Band gap of vacuum evaporated CdS thin films

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Thin films of cadmium sulphide (CdS) have been deposited in a low atmosphere of H₂S obtained by thermal decomposition of thiourea inside the vacuum chamber. The substrate is kept at an elevated temperature to eject any sulphur atoms deposited due to thermal decomposition of CdS during evaporation. The cadmium ions would promptly recombine with the H₂S to give better stoichiometry of the films. This results in better growth of films which are more uniform, more adherent, pin holes free and have better crystallinity as have been inferred by the sharpness of the absorption spectra. Such films are inherently better suited for device fabrication.

Cadmium sulphide (CdS) is a useful opto-electronic piezo-electric and semiconducting material. Thin films have been prepared by different techniques including sputtering and laser deposition. The vacuum evaporated thin films of CdS are usually polycrystalline and have excess of cadmium owing to the dissociation of CdS during evaporation. The stoichiometry can be restored by codeposition of sulphur together with CdS or by annealing the film in CdS powder. However, compensation for sulphur deficiency can also be accomplished by exposing the film to a hydrogen sulphide atmosphere during growth. The higher reactivity of hydrogen sulphide will ensure a better conversion of the dissociated Cd ions into CdS and also will not produce any excess of sulphur at the substrate. From the point of view of vacuum evaporation, the thermal decomposition of thiourea is a convenient source of H₂S which can be controlled by regulating the temperature of the electrically heated borosil test tube in the evaporation chamber. This communication describes the energy band gap of vacuum evaporated CdS thin films “with and without” thiourea.

Experimental Procedure
Cadmium sulphide powder of 9N purity was evaporated at about 850°C from a deep narrow mouthed molybdenum boat. Deposition was made onto glass substrates held at 200°C in a vacuum of the order of 10⁻⁵ torr. The substrates were cleaned in aqua regia, washed in distilled water and isopropyl alcohol (IPA). A borosil test tube was used for the thermal decomposition of thiourea at 150°C, this was separated from the CdS molybdenum boat by a stainless steel heat shield for comparison films were deposited both “with and without” thiourea.

Absorption spectra of vacuum evaporated cadmium sulphide films both “with and without” thiourea were taken at room temperature with the help of “Hitachi spectrophotometer model U-3400” as shown in Fig. 1.

Results and Discussion
Energy band gap
The energy band gap of these films has been calculated with the help of absorption spectra (Fig. 1). To measure the energy band gap from absorption spectra the Tauc relation is used.

Note

Fig. 1—Absorption spectra of vacuum evaporated CdS films for both “with” and “without” thiourea.
\[ \alpha h \nu = A (h \nu - E_g)^n \]

where, \( h \nu \) = photon energy, \( \alpha \) = absorption coefficient, \( E_g \) = energy band gap, \( A \) = constant, and \( n = 1/2 \) for direct band gap.

To measure the energy band gap from 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. Figs 2 and 3 show the plot of \((\alpha h \nu)^2\) vs \( h \nu \) for the vacuum evaporated CdS thin film 'without and with .' thiourea respectively. From these graphs, the value of energy band gap of CdS with and without thiourea comes out as 2.47 eV and 2.39 eV respectively. It was found that the films with thiourea were of dark yellow colour and of excellent uniformity. They have better adhesion to the substrate and better transparency than films deposited without thiourea.

The thickness of these films was measured by the "Hitachi spectrophotometer model U-3400" and the values are 4.2, 3.9 micron for both films with and without thiourea respectively. The time of deposition for both films is 15 min.

Nature of band gap

For the nature of band gap, a graph in \( \ln (h \nu - E_g) \) vs \( \ln (\alpha h \nu) \) has been drawn and is shown in Fig. 4. From Fig. 4, slope

\[
\ln (\alpha h \nu) = (y_2 - y_1)/(x_2 - x_1)
\]

\[
= (3.273 - 2.819)/(-1.2729 - (-2.2072))
\]

\[ = 1/2 \]

This shows the band gap to be direct.

Conclusion

It is concluded here that the CdS films with thiourea were of dark yellow colour and of excellent uniformity. They had better adhesion to the substrates.
and better transparency than films deposited without thiourea. The band gap of films prepared with thiourea shows good results than that without thiourea.

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References