SECTION IV
CHAPTER 4.1

Conclusions and scope for the future work

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I INTRODUCTION

This thesis described the growth and photo-electrochemical characterization of thin films of copper indium diselenide (CuInSe$_2$) and tungsten sulfo-selenide (WSSe) single crystals. Important conclusions drawn from the reported work are presented below. A scope for the future work has also been suggested.

II CONCLUSIONS

The I-III-VI$_2$ chalcopyrite compounds are the three element analogues of the extensively studied II-VI
semiconductors and have recently attracted extensive basic and applied research interest. The virtually unique absorbing properties of CuInSe$_2$ coupled with its appropriate band gap has resulted in about a decade of research and development activity designed to develop an efficient and economic photovoltaic convertor. The opto-electronic structural and morphological properties of CuInSe$_2$ and the corresponding device performance, are highly dependent on film composition, defect chemistry and growth parameters, such as substrate temperature.

With this thing in mind the preparation of thin films of CuInSe$_2$ at various substrate temperatures using thermal evaporation technique and their characterization using electron and X-ray diffraction technique have been done.

It is seen that single source deposition is adequate to produce single phase CuInSe$_2$ thin films. Improvement in the crystallinity and orientation is observed at higher temperature.

Among the layered compounds of transition metal dichalcogenides, all research activities of solid state photovoltaic cells have been limited to WSe$_2$ and
Both these compounds have been successfully used as photoelectrodes in PEC solar cells. By suitable adjustment of sulphur and selenium content in \( \text{WS}_x\text{Se}_{2-x} (0 \leq x \leq 2) \) the band gaps can be altered and a material suitable for solar energy conversion can be prepared.

By taking equal portions of sulphur and selenium in \( \text{WS}_x\text{Se}_{2-x} (0 \leq x \leq 2) \), single crystals of tungsten sulphoselenide (WSSe) were grown by the DVT and CVT techniques.

These crystals possess proportionate elemental composition and are stoichiometrically pure and perfect. X-ray diffraction studies indicate that all of them are single phase compound isomorphous with MoS\(_2\) type structure.

It is observed that resistivity of the crystals grown at higher temperature [i.e. by direct vapour transport] exhibit lower resistivity where as crystals grown by chemical vapour transport at lower temperature have high resistivity. Measurements of Hall coefficient point out that crystals grown by direct vapour transport are p-type, while those grown by
chemical vapour transport possess n-type semiconducting nature.

In all the different electrolytes, the Iodine/Iodide electrolyte gives better results with n-WSSe electrodes while the ferric/ferro cyanide electrolyte gives better results with p-WSSe electrodes.

The photocurrent (I) vs voltage (V) curves shift outwards with increase in intensity of illumination. The efficiency and fill factor decrease with increase in intensity of illumination. The photoresponse was found to decrease when crystals showing the presence of screw dislocations were used in the fabrication of PEC cells.

p-CuInSe₂ electrodes have been characterized in terms of the energetic location of the valence and conduction band positions, which suggests that couples with redox potentials between -0.8601 V and +0.1798 V vs SCE should be appropriate for PEC solar cells of p-CuInSe₂ single crystal electrodes in electrolyte.

It has been observed that the photocurrent and efficiency of PEC cells can be improved considerably
by chemical etching.

III SCOPE FOR FUTURE WORK

Resistivity and Hall coefficient observations at higher temperature have not been reported in this thesis because of the lack of facilities for the high temperature work. In order to understand the nature of carriers, their behaviour and conduction mechanism transport studies at high temperature need a worth while consideration.

It is seen that PEC cells fabricated using CuInSe₂ crystals have very low values of efficiency (n ≈ 1%). This is because the crystals of CuInSe₂ grew in the form of a rod from which sufficiently thin flakes could not be obtained in the absence of availability of a diamond knife. Therefore it is desirable to carry out the growth of single crystals of CuInSe₂ in the form of needles or thin flakes. Such attempts by author did not yield useful results. However, author is quite optimistic, and if different growth conditions are tried one should be in a position to achieve success.

Studies leading to a suppression of photocorrosion in different aqueous and non-aqueous
electrolytes can be carried out by using Rotating Disc Electrode (RDE), Rotating Ring Disc Electrode (RRDE), Sinusoidal Hydrodynamic Modulation (SHM) at RDE and by Rotating Split Ring - Disc Electrode techniques. Photocorrosion of the photoactive material is still an unsolved problem which can be studied with the help of a potentiostat/Galvanostat system. It can also be studied in detail to understand mechanism of charge transfer of the semiconductor-electrolyte interface.