CHAPTER 10

CONCLUSION AND SCOPE
FOR FUTURE WORK
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10.1 INTRODUCTION

Since last few decades, there has been a great deal of interest in the study of properties of materials having layered structures. The layered materials are in practical use in widely differing areas of physics and chemistry. The layered compounds have drawback that they have not yet found a large scale practical applications in electronic devices. This is due to the fact that only limited material research has been carried out in relation to the device potential of these layered semiconductors. On the other hand they are quite promising and the studies reported so far, though exploratory in nature, serve to bring out the potential of these materials for photovoltaic devices.

Among the group VI compounds, MoS$_2$ and MoSe$_2$ form a very interesting class of layered semiconductors. These layerlike chalcogenides crystallize in an Hexagonal crystal structure $P_{6_3}/mmc$. The MoS$_2$ and MoSe$_2$ crystal structure consists of hexagonal stacking of S-Mo-S and Se-Mo-Se sheets in which every 'Mo' atom is surrounded by six 'S' atoms and 'Se' atoms in MoS$_2$ and MoSe$_2$. A layers is composed of alternately occupied prisms, placed side by side. Thus each 'S' and 'Se' shares itself with three 'Mo' atoms in the same layer and no strong bond exists across the gap between the layers. This accounts for the easy mechanical cleavage along the basal plane.

Recently MoS$_2$ and MoSe$_2$ have attracted considerable attention because of their use in optoelectronics, holographic recording systems, electronic switching and infrared generation and detection systems. The interest in
the properties of these materials either in the form of a single crystal, polycrystal or a thin film with large dimensions for an optimum photoconversion has been shown several times.

However, in order to obtain variable conduction properties, MoS$_2$ and MoSe$_2$ must be grown in form of single crystals. Although MoS$_2$ and MoSe$_2$, very few experimental results are available at present. The authors has therefore, investigated the feasibility of growing MoS$_2$ and MoSe$_2$ in form of single crystals and study their various properties. Author has made an attempt to study the photoelectrochemical behavior of MoS$_2$ and MoSe$_2$ single crystals by preparing a photoelectrochemical solar cell, with MoS$_2$ and MoSe$_2$ single crystal acts as a photoelectrode.

The entire work carried out in the above manner has been described in the present thesis. Attempts have been made here to come to some important conclusions on the basis of the present work and to find out scope for future work.

**10.2 CONCLUSIONS**

The large size of MoS$_2$ and MoSe$_2$ crystals were successfully grown by chemical vapor transport technique with transporting agent. The growth conditions for MoS$_2$ and MoSe$_2$ were determined. The stoichiometries of the MoS$_2$ and MoSe$_2$ crystals were confirmed from the EDAX analysis.

The results from the X-ray diffraction analysis indicate hexagonal crystal structure of the crystals. The values of the lattice parameters $a$, $b$, $c$,
and c of the crystals are in agreement with those obtained by previous workers. The microscopic examinations of the surfaces of the crystals have revealed layered growth mechanism for their growth. The presence of growth layers initiating from edges and corners and spreading across the face clearly support this conjecture.

The variation of conductivity and thermoelectric power with temperature confirms the semiconducting nature of the single crystals of the MoS$_2$ and MoSe$_2$. The positive value of Hall coefficient and Seebeck coefficient indicate that all crystals are p-type and majority charge carriers in them are holes.

The optical absorption study has clearly shown that MoS$_2$ and MoSe$_2$ compounds have direct as well as indirect band gaps. An accurate analysis of the absorption data has shown that the indirect transitions represented by the absorption curves are indirect allowed. The optical properties of molybdenum disulphide and molybdenum diselenide has been successfully described using two dimensional as well as three dimensional models, earlier by various workers.

Recent studies on the effect of pressure and temperature on the electronic transitions in MoS$_2$ and MoSe$_2$ semiconductors inspired the author to carry out the studies under pressure. The electrical resistance in these crystals was found to be pressure dependent. No phase transition observed
in these crystals up to 6.5 GPa. However the electrical resistance decrease with increase in pressure showing a shift from being predominantly two dimensional material to a three dimensional one.

Although, number of investigators have shown the utility of layered transition metal dichalcogenides as an efficient electrode material in the photoelectrochemical devices, some work has been reported so far on the PEC behavior of MoS$_2$ and MoSe$_2$ single crystals grown by different techniques. The author therefore undertook the photoresponse study of MoS$_2$ and MoSe$_2$ in order to see the possibility of their use in a PEC solar cell. The conversion efficiency of the PEC solar cell prepared with MoS$_2$ and MoSe$_2$, as a photoelectrode was calculated.

10.3 SCOPE FOR FUTURE WORK

The author has the relief of satisfaction that undoubtedly efforts have been made by her in this direction and to a certain extent has achieved success, there are a considerable number of aspects remained untouched and deserves further investigations.

The resistivity measurements along the basal plane of the crystals were carried out up to a temperature of 473 K. In order that the energy gaps obtained from the resistivity measurements with the data obtained from the optical absorption studies, the experiments on basal plane resistivity should be taken in the higher temperature range i.e. from room temperature to about 1073 K.
The author feels that the dependence of carrier concentration and mobility upon temperature as well as requires to be studied at different temperatures and magnetic fields. This demands the detailed work on Hall effect measurements. This will enable one to understand the nature of charge carriers, their behavior and conduction mechanism in different temperature ranges.

The resistivity and TEP measurements under pressure have been measured along the basal plane of the crystals. Looking to the highly anisotropy character of these crystals it is very much desirable that these measurements be carried out in a direction normal to the basal plane of the crystals. Such studies will help us better to understand the anisotropic behavior of these layered materials under high pressure.

The study of PEC behavior of MoS$_2$ and MoSe$_2$ was an attempt to see the possibility of fabricating a PEC solar cell with this material. The results obtained suggest that for optimum performance MoS$_2$ and MoSe$_2$ crystals with absolutely plane faces should be used as photoelectrode in the photoelectrochemical solar cells. For obtaining better photoresponse the surfaces of the photoelectrode should be given a pretreatment to reduce the surface states as well as corrosion effect. The effects of surface treatments such as chemical etching, photoelectrochemical etching and dye layer applications can also be undertaken to improve the efficiency considerably.

Thin films of layered materials are preferred for practical solar energy conversion devices, for lubrication and for electrochemical energy storage.
The film characteristics required for each of these applications are different. The structural defects, impurities, size and orientation of the crystallites strongly influence the photoelectronic properties. In case of layered materials, due to high levels of recombinations at the edge planes (i.e. parallel to c-axis) it is essential that these planes be not exposed to the junction. All these work can form a guideline for the future PEC investigations of these materials.

Recently, various applications of MoS$_2$ and MoSe$_2$ have been reported. The MoS$_2$ are used as cathodic materials in lithium intercalation batteries, switching behaviour and conductivity measurements could be carried out in these specimens.

A lot of work has been reported in the field of crystal growth, physical and structural characterization of layered semiconducting compounds, revealing their unique and distinguished characteristics in comparison to those of normal semiconductors. However, comparatively very little work is reported in the direction of their applications utilizing their unique characteristics.

The author feels that attention should now be more focussed in this direction particularly on the preparation of good quality crystals of this class. Research on all these aspects will certainly add something to the existing knowledge on these important compounds.