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TEMPERATURE DEPENDENT TRANSPORT AND BARRIER PROPERTIES OF DVT GROWN WSe_2CRYSTALS AND SCHOTTKY DEVICES

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ABSTRACT

Single crystals of Tungsten diselenide (WSe_2) have been grown using direct vapour transport technique (DVT). Measurements of thermoelectric power in temperature range 300 – 673K confirms that WSe_2 possess a p-type conductivity. The Ohmic cotacts were developed using Ag-paste and the Hall effect measurements have been carried out in the temperature range 10 - 300 K to determine some essential parameters such as the hole mobility (μ_h), carrier concentration (*n*), Hall coefficient (R_H). The DVT grown crystals were also used to fabricate Schottky junction with thermally evaporated Indium contacts and the diode behavior was characterized over temperature in range 200 – 310K. The thermoelectric and electrical properties variation with temperature and temperature variation of diode parameters are discussed.

Key words: *TMDC crystals, Thermoelectric power, Hall effect, In/WSe_2 Schottky diode.*

INTRODUCTION

TMDC have a general formula MX_2, where *M* is usually a transition metal atom from group of *IVB, VB, VIB* of the periodic table and *X* is one of atoms from sulfur, selenium, or tellurium. The layered structure of TMDC can be regarded as stacking of two-dimensional *X-M-X* sandwiches. The bonding within each sandwiched layer is covalent, while the bonding between them is weak van der Waals type. The crystal structures of the layered TMDC are usually described as belonging to *1T, 2H, 3R,* $4H_2$, $4H_b$, *6R* phases [1, 2]. TMDCs have been used for many years as solid state lubricants [3], photovoltaic/photocatalytic solar energy converters [4], Schottky and liquid junction solar cells [5, 6], catalysts in many industrial applications and in secondary batteries etc. Increasing potential for use of transition metal dichalcogenide materials in Schottky devices, photovoltaic and photoelectrochemical (PEC) solar cells is because of their inherent resistive nature to photo corrosion. They have also found use in Schottky barrier devices, photovoltaic and photoelectrochemical solar cells as a flexible electronic material in recent years [7].

Looking to potential for such diverse applications of TMDCs, we have chosen to study WSe_2 semi-conducting materials of group *VI*. Successful growth of single crystals of WSe_2 has been reported earlier [8] for the measurements of photoelectric and electrical properties. Here we report the electrical transport properties of WSe_2 crystals evaluated from the high temperature thermoelectric power and Hall effect measurements. These investigations can yield valuable information about their electronic properties. The Schottky diode, fabricated on WSe_2 single crystal with Indium thin films has also been characterized to estimate the Schottky barrier parameters in the temperature range 200 – 310K.

EXPERIMENTAL

The single crystals of WSe_2 were grown by direct vapour transport technique using a two zone horizontal furnace. The crystals grown were found to be in the form of thin platelets having opaque appearance with perfectly shining surfaces. These grown crystals were first characterized by thermoelectric power measurement in 300 – 673K temperature range using a setup developed for this purposes. These crystals were also characterized using Hall effect measurement setup (Lake*s*hore - 7504) in temperature range 10 – 300K to estimate the carrier concentration, hole mobility, Hall coefficient and resistivity.

Indium thin film of 500Å thickness was deposited through a thin metal mask having area around of 0.186 cm^2 on well cleaned WSe_2 single crystals using vacuum evaporation technique with pressure better than 10^{-5} torr. Low temperature I – V characteristic of Schottky diode was measured using Keithley 2400 SMU and a liquid nitrogen cryostat in temperature range 200 – 310K.

RESULTS AND DISCUSSIONS

Thermoelectric Power measurement

The variation of thermoelectric power '*S*' for WSe_2 crystals as a function of inverse temperature in the range of 300 K to 673 K is shown in Fig. 1. It is observed that TEP increases with temperature, indicating the typical semiconducting behavior of the WSe_2. Moreover, the sign of TEP is found to be positive for WSe_2 indicating that grown crystals possess *p*- type semiconducting character.

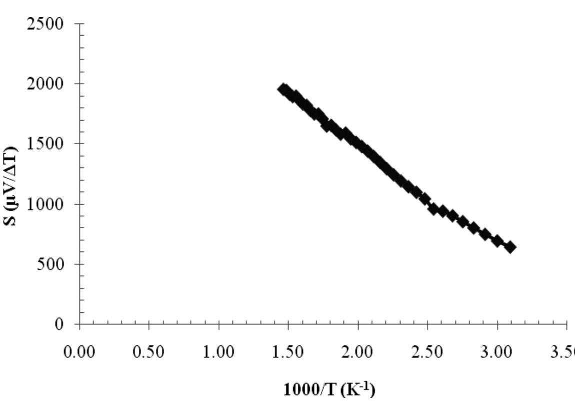

Fig. 1 Thermoelectric power variation with inverse of temperature for DVT grown WSe_2 crystals.

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To analyze the temperature dependence of the thermoelectric power of a *p*-type semiconductor, the expression given by Mohanchandra and Uchil [9] and Goldsmid [10] given below has been used:

$$S = -\frac{k}{e}\left[A + \frac{E_F}{kT}\right] \qquad (1)$$

here k is the Boltzmann constant, e is the electronic charge, A the constant determined by the dominant scattering process and E_F is the separation of the Fermi level from the top of the valance band. Table - 1 shows the calculated thermoelectric parameters from these measurements.

Table – 1 Parameters from TEP measurement on DVT grown WSe_2 crystals.

Majority carrier conductivity Type	**Fermi energy E_F (eV)**	**Effective Density of State N (m^{-3})**	**Effective Mass M_h* (Kg)**	**m_h^*/m_h**	**Scattering Parameter s**
p - Type	0.0521	6.683×10^{24}	7.600×10^{-31}	0.83	2.48

Low Temperature Hall Effect

The Ohmic nature of contacts prepared for van der Pauw geometry in case of various pairs of contacts at 300 K is shown in the Fig. 2. It is seen from here that Ag-paste contacts exhibit good Ohmic nature for both polarity in a large current range. The average van der Pauw factor for a set of four contacts is found to be 0.7. This deviation from ideal requirement of unity probably originates from the anisotropic nature of WSe_2 and not from other conditions required for measurements using van der Pauw technique.

The resistivity (ρ), Hall coefficient (R_H), carrier density (n) and mobility (μ) of WSe_2 single crystals were calculated from the measured I – V values under magnetic field of 3kG using the standard formula over the temperature range of 10K to 300K and the results are tabulated in Table - 2.

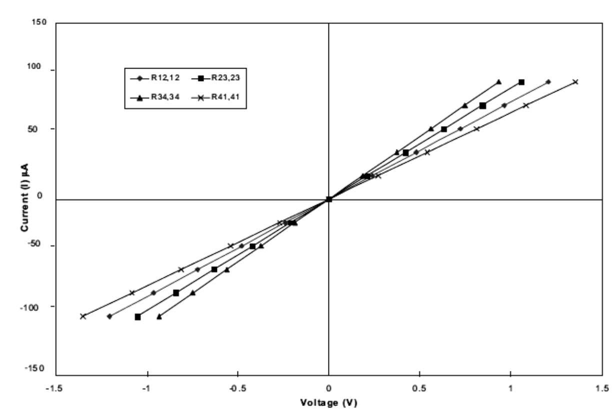

Fig. 2 I - V Characteristics of the Pair of ohmic contacts (12,12), (23,23), (34,34) and (41,41) prepared by Ag paste (Elteck-1228) on DVT grown WSe_2 crystals.

Figs. 3 and 4 show the variation of Resistivity, Hall Coefficient and Carrier concentration with respect to inverse of temperature. From these figures it is clearly seen that resistivity is decreasing monotonically with increasing temperature above around 90K which confirms the semiconducting nature of WSe_2 crystals. The anomalous semiconducting behavior below 90K is reflected in mobility also and seems to be related to changes in the carrier scattering mechanism. However carrier concentration is increasing with increasing temperature.

Table - 2: Hall parameters of DVT grown WSe_2 crystals.

Temp. T(K)	**Resistivity ρ (Ω.cm)**	**Carrier Density n (cm^{-3})**	**Hall coefficient R_H (cm^3/C)**	**Mobility μ(cm^2/Vs)**
300	2.797	1.032×10^{18}	6.049	2.141
290	2.918	$6.554\times10P^{17}$	9.524	3.266
270	3.077	2.924×10^{18}	2.135	0.695
250	3.309	5.443×10^{17}	11.47	3.464
230	3.639	1.297×10^{17}	48.12	13.22
210	4.259	8.187×10^{16}	76.25	17.91
190	5.101	5.410×10^{16}	115.4	22.65
170	6.557	9.967×10^{16}	62.63	9.632
150	8.913	2.226×10^{16}	280.5	31.46
130	13.02	9.088×10^{15}	686.9	50.85
110	18.447	9.215×10^{15}	677.4	2.852
90	19.734	1.147×10^{15}	5444	113.7
70	1.624	1.085×10^{15}	5754	185.7×10^2
50	1461	9.81×10^{13}	63630	183.8
30	1754	5.324×10^{12}	1173×10^3	67.58
10	5938	2.363×10^{11}	26420×10^3	3205×10^2

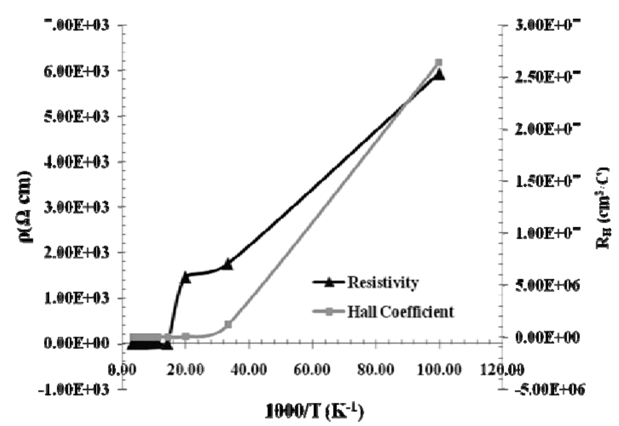

Fig. 3: R_H and ρ of *p* - WSe_2 Crystals as a function of 1000/T.

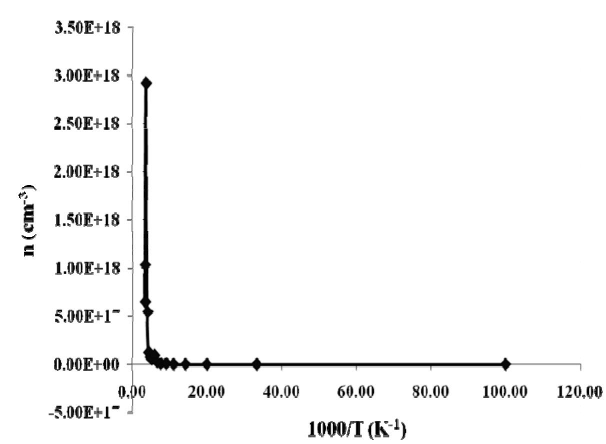

Fig. 4: Carrier concentration vs. 1000/T for *p*-WSe_2 Crystals.

I – V characteristics of In/p-WSe_2 Schottky diode

The nature of the I-V characteristics of one of the In/$p$$WSe_2$ Schottky diodes at different temperatures is shown in Fig. 5.

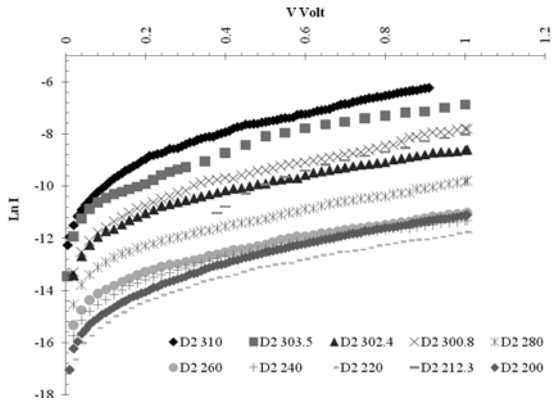

Fig. 5 I-V Characteristic of In/$p$$WSe_2$ Schottky diode at different temperatures.

Based on thermionic emission theory, the current–voltage characteristic of a metal-semiconductor contact is given by [11]

$$I = I_0 \exp\left[\frac{q\left(V - IR_s\right)}{\eta kT}\right]\left[1 - \exp\left(\frac{-q\left(V - IR_s\right)}{kT}\right)\right] \quad (2)$$

where I_0 is the saturation current given by,

$$I_0 = AA^*T^2 \exp\left[\frac{q\phi_{b0}}{kT}\right] \quad (3)$$

Here symbols have their usual meaning and A^* is the Richardson constant which is equal to 27.6 $Acm^{-2}K^{-2}$ for p-type WSe_2 [12]. From Eq. (2), ideality factor η and zero bias barrier height (Φ_{b0}) can be calculated using standard relationship. The flat band barrier height can also be calculated using the following equation,

$$\phi_{bf} = \eta\phi_{b0} - \left(\eta - 1\right)\frac{kT}{q}\ln\left[\frac{N_V}{N_A}\right] \quad (4)$$

where N_v and N_A $(=n)$ are effective density of states and carrier concentration. The experimental values of η, Φ_{b0} and Φ_{bf} were determined from intercept and slope of the forward-bias ln I vs V plot (Fig. 5) at each temperature. It is found that the value of η increased and the value of Φ_{b0} decreased with decrease in temperature (Fig. 6).

Since current transport across the MS interface is a temperature activated process, electrons at low temperatures are able to surmount the lower barriers and therefore current transport will be dominated by current flowing through patches of the lower Schottky barrier heights (SBH) that results in larger ideality factor [13]. Series resistance of diode is seen to be contributing in deterioration in the nature of I – V characteristics at higher voltages and the variation of series resistance is shown in Fig. 7.

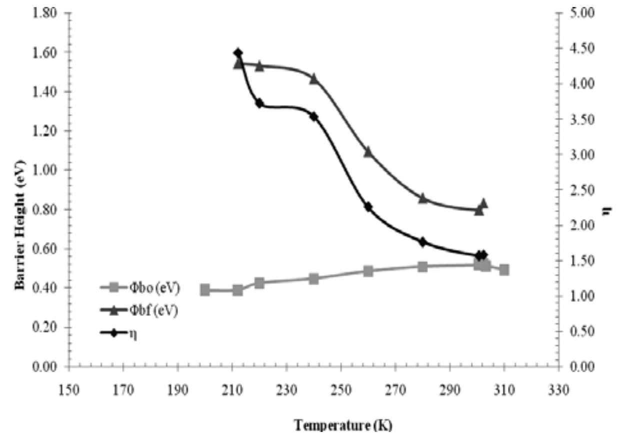

Fig. 6 Variation of Φ_{b0}, Φ_{bf} and η with temperature for In/$p$$WSe_2$ Schottky diode at different temperatures.

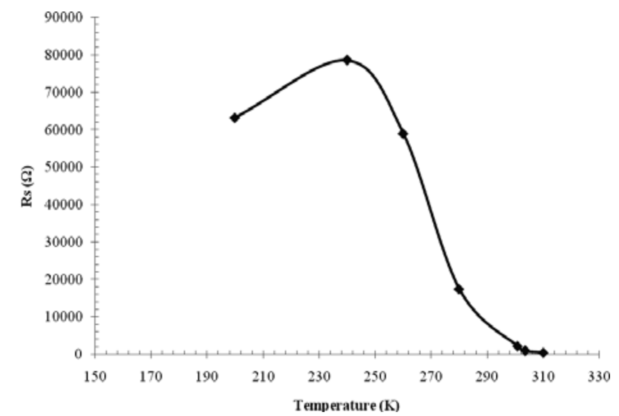

Fig. 7 Variation of Series resistance for In/$p$$WSe_2$ Schottky diode at different temperatures.

CONCLUSION

The single crystals of WSe_2 grown by a direct vapour transport technique are found to have a p- type (WSe_2) semiconducting nature. The value of scattering parameter is nearly ≈ 2.48 which shows that the defect scattering dominates the charge transport mechanism in the grown crystals. The value of effective density of states is found to be around 6.68×10^{24} m^{-3}. The effective mass of charge carriers m_h^* was calculated and is found to be around 7.6×10^{-31} Kg. All these estimated parameters are in good agreement with the reported values in the literature [14-17].

The sign of Hall coefficient remains positive in the entire range of measurement temperature, indicating the conductivity type of the crystals as p-type and it is in agreement with the TEP measurements. This again shows that the quality of ohmic contacts made for present investigations is good and stable throughout the range of reported measurements. The conductivity of the sample decreases with the temperature and thus again confirms the semiconducting nature of the grown WSe_2 crystals. The measured carrier concentration at room temperature is 1.032×10^{18} cm^{-3}. This is in agreement with the reported value of 3.5×10^{18} cm^{-3} [18].

In/$p$$WSe_2$ Schottky diodes have been fabricated and studied in the temperature range of 200 - 300 K for their I-V characteristics. The zero bias barrier height decreases while the ideality factor increases with temperature. The increment in series resistance with decreasing temperature also exhibits a semiconducting nature of DVT grown crystals as contacts are seen to be Ohmic.

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