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Study of Electrical Resistivity and Mobility of Single Crystals of W0.85Se2 Grown By DVT Method

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ABSTRACT

The photo-voltaic criteria established by solar cell base materials like WSe_2. Single crystals of $W_{0.85}Se_2$ belonging to transition metal dichalcogenides MX_2 group are synthesized in the laboratory. Since the crystals are grown by Direct Vapor Transport (DVT) technique. The electrical transport properties of $W_{0.85}Se_2$ single crystal are studied and resistivity through Van der Pauw method in the high temperature range (313K–388K) is obtained. Employing the Hall Effect measurements, Hall coefficient, mobility as well as carrier concentration have been studied. The Van der Pauw technique is also used to evaluate the type, mobility and carrier concentration of $W_{0.85}Se_2$ single crystals.
Keywords: Temperature, Decompose, Carrier Concentration, Resistivity

I. INTRODUCTION

The recent photo electrochemical studies on the transition metal dichalcogenides, $W_{0.85}Se_2$ single crystals have emerged as the most efficient photo electrode materials used in the photo electrochemical solar cells. Among the layered compound group VI transition metal dichalcogenides, WSe_2 is the most promising semiconducting material for the photo electrochemical (PEC) conversion of solar energy to electricity, because of its high absorption coefficient in the visible and near infrared [1] and its excellent output stability as photo electrodes in polyiodide electrolytes [2,3]. A large number of investigators [3] have therefore focused their attention on the PEC studies of WSe_2. However, very little work appears to be done on off-stoichiometric crystals of Tungsten diselenide. The author has therefore decided to concentrate his attention on off-stoichiometric $W_{1-x}Se_2$ single crystals. Since these materials exhibit semiconducting behavior, it is worth studying them from the point of view of transport properties. It is obvious that these properties are of primary importance in the evaluation of these semiconducting materials for device fabrication. Since the material of $W_{0.85}Se_2$ possesses a semiconducting nature, the author decided to study its transport properties like the resistivity (μ), Hall coefficient (R_H), as well as carrier concentration (n).

II. METHODOLOGY

Depending upon the phenomena involved, the vapour phase method is classified in the following two categories: (i) Chemical vapour transport and (ii) Direct vapour transport. Single crystals of $W_{0.85}Se_2$ have been grown using a direct vapour transport technique. A stoichiometric mixture of 99.999% pure tungsten powder and 99.95% pure selenium powder were sealed under a pressure of 10^{-5}Torr in 2.5 cm bore x24 cm long high quality fused quartz ampoules. The sealed ampoule containing the mixture was then introduced into a two zone furnace at a constant-reaction temperature to obtain the charge of $W_{0.85}Se_2$. The charge so prepared was rigorously shaken to ensure proper mixing of the constituents and kept in the furnace under appropriate conditions to obtain single crystals of $W_{0.85}Se_2$. The growth conditions used for the synthesis are given in Table 1 and 2. The resulting crystals from the growth were black opaque and plate like with c-axis normal of the plates.

Table 1. Growth Parameters used to Synthesis Single crystals of $W_{0.85}Se_2$

Material	**Reaction**	**Growth**	**Growth Time**	**Crystal Size** (maximum)	**Appearance**
Growth Parameters	**Temperature**	**Temperature**			
$W_{0.85}Se_2$	1073 K	1248 K	212 hrs	7mmX6 mmX 0.2 mm	Black Opaque

Table 2. STRUCTURAL DATA OF $W_{0.85}Se_2$

Material	Lattice Parameters	
	a	c
$W_{o.85}Se_2$	12.975 $\pm$ 0.01	3.291 $\pm$ 0.001

Experimental Techniques

The resistivity measurements perpendicular to c-axis (i.e. along the basal plane) can be investigated using following techniques: (i)Van der Pauw Method and (ii) Four Probe Resistivity Method. The room temperature resistivity measurements were made using Van der Pauw method. The resistivity of $W_{o.85}Se_2$ single crystals can be measured at different temperatures in the temperature range (313K -388K) by a four probe method. The high temperature resistivity measurements were evaluated using the Four Probe Method. The four probe set up (Scientific Equipments, Roorkee, India) consists of probe arrangement, oven, constant current source, milliammeter and electronic voltmeter. Large size crystals having proper shape were used for the study of variation of resistivity with temperature using the four probe method.

III. RESULTS AND DISCUSSION

3.1 Resistivity Along the basal plane by van der Pauw method

The room temperature resistivity of $W_{0.85}Se_2$ single crystals, perpendicular to c - axis (i.e. along the basal plane) was investigated using van der Pauw method. The results of such measurements for representative samples are given in Table 3. Using the values of R_1 and R_2, resistivity can be calculated. The basal plane resistivity for $W_{0.85}Se_2$ crystals were evaluated and are reproduced in Table 6. From Table 3, average R_1 = 3.96 Ω and R_2 = 6.54 Ω.

Table: 3 Measurement of Resistivity through Vander Pauw Method.
Sample: $W_{0.85}Se_{2,}$ Thickness t = 0.004 cm, Length ℓ= 0.7cm Breadth b= 0.5cm

Current I_{AB} mA	**Voltage V_{DC} mV**	**Resistance R_1 Ω**	**Current I_{BC} mA**	**Voltage V_{AB} mV**	**Resistance R_2 Ω**
0.5	1.62	3.24	0.5	2.5	5.0
1.0	3.71	3.71	1.0	6.1	6.1
1.5	6.07	4.04	1.5	10.01	6.73
2.0	8.37	4.18	2.0	13.3	6.65
2.5	10.36	4.14	2.5	17.2	6.88
3.0	11.36	3.78	3.0	21.0	7.0
3.5	14.70	4.20	3.5	24.4	6.97
4.0	17.60	4.40	4.0	28.2	7.05

3.2. High Temperature Resistivity Measurement Perpendicular to c-axis

The high temperature resistivity measurement perpendicular to c-axis i.e. along the basal plane was carried out on single crystals of $W_{0.85}Se_2$ using the four probe technique as described earlier. Table 4 show the variation of resistivity with temperature (313K - 388K) for representative samples of $W_{o.85}Se_2$.

Table 4. Result of High Temperature Resistivity Measurement

Sample: $\mathbf{W_{0.85}}Se_2$ thickness t=0.004cm length ℓ=0.5cm breadth b=0.3cm

Temp (°C)	Temp T K	$\frac{1}{T}$ x 10^{-3} (k^{-1})	Resistance R k Ω	Resistivity $\rho = \frac{Rbt}{\ell}$ Ω cm	log ρ
40	313	3.19	64.4	154.56	2.18
45	318	3.14	58.3	139.92	2.143
50	323	3.09	57.8	138.72	2.142
55	328	3.04	55.4	132.96	2.12
60	333	3.00	53.7	128.88	2.11
65	338	2.95	47.7	114.48	2.05
70	343	2.91	44.3	106.32	2.05
75	348	2.87	40.2	96.48	1.98
80	353	2.83	39.4	94.56	1.97
85	358	2.79	34.6	83.04	1.91
90	363	2.75	28.5	68.40	1.83
95	368	2.71	27.30	65.52	1.81
100	373	2.68	25.60	61.44	1.78
105	378	2.64	22.10	53.04	1.72
110	383	2.61	19.10	45.84	1.66
115	388	2.57	18.00	43.20	1.63

3.3 Hall effect measurements

A modification of Van der Pauw technique has been used to evaluate the type, mobility (μ) and carrier concentration (n). The phenomenon in which the production of voltage difference across an electrical conductor transverse to and electric current in a conductor placed in a magnetic field perpendicular to the current is know as hall effect. Hall Effect measurement is the only tool to provide basic electrical parameter of material. The sample $W_{0.85}Se_2$, for this measurement is kept in known magnetic field produced by an electromagnet (Type EMPS-5 Omega Electronics, Jaipur, India). This magnetic field modifies the path of electrons producing the Hall voltage. By knowing the values of difference in resistance (△R), magnetic field (△B) and the thickness of the sample t, the mobility of carriers was evaluated using the following equation

$$\mu_H = \frac{t\Delta R}{\Delta B \rho} \qquad (1)$$

Where ρ is the room temperature resistivity of the samples. The Hall coefficient (R_H) and carrier concentration (n) were calculated using the following formula

$$R_H = \mu_H \times \rho \qquad (2)$$

$$n = \frac{1}{R_H e} \qquad (3)$$

From the sign of Hall coefficient, the nature of the charge carriers in the grown samples could be ascertained. The calculated values of R_H and carrier concentration (n) for each case are represented in Table 6. The result obtained from Hall Effect Measurement for sample is given in Table 5.

Table 5. Result of Hall Effect Measurement

Sample: $W_{0.85}Se_2$ Thickness t = 0.004 cm. Constant current I= 2 mA

Magnetizing Current I Amp	Magnetic Field B K.Gauss	Hall Voltage mV	Resistance R = V/I Ω	△ R	△ B	Hall Coefficient R_H Cm³/coul	Mobility U cm²/V.sec	Carrier Concentration n cm³
0.5	2.58	-10.05	5.025	0.25	2.26	44.24	484.02	1.41 x 10E+17
1.0	4.84	-9.55	4.775	0.04	1.89	8.46	92.56	7.38 x 10E+17
1.5	6.73	-9.47	4.735	0.035	1.55	9.032	98.81	6.91 x 10E+17
2.0	8.28	-9.40	4.700	0.045	1.24	14.51	158.75	4.30 x 10E+17
2.5	9.52	-9.31	4.655	0.055	0.92	23.91	261.59	2.61 x 10E+17
3.0	10.44	-9.22	4.610	0.025	0.75	13.33	145.84	4.68 x 10E+17
3.5	11.19	-9.17	4.585	0.04	0.52	30.76	336.54	2.03 x 10E+17
4.0	11.71	-9.09	4.545	---	--	---	---	----

Table:6 Result Of Measurement on off-stoichiometric Crystals of $W_{0.85}Se_2$

Sample Examined	Resistivity ρ Ω.Cm	Hall coefficient R_H Cm^3/coul	Mobility μ cm^2/V.sec	Carrier Concentration n cm^{-3}
$W_{0.85}Se_2$	0.0914	13.86	151.51	5.17×10^{17} (n)

IV. RESULTS AND DISCUSSION

The variation of resistivity along the basal plane with temperature clearly brings out the classical semiconducting nature of $W_{O.85}Se_2$ single crystals. Whereas the negative values of Hall coefficient for W0.85Se2 reveal their n-type character. Hall Effect measurements shown in respective tables. Following are the main results:

(1) The resistivity measurements point out that the samples of $W_{0.85}Se_2$ indicate a classical semi-conducting behavior.

(2) The off-stoichiometric crystals of tungsten diselenide show a semiconducting behavior in the temperature range 313K to 388K.

(3) The positive values of Hall coefficients for $W_{o.85}Se_2$ confirm that they are n-type semiconductors.

V. CONCLUSION

The electrical transport property measurements are carried out on $W_{0.85}Se_2$ single crystals. The experiments may be carried out on their photo electrochemical characterization. This can be done by preparing liquid junction Solar cells with them. The suitability of cells so fabricated should be decided in different electrolytes. The Photo electrochemical studies will clearly indicate the effect of non-stoichiometry on the photo electrochemical performance of WSe2 solar cells.

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VII. REFERENCES

[1]. Buckley, H.F., Crystal growth, John Wiley & Sons, New York, 1951.

[2]. Lawson, W.D. & Nielson, S., Preparation of single crystals, Butter worths Scientific publ. London, 1958.

[3]. Lawson, W.D., Nielson, S. & Gilman, J.J. The Art and Science of Growing Crystals, John Wiley & Sons, New York, London, 1963.

[4]. White, E.A.D., Brit. J. Appl. Phys., 1970, 25, 151

[5]. Laudise, P.A., The Growth of Single Crystals, Prentice Hall Inc., New Jersey, 1970.

[6]. Perker, R. K., Solid State Physics, 1970, 25, 151

[7]. Mullin, J.W. Crystallization, Butterworths Scientific Publication, London 2nd Edition,1972.