 nm for CdS film. The particle size shows change in case of the Pb doped film. The bandgap for CdS film as determined from the absorption spectrum is found to be 3.82 eV for CdS film, which decreases on doping with Pb.

Keywords: Nanoparticles, cadmium sulfide, UV-VIS spectroscopy, XRD.

Introduction

Thin films of polycrystalline semiconductors are of great scientific interest owing to their applications in various electronic and optoelectronic devices. The technological interest in the devices based on polycrystalline semiconductors is mainly caused by their low production cost.

Cadmium sulfide (CdS) polycrystalline thin films is a representative of II-VI semiconductor materials with many applications such as large area electronic devices and solar cells. It is a wide direct band gap (2.42 eV) material and has been used as a window material together with several semiconductors such as CdTe, Cu2S and CuInSe2. The interest in CdS thin films can be attributed to its piezoelectric properties and potential laser applications.

Many techniques have been used for depositing CdS thin films. These include evaporation, sputtering, photochemical deposition, molecular beam epitaxy (MBE) technique, spray pyrolysis, successive ionic layer adsorption and reaction (SILAR) method. The chemical bath deposition (CBD) method appears to be a relatively simple method to prepare a homogenous films with controlled composition. In particular CBD is widely used for achieving good-quality CdS thin films. The films deposited by this method better photoconductivity and improved morphological properties such as roughness and pinhole density as compared with films processed other techniques. In this paper, chemical bath deposition has been carried out to prepare CdS thin films by using cadmium chloride as a source of cadmium ions (Cd2+) and thiourea as a source of sulfur ions (S2-) and ammonia solution acts as a buffer solution. The structural and optical properties of CdS thin films as well as Pb doped CdS films were studied and the results described in this paper.

Experimental details

The CdS films were prepared using solutions of cadmium chloride [CdCl2] thiourea ([NH2)2CS] and ammonia solution. For preparing Pb doped CdS films lead nitrate PbNO3 was also added to CdCl2 solution in appropriate amount. The pH of the solutions play major role in reaction. The pH of the bath solution during deposition was maintained 9-10. CdS films have been prepared by chemical bath deposition (CBD) method on glass substrates at room temperature. Cadmium chloride was used as a source of Cd2+ and thiourea as a source S2- and lead nitrate as a source of Pb2+.

Clean glass substrates were mounted vertically in the solution at room temperature for 10 min and two samples – pure CdS and Pb doped CdS thin films were prepared on glass substrate. After the formations of the films the substrates were removed from the bath and rinsed several times in distilled water to remove any adherent particles and unreacted material. Samples were dried at room temperature. Adequate precaution was taken to protect the films from dust.

The XRD patterns were recorded using D8 Advanced X-ray diffractometer from Bruker. UV-Vis absorption spectra were recorded using Shimadzu 2450 double beams spectrophotometer.

All the experiments were performed at room temperature.
Results and Discussion

3.1 XRD studies: The X-ray diffraction patterns of the CBD-CdS thin films are reproduced in Figure 1a. It can be seen that CdS nanostructures are polycrystalline in nature and possess hexagonal structure. CdS can exist in three crystalline phases, hexagonal, cubic (zincblende) and cubic (rock salt). The first two phases have been reported for CdS thin films prepared by CBD method. The crystal structure of CdS films in the present study are in agreement with the observation of earlier researchers. There are many variables which affect the crystal structure of CdS films including the nature of the starting material, the substrate etc. Lee studied the effect of substrates on the structure and phase of CBD CdS thin films and observed that different substrates led to hexagonal or cubic phase which agrees with our result.

The interplanar distance \( d \) were calculated using Bragg’s law
\[
n_\lambda = 2d \sin \theta
\]
where \( n \) is the order of diffraction, \( \lambda \) is the wavelength of the incident x-ray, \( d \) is the interplanar distance, \( \theta \) is the Bragg angle

The \( d \)-values corresponding to prominent peaks are reproduced in table 1. The interplanar spacing \( d \) of the CdS film under study match well with those reported by JCPDS files (JCPDF#892944, 890440). The XRD pattern of Pb doped CdS film. The interplanar distance of the prominent peaks are reproduced in table 1. The shift in the peak positions can be attributed to doping of Pb in the CdS structure.

X-ray diffraction peak profiles as seen in figure 1a and 1b are broad which can be attributed to small crystallite size.

The crystallite size of the nanoparticles is estimated by using Scherrer’s formula
\[
D = \frac{k\lambda}{\beta\cos \theta}
\]
Where \( k \) is constant, \( \lambda \) is the wavelength of X-Ray used, \( \beta \) is the full width at half maximum (FWHM).

<table>
<thead>
<tr>
<th>Table 1</th>
<th>XRD data and crystallite size of pure and Pb doped CdS films</th>
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<tbody>
<tr>
<td>For Pure CdS</td>
<td>S.No.</td>
</tr>
<tr>
<td>01</td>
<td>27.21</td>
</tr>
<tr>
<td>02</td>
<td>31.43</td>
</tr>
<tr>
<td>03</td>
<td>34.36</td>
</tr>
<tr>
<td>For Pb-doped CdS</td>
<td>01</td>
</tr>
<tr>
<td>02</td>
<td>28.47</td>
</tr>
<tr>
<td>03</td>
<td>29.90</td>
</tr>
<tr>
<td>04</td>
<td>30.94</td>
</tr>
<tr>
<td>05</td>
<td>31.48</td>
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<tr>
<td>06</td>
<td>31.76</td>
</tr>
<tr>
<td>07</td>
<td>32.70</td>
</tr>
<tr>
<td>08</td>
<td>33.25</td>
</tr>
<tr>
<td>09</td>
<td>33.89</td>
</tr>
</tbody>
</table>

a: JCPDF#892944 (Hexagonal)  
b: JCPDF#890440 (Cubic)
Absorption studies: The absorption spectra of pure CdS and Pb doped CdS thin films were recorded at room temperature and are reproduced in figures 2a and 2b respectively. Absorption edge of CdS thin film shows a clear shift to the lower wavelength as compared to its bulk counterpart. This blue shift of the absorption edge indicates decrease in the crystallite sizes and confirms the formation of nanostructured CdS film. Similarly, the Pb doped CdS film is also nanostructured in nature.

A graph between $h\nu$ vs. $(\alpha h\nu)^2$ is plotted and is reproduced in figure 3a. for CdS film and in figure 3b for Pb doped CdS film. The extrapolation of straight line portion of the graph to $(\alpha h\nu)^2 = 0$ axis gives the value of the energy band gap of film materials. The band gap of the films has been determined from the plots which are found to be 3.82 eV for pure CdS and 3.5 eV for Pb doped CdS. This is in confirmation with the XRD results, which shows that doping increases the particle size. The decrease in the bandgap as a consequence of the increase in particle size is in conformation with the earlier studies.

Conclusion
CdS films and Pb doped CdS films were prepared using Chemical Bath Deposition technique onto glass substrates. The energy gap, and particle size have been evaluated, which shows that the particle size of CdS increases in Pb doped film, while the bandgap decreases as a result of doping Pb in the CdS film.

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References