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Growth, Structural and Thermoelectric Properties of Tungsten Diselenide Crystals

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Abstract: *Crystals of Tungsten diselenide (WSe_2) have been grown by direct vapour transport (DVT) technique using micro processor controlled dual zone horizontal furnace. The chemical composition and structure of grown crystals were confirmed using energy dispersive analysis of X-ray (EDAX) and X-ray diffraction (XRD). In the present investigation thermoelectric power measurements (TEP) have been carried out on the grown crystals. Different electrical transport parameters of semiconductors have been determined and discussed in the paper.*
Keywords: *WSe_2, Structural, Electrical, EDAX, XRD.*
PACS: *71.18+y, 71.20.-b, 71.20 Nr. , 73.90+F*

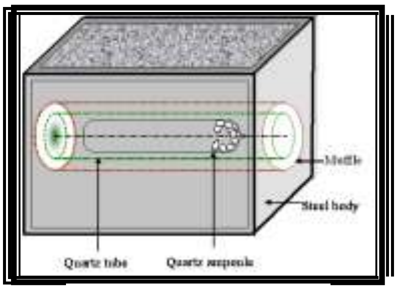
I. Introduction

In recent years, group- *VI* semiconductors have attracted much interest in their applications particularly in the area of solar cells. WSe_2 is a member of the compounds of *VI-A* and *VI-B* group. It has stacked layer structure of M-X-M type which is an extra incentive for device research. Here M is transition metal e.g. tungsten and X is chalcogen e.g. Selenium [1,2]. Amongst layered TMDCs, DVT grown WSe_2 crystals have been less studied for their thermoelectric properties in a wide temperature range.

In the present investigation thermoelectric properties of the well characterized grown crystals of WSe_2 have been done. Electrical transport parameters like carrier concentration, Fermi energy, density of states and effective mass of carriers have also been determined and discussed in the paper.

II. Experimental

Crystals of Tungsten diselenide (WSe_2) have been grown by direct vapour transport (DVT) technique using dual zone horizontal furnace [3]. The chemical composition was identified using energy dispersive analysis of X-ray (EDAX). XRD analysis was carried out by X-ray Diffractometer for the determination of structure. The thermoelectric power measurements (TEP) have been carried out on the grown crystals with the help of TEP measurement setup developed in our laboratory.



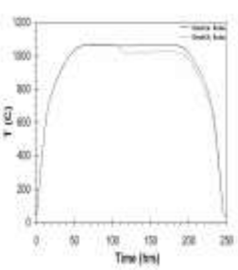
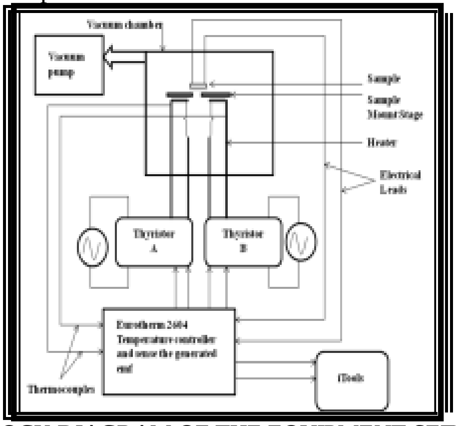


Fig.1. The temperature profile used for the growth of WSe_2.

The thermoelectric power measurements (TEP) have been carried out on the grown crystals with the help of TEP measurement setup developed in our laboratory. The sample with area 3x3 mm^2 was used.. The measurements were taken in the temperature range of 333K to 473K and the temperature difference (ΔT) between the ends of the sample was kept to be 10K.



BLOCK DIAGRAM OF THE EQUIPMENT SETUP

III. Results And Discussions

The stoichiometry of the grown crystals was analyzed by EDAX and it is found that the grown crystals posses nearly perfect stoichiometry with chemical formula WSe_2..

Fig.1 shows the X-ray diffractogram of WSe_2. crystal. XRD analysis shows that crystals posses hexagonal structure. For this hexagonal structure lattice parameters a, b and c were determined. The obtained values are a=b=3.28 Å, and c=13.00 Å. These observed lattice parameters of as grown crystals are in good agreement with reported JCPDS data [4].

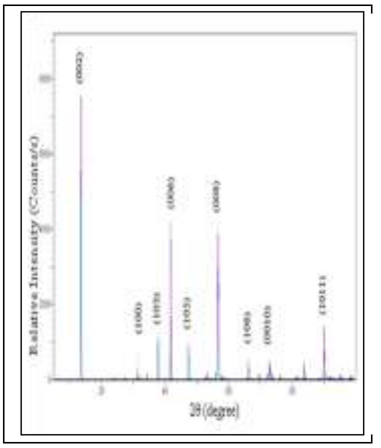


FIGURE 1. X-ray diffractogram of WSe_2 crystal.

The results of TEP measurements as shown by variation of thermoelectric power (S) with temperature in the range 333K to 473K have been shown in fig 2(a).The positive values of 'S' shows that the crystals possess p-type conductivity. To analyze the temperature dependence of thermoelectric power of a p-type semiconductor, the expression given by Mohanchandra and Uchil [5] and H. J. Goldsmid [6] has been used. It is given as

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

where k is Boltzmann constant, e is electronic charge, A=(5/2-C) is the scattering coefficient which varies from 0 to 4 depending on the scattering process , *C* is the scattering parameter and E_F is the separation of Fermi level from the top of the valance band.

As the carrier concentration depends on E_F in the crystal and for a small temperature range, E_F can be considered as fairly constant, equation (1) can be expressed as

$$S = \frac{k}{e}\left[A + \ln\frac{N_A}{p}\right] \quad (2)$$

Here $N_A = [2\pi m_h^* kT/h^2]^{3/2}$ is the effective density of states in which m_h^* is the effective mass of holes and h is the Plank's constant.

Considering constant E_F, the plot of thermoelectric power (S) against the reciprocal of temperature gives a straight line as shown in fig.2 (b).

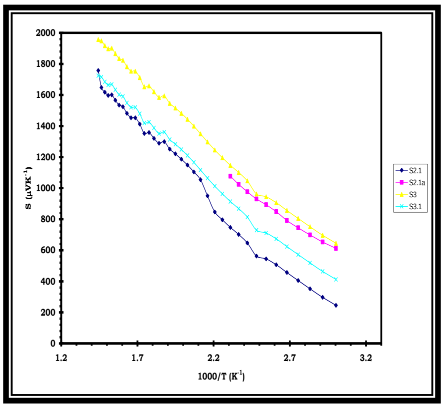


FIGURE 2 (a). Variation of thermoelectric power vs temperature and **(b).** Variation of thermoelectric power as a function of inverse of temperature

From the slope the value of E_F is found to be 0.0368 eV. Using the value of carrier concentration ($6.67x10^{18}cm^{-3}$) obtained from Hall Effect measurement, effective density of states N_A was also calculated and is found to be 6.679 $x10^{24}$ m^{-3}. Using this value the effective mass was calculated and is found to be7.597$x10^{-31}$ kg. These calculated values for DVT grown WSe_2 crystal are close to the values reported in the literature [7].

IV. Conclusions

The EDAX analysis shows that the grown crystals are nearly perfect in stoichiometry. The X-ray analysis shows that crystals posses hexagonal structure. The values of the computed lattice parameters for the grown crystals are a= b=3.28Å and c=13.00 Å. The positive values of thermoelectric power show that the crystals possess p-type conductivity. The values of Fermi energy E_F, Density of states N_V, effective mass m_h* obtained for crystal are close to the values reported in the literature.

Sample	E_F (eV)	A	s
WSe_2	0.019	4.20	-1.71

Table 1.E_F and values of scattering parameter *s* for W.Se_2 crystals

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