PREFACE

“INVESTIGATIONS OF TMDCs AND USE IN SOLAR CELL”

Solar energy is the blessings of almighty to the mankind. Solar energy is an unlimited, renewable, pollution free and easily available source of energy. The surface of the earth attains approximately 6000 times the solar energy then our total energy demand. The energy demands of the present era increases quite swiftly due to improvement in a human standard of living and increase in human population. Thus the efficient, cheaper and commercially feasible solar energy conversion technology is the urgent requirement of the present era. In India intense solar radiation is found in almost all part of the country. We also have very vast non agricultural land like desert of Rajasthan and Kutch. Hence the well-organized solar energy conversion technology is very vital for countries like India. Solar cells are solid state electronic devices which can convert the solar energy directly into electrical energy. Injection of the solar radiation on the PV cells develops electron hole pairs that diffuse through the junction. This phenomenon produces the electric current in external circuit and hence produces electrical power.

On the other hand, there exist several disadvantages of the silicon based PV solar cells. The high production cost of the PV solar panel is the main hurdle for their commercial utilization. The toxic characteristic of PV solar cell is another disadvantage. The disadvantages of conventional PV solar cell and increasing demand of the energy ignite the search of the new solar energy conversion technology. The transition metal dichalcogenides (TMDCs) are group of materials which are found to be very promising with respect their solar energy conversion ability. The optical band gaps of these materials are found to be in the range of 1eV to 2 eV. The maximum of solar radiation falls in this region. The
absorption coefficient of these materials is found to be very high. TMDCs materials are also very useful in the field of optoelectronics, holographic recording coordination, electronic controls, infrared creation, detection, lubrication etc. The TMDCs acquire semiconducting property with explicit individuality of layered structure.

They form a coherent family of compound semiconductors. These layers are separated from each other by the week Van der Waals forces. These materials found to be highly stable against photo corrosion and photo decomposition due to d→d transitions. Hence the investigations of TMDCs are incredibly vital as it is useful in the multiple fields.

In the present research work TMDCs materials WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ have been investigated in detail. Direct vapour transport technique (DVT) have been utilized to grow single crystals of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$. The complexity of contamination inclusion in the grown crystal has been resolved effectively by the use of direct vapour transport technique (DVT). It has been found that this crystal growth method is more suitable for the growth of high purity & contamination free single crystals. The structural and elemental investigations have been carried out using standard techniques like Energy Dispersive Analysis of X-rays (EDAX), X-ray Diffraction (XRD). The optical investigation has been carried out using UV-VIS-IR absorption technique. The DVT grown crystals of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ have been utilized to construct the PEC solar cells. The characteristic efficiency of the TMDCs based PEC solar cells have been analyzed in detail in present investigation. Various combinations of electrolyte, reference electrode and semiconducting electrode have been analyzed to get a better response of the PEC solar cell. The different parameters like fill factor, maximum power and efficiency have been analyzed in detail.
The work carried out on the INVESTIGATIONS OF TMDCs AND USE IN SOLAR CELL has been presented in the form of seven chapters in this thesis. The methodical distribution of the work covered in all the chapters has been described below.

In chapter 1 the basic properties and application of TMDCs are discussed. The crucial elemental information of materials used in the present investigation is also covered in this section. The application and significance of individual element utilized in the present studies are disused in this chapter. The existing information on structural properties, electrical properties and optical properties of TMDCs are briefly reviewed in this chapter.

Chapter 2 comprises essential information about growth of WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals using direct vapour transport (DVT) technique. Different crystal growth techniques have been discussed briefly in chapter 2. The crucial parameters of direct vapour transport (DVT) technique have been described in this chapter. The various aspect of ampoule preparation and function of the two zone furnace have been explained in this section. The entire crystal growth process of TMDCs material has been discussed in detail in this section.

In the present investigation Energy Dispersive Analysis of X-rays (EDAX) technique has been utilized to verify the elemental proportion in the grown crystals. The fundamental aspects of EDAX technique and outcome of the experiments have been described in detail in the chapter 3. The investigations of structural properties of the grown crystals have been completed with the help of X-ray diffraction (XRD) technique. The essential features of X-ray diffraction (XRD) techniques and analysis of the results have been discussed in this chapter. The microstructural analysis of the DVT grown crystals have been carried out with the help of the powerful microscope. The fundamental information about the microscope and analysis of microtopography of crystal surfaces have been described in this section.
Chapter 4 includes essential information about electrical properties of all the samples under investigation. The electrical resistivity of $\text{WSe}_2$, $\text{W}_{0.9}\text{Se}_2$ and $\text{MoSe}_2$ single crystals have been carried out using two probe method. The resistivity parallel to C-axis and perpendicular to C-axis has been analyzed in this chapter. The graphical interpretation of resistivity plots and calculation of activation energy have been explained in detail. The anisotropic behaviour of all the samples under investigation has been discussed here. The investigations of thermo electric power of all the samples have been carried out and described in this chapter. The graphical interpretation of TEP plots and calculation of Fermi energy have been described in detail. The Hall Effect experiment was also carried out for all the samples under investigation. The vital parameters like charge carrier density, resistivity, hall coefficient and type of conductivity have been analyzed in this chapter. The different hall parameters have been calculated and the results are presented in this chapter along with the discussions.

The optical properties of grown single crystals of $\text{WSe}_2$, $\text{W}_{0.9}\text{Se}_2$ and $\text{MoSe}_2$ have been investigated in chapter 5. The UV-VIS-NIR spectrometer has been utilized to get absorption spectra of all the samples under investigation. The value of optical energy band gap ($E_g$) is calculated from the plots of $(\alpha h\nu)^x$ vs. $h\nu$ for all the samples. The two and three dimensional models for direct and indirect transitions of photo-generated carriers have been analyzed. The detail studies of optical absorption spectra have been described in this chapter. It is established that all the samples under examination acquire the direct as well as indirect band gap. Different optical parameters have been obtained using optical absorption spectra and analyzed in this chapter.
The chapter 6 accounts for the necessary preamble to PEC solar cells. Various types of solar cells have been described and discussed here. The advantages of PEC solar cells over its solid state counterpart have also been explained. This chapter also describes author’s attempt to fabricate PEC solar cells using WSe$_2$, W$_{0.9}$Se$_2$ and MoSe$_2$ single crystals. Various parameters of PEC solar cell like short circuit current, open circuit voltage, fill factor and efficiency have been analyzed here. The graphical analyses of experimental results have been discussed in this chapter.

The brief appraisal of the conclusions of all the analysis covered in above chapters is presented in Chapter 7. It deals with the conclusion established from the entire effort and scope for the future work.