Chapter 7

Conclusions and scope of future work
7.1 CONCLUSIONS OF THE PRESENT INVESTIGATION

The present research work is centered on the growth, characterization and photoelectrochemical investigation of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals. All these compounds belong to transition metal dichalcogenides (TMDCs) family. The structural, electrical, optical and photoelectrochemical properties of all the compounds were investigated in detail in the present research work. The conclusions of various analytical investigations were briefed in the following section.

Chapter 1 comprises essential elemental information of tungsten, molybdenum and selenium. The vital aspects of literature survey were analyzed with respect to present research work. The parameters associated with direct vapour transport technique (DVT) were discussed in detail in the chapter 2. The analysis reveals that good quality crystal can be grown by the appropriate use of direct vapour transport technique. The Energy Dispersive analysis of X-rays (EDAX) has verified that elemental proportion found in the grown crystal is almost similar to that taken for the crystal growth process. EDAX analysis also confirms that grown crystals are pure and no impurity elements are present in the developed crystals.

Investigation of X ray diffraction (XRD) analysis disclose that all the compound possess hexagonal structure. Lattice parameters, volume of unit cell, density of unit cell and particle size distribution have been carried out and are reported in the present research work. The facial appearances of the grown crystal were analyzed using prominent optical microscope. The hexagonal spirals were observed in the microtopography of crystals faces in all the samples under investigation. The observation confirms that well known screw dislocation mechanism was in action during the crystals growth process.

The investigation of high temperature electrical resistivity of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals were discussed in detail in Chapter 4. The analysis of resistivity plots notify that the resistivity exponentially decreases with the temperature. The resistivity plots confirm
that all the samples are semiconductor. The electrical resistivity along c-axis is observed to be higher than that of along a-b axis. The observation confirms anisotropic nature of all the samples under investigation. The presence of weak van der Wall forces between crystal layers along c-axis and strong covalent bonding between the atoms along a-b axis results in an anisotropic behavior of the material. The anisotropic nature of the materials confirms that WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals have layered structure. The activation energy in the different temperature ranges were determined and have been reported in the same section. The variation of Thermo electric power with temperature was also analyzed for the sample of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals. The Seebeck coefficients are observed to be positive for all the samples. The observation indicates that all the samples are P type semiconductor. The positive values of Hall coefficient were found in the Hall Effect experiment. The results point out that all the samples are P type semiconductor and they contain holes as a majority charge carriers.

The optical response of the sample of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals were analyzed and discussed in detail in chapter 5. The direct and indirect band gaps were achieved using graphical analysis for all the samples under investigation. The absorbance, reflectance and transmittance were carried out and plotted against the photon energy of the incident radiations. The variation in extinction coefficient and refractive index were also analyzed and reported in the same section.

The photoelectrochemical solar cells were fabricated using sample of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals. The photo response of PEC solar cells were investigated using various electrolytes. The combination of 0.5M NaI + 0.025M I$_2$ + 0.5M Na$_2$SO$_4$ was found to be most appropriate electrolyte in the present investigation. The sample of W$_{0.9}$Se$_2$ shows highest efficiency among the three samples. The lowest resistivity and higher carrier density of the compound are responsible for the observed outcome. The trapping centers density and ideality factor were also carried out and are reported in the same section. The W$_{0.9}$Se$_2$ based PEC solar sell turn out be most ideal among the three solar cells.
7.2 SCOPE FOR THE FUTURE WORK

The author feels privilege to work in the sector of solar cell investigation. The single crystals of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ have been investigated in detail in the present research work. The efforts have been made to develop chip and efficient solar cell in the present investigation. There is a lot yet to be discovered in the field of solar energy conversion. The numbers of semiconductor compounds that can be develop and should be investigated for their solar cell application. The investigation of the present research work shows that all the grown compounds have optical band gap between 1.26eV to 1.4eV. Consequently efforts should be made to develop compounds which have optical band gap much close to maxima of the solar radiation.

With the help of direct vapour transport technique a good quality crystal can be developed. The problem of contamination inclusion in the grown crystals is successfully resolved by the direct vapour transport technique (DVT). Slow heating and cooling rate of furnace are the crucial aspect of DVT technique. By making proper use of DVT technique high quality crystal can be developed.

The efforts have been made to increase the efficiency of the PEC solar cell. The various reference electrode and number of electrolyte have been investigated to achieve higher efficiency in the PEC solar cell. Further investigation should be made to achieve best possible efficiency of PEC solar cells. The use of solid electrolyte in the PEC solar cell should be investigated in detail. Author feels that solid electrolyte may offer lot more advantage than the liquid electrolyte. The efficiency of the PEC solar cells is affected by the reflectivity of the semiconducting electrode, corrosion of the counter electrode, hole electron recombination rate, resistivity of the crystal samples and absorption losses in the electrolyte. The right combination of all these parameters may result in the best possible efficiency of the PEC solar cell.