Chapter 7
Final Remarks And Future Direction

This chapter summarizes the work done, presents the results and makes certain conclusions. It may be mentioned that some of the results corroborate the work done earlier by other research groups, as referred in chapters 3, 4, 5 and 6; but other results demand new explanations. In certain cases further pursuit is needed to give a definite conclusion and finally there are a few situations where the investigations can be extended to another level. However, all these do not come under the purview of the present study; but are mentioned in this chapter appropriately.

Electrical characterization of the metal – WSe_2 thin film contacts is the main objective of this thesis. In this context various barrier parameters of Schottky diodes and finally current transport mechanisms were studied in detail. Besides, structural, optical and electrical characterizations were made on thin WSe_2 films to assess the film parameters for their suitability required for device production.

7.1 Final Remarks

In this present study structural, optical and electrical properties of thin films and junctions of metal with semiconductors have been studied. The films of tungsten diselenide (WSe_2) with different thicknesses were used to prepare Schottky junctions with evaporated thin aluminum films. All the films as well junctions were prepared by vacuum evaporation technique (i.e. thermal evaporation technique for metal thin film and ē – beam evaporation technique for semiconductor thin film).

Considering the importance of TMDC materials of group *VIA* and *VIB* in various electronic applications as described in chapter 1, author has chosen the tungsten diselenide (WSe_2) in thin film form which is a member of this group for its structural, optical and electrical properties and its use in junction devices.

As WSe_2 is a compound semiconductor having melting point of 1200 °C, initial efforts were made to deposit device quality films using different techniques e.g. thermal evaporation, flash evaporation and ē - beam evaporation. It is concluded from the EDAX results that the ē - beam evaporation technique could yield in to relatively good quality thin films with only little deviation from the stoichiometry.

The deposited WSe_2 thin films of different thicknesses were then characterized for their structural and microscopic properties using XRD, ED, SEM and AFM. Structural studies by XRD and ED indicated the polycrystalline nature of the films. The data are in good agreement with JCPDS file with their respective code. The average grain sizes of deposited WSe_2 films were found to be 55 Å, 50Å and 100Å respectively for 1000Å, 1732Å and 3226Å thin film. It is further found that all the deposited films posses hexagonal structure and calculated lattice parameters are in good agreement with the reported values. From XRD spectra of WSe_2 films, the strain and dislocation density of the prepared films were calculated and these values were found to be decreasing with increase in film thickness. The topography of the surfaces of the prepared WSe_2 films were studied using the SEM micrographs for all three films. The films were found to be continuous on the glass substrates and the films deposited with higher thickness were fairly uniform and polycrystalline in nature. There were no macroscopic defects like void, pinhole, peeling or cracks. AFM photographs also show the structural improvement with film thickness.

Optical absorption study of deposited WSe_2 thin films were made in the wavelength range 200 - 3200 nm. It is revealed that the direct allowed transition of charges due to strong absorption has been found as a dominant carrier transition mechanism. The values of optical bandgap for all deposited thin films decrease with increase in thickness of thin film. Further, the value of refractive index is also calculated and it is found to be decreasing with increase in film thickness. Moreover, extinction coefficient and dielectric constant are also obtained.

Electrical properties of ē - beam evaporated WSe_2 thin films have been studied using two methods viz. temperature dependent Hall effect by van der Pauw geometry and thermoelectric power measurement with fixed temperature gradient. Room temperature I – V characteristics show the ohmic nature of silver with all three deposited thin films. The sign of Hall coefficient is found to be positive and it remains the same throughout the measurement in the temperature range 300K to 70K which confirms the p type nature of WSe_2 thin films. The positive sign of Seebeck coefficient also gives the support to the Hall effect results. The increasing nature of resistivity with fall in temperature and increasing nature of Seebeck coefficient with rise in temperature show the typical nature of semiconductor. Using the Hall effect and thermoelectric power measurement mobility, carrier concentration, effective density of states, Fermi energy, activation energy, effective mass of charge carrier have been obtained. Finally, it is found that the thickness dependent structural changes are reflected in electrical properties of deposited films. However, this study could not be extended for large variation of film thickness due to limitations of ē - beam evaporation technique.

Looking toward the higher value of mobility and electrical properties of thin films, it is then decided to fabricate the thin film Schottky diode by evaporating aluminum film on pre deposited WSe_2 thin films on glass substrate. I – V characteristics of these diodes have been observed in the temperature range 310K - 100K. From the detailed and careful analysis of observed I – V characteristics following conclusions have been drawn.

All the SB interfaces exhibit fairly good rectification properties. The values of parameters like barrier height, flat band barrier height and ideality factor for each diode were determined over a wide range of temperatures. Other important barrier parameters e.g. 'α', 'E_{a}', 'A^{*}', 'A^{**}', 'σ_{0}', 'σ_{s}', 'ρ_{2}' and 'ρ_{3}', percentage of inhomegenitites etc. were also determined for diode.

It has been observed that the ideality factor increases with decrease in temperature for all three rectifiers. On the other hand, the zero-bias barrier height decreases with decrease in temperature.

The ideality factor is simply a manifestation of the barrier uniformity and it increases for an inhomogeneous barrier. An apparent increase in ideality factor and decrease in BH at low temperature are possibly caused by inhomogeneities of thickness and composition of the layer, non-uniformity of the interfacial charges or the presence of any thin insulating layer between the metal and the semiconductor. Since the current transport across the MS interface is a temperature-activated process, at low temperature the current will be dominated by the current through the patches of low barrier height. Therefore at low temperature, electrons are able to overcome the lower barriers, and hence current transport will be dominated by current flowing through the patches of lower BH and result into a larger ideality factor. As the temperature increases, more and more electrons have sufficient energy to overcome the higher barriers. As a result both BH and n are strongly dependent on temperature.

The value of mean barrier height for aluminum has been found to be close to their Schottky model values of $0.92eV$. This suggests that there is not any sandwiching oxide layer formation across the interface. In other words the faces of the metal and the semiconductor make direct and intimate contact and this happens mainly because WSe_2 surfaces are smooth and inert.

We can also see that the percentage of inhomogenity in case of Al/pWSe$_2$(1732Å) diode and Al/pWSe$_2$(3226Å) diode is around to be 7.0% which is very small compared to the Schottky diode prepared using DVT grown single crystal and this indicates the good quality of thin film Schottky diodes. The calculated Richardson constant and modified Richardson constant are found to be in good agreements with reported values.

7.2 Future Direction

The main aim of present thesis is to investigate various properties of WSe_2 thin films and its application as a thin film Schottky diode. The notable investigations on thickness dependent properties of WSe_2 thin films grown successfully by ē - beam evaporation technique and that on Schottky barrier devices have been chapterized in the present thesis. However, the outcome of the present research efforts has opened new directions of further studies in future. Following is a brief note on important outcome which leads to scope for future work.

- Since ē - beam evaporation technique is well known for depositing a good quality and pure thin films, it is too difficult to deposit on large area substrate uniformly with controlled rate of deposition.
- To achieve higher thickness of the film of a compound semiconductor is probably a challenging task in the case of ē - beam evaporation technique.
- To reduce and avoid the above mentioned limitations, one can use other deposition techniques like RF sputtering, Magnetron sputtering, chemical vapour deposition e.g. chemical bath deposition, electro-deposition etc. to deposit on large scale substrates with higher thicknesses.
- In present investigation various properties of deposited thin films and devices were examined as an effect of film thickness successfully. It will be investigated to study them with higher thickness and also study the effect of substrate temperature variation on it.

- Prepared Schottky diodes have been characterized with $I - V - T$ method to evaluate their barrier parameter using thermionic model with assumption of Gaussian distribution of barrier height at the junction of devices. However 1st order Gaussian distribution has been applied to estimate the barrier parameters of prepared diodes. One can apply at-least 2nd order Gaussian distribution to evaluate the barrier parameters.

- Capacitance - Voltage method, which is again an important method to evaluate the barrier parameter, can be used for such devices in wide range of temperature.

- In this work $p$$WSe_2$ thin film Schottky junctions with aluminum thin film are studied. As this system of metal-semiconductor is less studied in thin film form, it will be further interested to study the effect of metal work function on terminal properties of Schottky barrier devices by depositing different metals on WSe_2 thin films.

- Also $p$$WSe_2$-$n$$MoSe_2$ thin film heterostructure and different metal film based MESFETs and MOSFETs as well as a thin film solar cell are interested and imported devices to be explored.

- Looking towards the bright future of nano technology, one can study the nano phase of WSe_2 and the results on nano-Schottky devices can be fully analyzed in light of the change in properties by acquiring nano phase.