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ELECTRICAL TRANSPORT PROPERTIES OF TUNGSTEN DITELLURIDE (WTe_2) CRYSTALS

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ABSTRACT

Tungsten Ditelluride (WTe_2) crystals having a layer structure grown by chemical vapour transport technique (CVT) using iodine as transporting agent are studied here. The electrical resistivity and thermoelectric power (TEP) of these crystals were carried out within the range 313K to 573K. The crystals were found to exhibit semiconducting nature in this range. The activation energy, Seebeck coefficient and scattering parameters were calculated for these crystals. The Hall coefficient, carrier concentration and Hall mobility were determined from Hall Effect measurements at room temperature. Also the measurement of Thermal conductivity and Electrical conductivity of WTe_2 crystals along the chain axis were carried out. The implications of the results have been discussed.

Key worlds : *Tungsten Ditelluride, thermoelectric power, Seebeck co-efficient, scattering parameter, thermal conductivity, electrical conductivity.*

INTRODUCTION

W and Te are the members of groups VIB and VIA respectively, which possesses layered structure. Tungsten Ditelluride constitutes a well defined family of compounds which crystallize in a layer type structure. The layered tungsten dichalcogenides also exhibits superconducting behavior when intercalated with alkali. The crystal structure of WTe_2 is orthorhombic with space group $P_{nm}21$ having lattice parameters a=3.38Å, b=6.27Å and c=14.16Å. The study of electrical properties of the layered compounds of the group IV-VI has aroused a widespread interest and attention of the material scientists all over the world during the last few decades [1-8]. Most of the semiconductor applications are governed by the electrical properties of the materials. Hence, electrical properties like resistivity, Hall coefficient, thermoelectric power, thermal conductivity and electrical conductivity along the chain axis were carried out on the WTe2 crystals. The study of thermo electric power provides an independent way to determine the charge carrier sign, density and position of Fermi level in semiconductors.

EXPERIMENTAL

Crystals of Tungsten Ditelluride (WTe_2) grown by [9] chemical vapour transport method using iodine as the transporting agent are studied here. In this report we present results on electrical resistivity and thermoelectric power measured in temperature range 313K to 573K and also on hall parameters, electrical conductivity and thermal conductivity[3,5].

RESISTIVITY MEASUREMENTS

In the present study, resistivity has been measured perpendicular to *c*-axis (along the chain axis).

Two- probe method and four- probe method are used for resistivity measurement.

TWO-PROBE METHOD

In the present study resistance has been measured along the cleavage plane with the help of multimeter (model 2700, Make: KEITHLEY). The measurements were carried out in the temperature range from 313K to 573K at an interval of 5K. The resistivity (ρ) of the samples was calculated by using the formula

$$\rho = RA/l \qquad (1)$$

Where A is the cross sectional area of the specimen in the direction of measurement, R is the resistance of the specimen and l is the length of specimen.

From the slopes of log ρ Vs 1000/T plots the values of activation energies were calculated using the formula,

$$E_a = 2.303 X k_B X 10^3 X slope (eV) \qquad (2)$$

Where $k_B = 8.602 X 10^{-5}$ eV/K

FOUR-PROBE METHOD

Electrical resistivity measurements along chain axis of WTe_2 single crystals were performed by four- probe method. Measurements were performed in the temperature range from 303K to 483K using the set up made in our laboratory. Expressions for resistivity and activation energy are same as two-probe method.

MEASUREMENT OF HALL PARAMETERS

Hall Effect measurement was performed along the cleavage plane of crystals of WTe_2 in order to determine the type of conductivity, mobility and carrier concentration. Ohmic nature of the contacts taken (by silver conducting adhesive) for these measurement was confirmed by I-V characteristics measurement using Van der Pauw technique. Knowing the value of difference in resistance (*R*), magnetic field (*B*) and thickness of the sample *t*, the mobility of charge carriers is evaluated using the relation

$$\mu_H = \frac{t}{\Delta B} \times \frac{\Delta R}{\rho} \qquad (3)$$

The Hall coefficient (R_H) and carrier concentration (*n*) are evaluated using the following formula;

$$R_H = \mu_H \times \rho \qquad (4)$$

$$n = 1/R_H.e \qquad (5)$$

THERMOELECTRIC POWER MEASUREMENT

The measurements of the thermoelectric power with temperature were carried out in the temperature range 313 K to 573 K. For the study of temperature dependent thermoelectric power S of a p-type semiconductor the expression is given by

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$$S = \frac{k}{e}[A + \frac{E_{FV}}{kT}] \quad (6)$$

Where k is Boltzmann constant, e is the electronic charge, $E_{FV} = E_F - E_V$ is the separation of the fermi level from the top of the valence band and A is the constant determined by the scattering process.

THERMAL CONDUCTIVITY

A simple method known as the divided bar method for thermal conductivity measurement is used. Here, thermal conductivity is measured at 100^{0}C. Assuming that the loss of heat by radiation from the surfaces is negligible compared to the heat transferred and the heat flowing through the metal block and the crystal, we get,

$$K_m A(dT/dX)_m = K_c A(dT/dX)_c \quad (7)$$

$$K_c = K_m (dT/dX)_m / (dT/dX)_c \quad (8)$$

Here, K_m, K_c, are co-efficient of thermal conductivity of metal and crystal respectively and $(dT/dX)_m$ and $(dT/dX)_c$ are thermal gradients of metal and crystal respectively[5].

ELECTRICAL CONDUCTIVITY

Electrical conductivity (σ) is given by

$$\sigma = 1/\rho \quad (9)$$

Where, resistivity,

$$\rho = R \times A / l \quad (10)$$

Here, electric conductivity is also measured at 100^{0}C.

RESULTS AND DISCUSSION

Variations of log ρ versus 1000/T for WTe_2 crystals for two-probe method and four- probe method are shown in Figures 1 and 2 respectively. The resistivity along the cleavage plane decreases with increase in the temperature which indicates the semiconducting behavior of these crystals. From the high temperature resistivity measurements we get the activation energy of WTe_2 crystals which is presented in Table 1. Variation of thermoelectric power (S) with an inverse of temperature for WTe_2 crystals is shown in Figure 3. From the variation of thermoelectric power with temperature gives the value of scattering parameter and fermi energy are given in Table 3. All the results obtained from the Hall Effect measurements are given in Table 2. Current-voltage characteristic of WTe_2 crystal is shown in Figure 4. Using Wiedemann–Franz law, we can find the Lorentz number of WTe_2 crystal which is the relation between thermal conductivity and electrical conductivity. The values of thermal conductivity, electrical conductivity and Lorenz number (L) are given in the table 4.

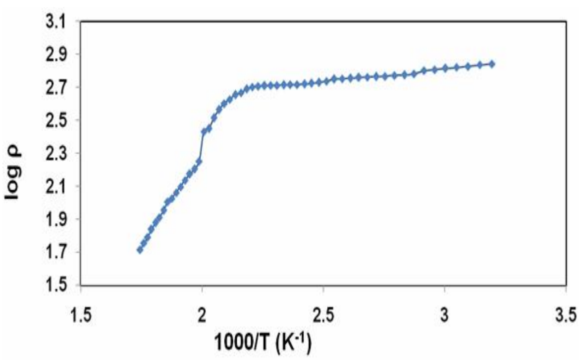

Fig. 1 Variation of log ρ vs 1000/T for WTe_2 crystal for two probe method

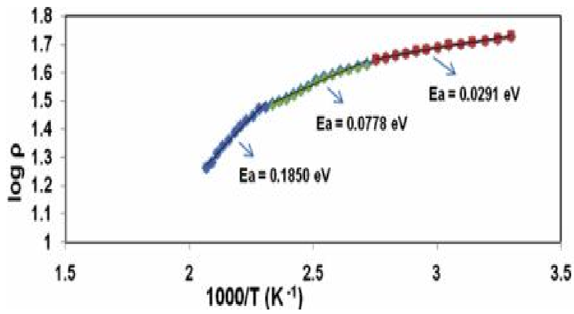

Fig. 2 Variation of log ρ vs 1000/T for WTe_2 crystal for four probe method

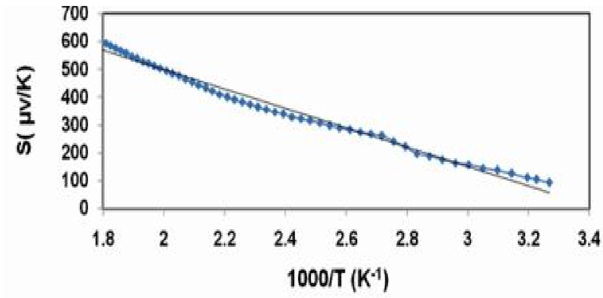

Fig. 3 Variation of thermoelectric power (S) with an inverse of temperature for WTe_2 crystals.

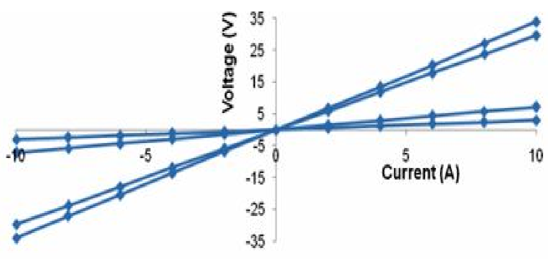

Fig. 4 Current-Voltage curve for WTe_2 crystal

Table - 1 Activation energies determined by high temperature resistivity measurement for WTe_2 crystals

Sample (method)	Temperature (K)	Activation Energy (eV)
WTe_2 (Two- Probe)	313-573	0.2542
WTe_2 (Four -Probe)	303-363	0.0291
WTe_2 (Four- Probe)	368-428	0.0778
WTe_2 (Four- Probe)	433-483	0.1850

Table- 2 Hall parameters for WTe_2 crystals

Sample	Resistivity ρ(Ω?m)	Conductivity σ(Ω?m)^{1}	Hall coefficient R_H (m^3/C)	Mobility μ?(m^2/V?s)	Carrier concentration $N_c \times 10^5$ $(m)^{-3}$
WTe_2	3.11	0.32	621	239	2.44×10^{16}

Table -3 Parameters A, E_{FV} and s for WTe_2 crystals

Sample	A	Scattering parameters	E_{Fv} (eV)
WTe_2	1.1970	1.3030	0.3480

Table- 4 Value of electrical conductivity, thermal conductivity and Lorentz number for WTe_2 crystals

Electrical conductivity	Thermal conductivity	Lorenz number
1.7288×10^{-3} (? cm) $^{-1}$	0.03134 W/cm K	0.048 W?K $^{-2}$

CONCLUSIONS

The resistivity along the basal plane decreases with increase in the temperature which indicates the semiconducting nature of these crystals and also we can use this material as a lubricant at high temperature. The positive values of the Hall coefficient and the Seebeck co-efficient of the crystals of WTe_2 indicate that all crystals are *p*-type in nature and majority charge carriers in them are holes. The values of thermal conductivity, electrical conductivity and Lorenz number confirmed that the crystal of WTe_2 has semiconductor nature.

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