CHAPTER V

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SUMMARY AND CONCLUSIONS

Summary of the Results :

Optical and electrical properties of thin films of molybdenum sulphide were studied in the present investigation by keeping a view of their use in electrochemical photovoltaic cells, as a working photoelectrode. Experimental results of these properties are reported earlier and discussed at length in the respective chapters. Here these results are summarised.

Molybdenum sulphide thin films were prepared by spray pyrolysis technique which involves spraying of stoichiometrically mixed solutions of ammonium heptamolybdate and thiourea on hot substrates. The films prepared are uniform and adhere tightly to the substrate. The films are bluish green at lower substrate temperatures but colour of the films changes to gray at higher substrate temperature. The films prepared at 300°C are found to be more uniform in nature.

The plots of log σ versus $\frac{1}{T}$ shows that there are two distinct regions corresponding to high and low temperatures. Two principle activation energies are evident. The activation energies in high temperature regions decreases with increase in substrate temperature whereas there is no systematic variation at low temperature regions. The conductivity increases as substrate temperature increases. The lower conductivities at low substrate temperature may be due to incomplete reactions of the initial ingradients and poor crystallinity of the films.

The polarity of the thermoelectric voltage developed in the films states that films are of n-type. This is in agreement with results reported by other workers. Thermoelectric power increases with increase in temperature which is attributed to an increase in the electron concentration with rise in temperature. Thermoelectric power is higher for the films prepared at higher substrate temperature which is due to better crystallinity of the films.

The absorption data [plots of $(\alpha h\nu)^2$ versus $h\nu$] shows that the transitions are direct and allowed which is in agreement with the fact that the material is known to be a direct band gap material due to this, molybdenum sulphide films have higher resistance to photocorrosion when employed in electrochemical photovoltaic cells. The bandgap value obtained is 1.9 eV which is also in fair agreement with the values reported in literature. The absorption co-efficient (α) is found to be of the order of 10^{+4} cm^{-1} for all the films. The absorption coefficient increases with increase in substrate temperature except at substrate temperature 400°C.

The reflectivity measurements show that

1) The reflectivity of the films decreases with the film thickness.
2) As angle of incidence of light beam increases, the reflectivity of the film increases.
3) The reflectivity also increases for the films prepared at higher substrate temperature.

Variation of reflection coefficients for parallel (p) and perpendicular (s) components of light indicates that at normal incidence ($\phi = 0$) the parallel and perpendicular components are not distinguishable and equally reflected. As angle of incidence increases R_p drops to minimum corresponding to Brewester angle while R_s increases first slowly and then rapidly. At grazing incidence ($\phi = 90^\circ$) both the components are totally reflected.

The pair of values of optical constants n and K are determined from the R_p/R_s values by a graphical method due to Avery. Pair of values of n and K are obtained for different angles of incidence. The real value of n and K is then determined by the intersection of curves of K versus n at different angles of incidence. The refractive index is found to be 3.7 and extinction coefficient K = 0.82 for molybdenum sulphide thin films.

The real (ϵ_1) and imaginary (ϵ_2) parts of the complex dielectric constants (ϵ^*) are evaluated from n and K values and are found to be 13.2 and 6.06.

Conclusions :

1) Uniform thin films of molybdenum sulphide can be prepared by spray pyrolysis technique.

2) The films prepared at 300°C substrate temperature are found to be more uniform.

3) The resistivity of the molybdenum sulphide films is of the order of $10^2 \times 10^3$ (ohm - cm).

4) Molybdenum sulphide thin films are of n-type.

5) The conductivity and thermoelectric power is higher for the films prepared at 400°C substrate temperature.

6) The material is direct band gap material and the transitions are direct and allowed.

7) The absorption coefficient is found to be of the order of 10^{+4} cm^{-1}. The absorption coefficient increases with substrate temeprature.

8) The reflectivity of the molybdenum sulphide films increases with angle of incidence of light beam and with substrate temperature but decreases with film thickness.

9) The refractive index (n) is found to be 3.7 and extinction coefficient (K) = 0.82 for molybdenum sulphide thin films.

10) Molybdenum sulphide thin films can be used as photoelectrode in electrochemical photovoltaic cells due to their higher resistance to photocorrosion.