CHAPTER 10

CONCLUSIONS AND FUTURE SCOPE FOR FURTHER RESEARCH

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10.1 Introduction

In this thesis the studies of growth, characterisation of $MoSe_xTe_{2-x}$ ($0 \leq x \leq 2$) single crystals and their uses in the fabrication of photoelectrochemical solar cells have been presented. Attempt has been made here to draw some important conclusions from the work reported in the thesis and also suggest scope for future work.

10.2 Conclusions

Single crystal growth of middle compounds of $MoSe_xTe_{2-x}$ ($0 \leq x \leq 2$) series is not reported till to-date. In the past, growth of the end compounds of the series $MoSe_xTe_{2-x}$, $0 \leq x \leq 2$, i.e. $MoSe_2$ and $MoTe_2$, has been reported by direct vapour transport and chemical vapour transport techniques using Br_2 or I_2 as transporting agents.

The lattice parameters 'a' and 'c' determined by X-ray studies show a linear variation with composition suggesting thereby a complete solubility of $MoSe_2$ in $MoTe_2$. Crystals possess the 2H

polytype structure. The microscopic examination of the crystals has revealed hexagonal spirals originating at screw dislocations. The observation of microstructures suggests that the crystals have been grown by two dimensional nucleation.

The electrical measurements made on the grown crystals indicate that the resistivity increases with the increasing selenium content in the series. In order to determine the type of charge carriers, their concentration and mobility, Hall effect measurements were made, which showed the crystals to be n-type materials. This was also confirmed by Seeback coefficient measurements.

The investigations on the $MoSe_xTe_{2-x}$ ($0 \leq x \leq 2$) were also carried out with a view to consider the possibility of using them in the fabrication of photoelectrochemical solar cells. The location of valence and conduction bandedges and Fermi level within the redox electrolyte suggest that the redox couple potentials within the bandgap, positive of -0.50 V and negative of + 0.9 V Vs SCE should be appropriate for

PEC cells based on $MoSe_xTe_{2-x}$ ($0 \leq x \leq 2$) single crystals. Flat-band potential measurements showed increasing trend in its value from selenides to tellurides of molybdenum. The spectral response studies were made to gain information regarding the behaviour of these electrodes. It is observed that the schottky barrier model can be applied and the electrodes obey the spectral dependence for this model. The direct band gap for the grown series was found to increase from 1.1 eV to 1.4 eV with increasing selenium content. Since iodide/iodine redox system was found to give good results, a variety of iodine concentrations were used to determine the effect of the redox electrolyte composition on the efficiency of $MoSe_xTe_{2-x}$ ($0 \leq x \leq 2$) photoelectrodes. The efficiency was found to decrease at higher concentrations of iodine due to increased light absorption by the solution.

It was observed that the properties of PEC cells depend on temperature and that there exists an optimum temperature at which power output (efficiency) of the cell reaches a maximum value. This optimum temperature for the operation of the cell with maximum

output was found to depend upon many factors such as the spectral response, conductivity of electrode, etc. The open circuit voltage was found to vary linearly with irradiation intensity, while the short circuit current varied linearly upto certain light intensities. A decrease in the conversion efficiency was observed with increasing light intensity due to decrease in fill factor. It is concluded that the solar to electrical conversion efficiency for $MoTe_2$ is not as high as that for $MoSe_2$. The PEC behaviour of mixed chalcogen crystals has been found to be similar to that of the pure phases.

The life time (τ) of charge carriers of $MoSe_xTe_{2-x}$ ($0 \leq x \leq 2$) single crystals was measured. It is observed that the life time (τ) decreases as the amount of tellurium in the series $MoSe_xTe_{2-x}$ is increased.

10.3 Scope for Future Work

In the family of transition metal dichalcogenides most of the compounds assume layer structure, where so many variations in stacking order

of the sandwitches may exist. Therefore, the phenomenon of polytypism can be studied in these crystals. It is an established fact that within the layer, the bonds are strong while between adjacent layers they are remarkably weak. As a consequence the crystals have facile basal cleavage. A detailed study of dislocations using transmission electron microscopy and weak beam technique may therefore be carried out.

Resistivity and Seeback coefficient observed at lower temperature are not reported in this thesis, hence their variation with composition (x) is worth considering in order to understand the nature of carriers, their behaviour and conduction mechanism at lower temperature. Study of resistivity with dislocation density will also be useful. Hall effect measurements at different temperatures for these compositions may also be studied on single crystals. to elucidate the conduction mechanism and mobility of charge carriers, which will supplement the resistivity and Seeback coefficient measurements.

The switching and lubricating properties