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ELECTRICAL PROPERTIES OF MULTILAYERED MOLYBDENUM DISULPHIDE SINGLE CRYSTAL

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Abstract *—Molybdenumdisulphideis alayeredtransitionmetaldichalcogenidesthathasrecentlyraised considerable interest due to its unique semi conducting and optoelectronicproperties. Although severaltheoreticalstudieshavesuggestedanelectronicphasetransitionin molybdenumdisulphide, there has been a lack ofexperimental evidence.The crystals have been characterized with the help of energy dispersive analysis by X-ray (EDAX). Electrical resistivity measurements have been performed on M_OS_2 Single in the temperature range 303-473 K. The crystals were found to be exhibit semiconducting nature in this range. The anisotropy measurements have been carried out for the grown crystals. The semiconducting behavior of both crystals is confirmed by smack coefficient measurements.*

Keywords-Transition Metal Dichalcogenides, CVT anisotropy, M_OS_2 Single crystals, thermoelectric power.

I. INTRODUCTION

Recent advances in the preparation of atomically thin layers of van der Waals (vdW) bonded crystalline solids by mechanical exfoliation or chemical synthesis have allowed for renewed investigations of two-dimensional (2D) materials beyond graphene but with a similar layered hexagonal structure[1–5]. Within this class of 2D materials are transition metal dichalcogenides (TMDs), such as molybdenum disulphide (MoS2), which have beenincreasingly explored toaccess a wealth of phenomena including optoelectronics[5], valleytronics[6], spintronics[7]and coupled electromechanics[8]. All of these phenomena arise from the complex thickness-dependent physical and electronic structures of the multilayered materials, in which the coupled electro-mechanics can be regarded as straintronics. Multilayered MoS2, having a band gap (Eg) of B1.2 eV, is composed of stacked triatomic sheets where each triatomic monolayer exhibits a sandwiched structure with a plane of transition metal molybdenum atoms covalently bonded to, and sandwiched between, two planes of chalcogensulphur atoms. Unlike monoatomic multilayered graphene with sp2 hybridization, the diatomic composition of multilayered MoS2 coupled with its d-orbital electronic states9 and the small 6.5 Å vdW interlayer gap raises the prospects of strong sulphursulphur interlayer interactions under axial compression that might lead to an electronic phase transition.Single crystals of molybdenum dichalcogenides, as p or n type semiconductors have been extensively studies.Single crystals of the transition metal dichalcogenides MOS2 and MOSe2 have hitherto only been prepared using helogenvapour transport technique. [10-14].The optical and electrical properties of transition metal dichalcogenodes have been investigated by several authors. [15,16]. Room temperature electrical resistivity and hall effect measurements as a function of pressure are reported in p- type MOS2 and n-type MOS2 and MOTe2 [17]. The Electrical conductivity and Hall coefficient perpendicular to the c-axis of hexagonal MOS2,MoSe2 and MOTe2 were Measured over the temperature ranges 120 to 1170 K are also reported [18].Considerable literature exists on the electrical properties of the semiconducting transition metal dichalcogenide layer crystals MX2 , where M is Mo and X is S, Se and Te [4,5,7-9]. The Electronic bands in the fundamental gap region of the layered semiconductors MOS2 and MOSe2 have been studied [4, 5] and band structures have also been studied [19]. Experimental data are available on U.V. Photoemission [20], on electrical [21], optical properties [22, 23] and on electron paramagnetic resonance [6] have been studied. In this paper, we report the growth, measurements of resistivity to identify any possible temperature induced transitions in them.

II. EXPERIMENT

With a view to allowing and faster transport of constituents to produce the necessary super saturation for crystal growth in a vapour phase system, the chemical (Iodine) vapour transport method was employed. Pure elements (99.95%) of molybdenum, sulpher and selenium (make: Aldrich, USA) in stoichiometric proportion were sealed in an evacuated quartz ampoule. Also filled a small capillary with I_2 (2mg/cc) of ampoule volume and placed in the ampoule for the compound preparation. The details of growth conditions are given in table 1. The resulting crystals were in the form of thin Platelets and were characterized by energy dispersive analysis of x-rays (EDAX). The Chemical composition of the grown crystals has been well confirmed by carrying out EDAX analysis as shown in table 2.

The High temperature resistivity measurements perpendicular to c- axis i.e. along the basal plane were carried out on single crystals of M_OS_2 and M_OSe_2 single crystals in the temperature range 303-473 K using the four probe set- up manufactured by scientific Equipment's, Roorkee. The graph of log $\rho_\perp$ vs. 1/T is shown in figure 1 for M_OS_2 and M_OSe_2 single crystals.

Resistivity measurements parallel to c-axis i.e. normal to the basal plane were carried out on an experiment set up designed and prepared by the university science and instrumentation center (USIC), Sardar Patel University, Vallabh Vidhyanagar. The graph of log $\rho_{\parallel}$ vs. 1/T is as shown on figure 2 (a) & (b).

Using the resistivity values parallel to c-axis, the anisotropy $\gamma = \rho_{\parallel} / \rho_{\perp}$ for both crystals has been determined in the temperature range 303-473 K is as shown in figure 3 (a) & (b).

Seeback coefficient measurements from room temperature to 308-368 K, has been carried out by Scientific solution's Mumbai was Using. The variation of Seeback coefficient with temperature is as shown in figure 4opto-electronic properties, Photoconductivity measurements have also been performed as a complementary means for understanding the opto-electronic properties of materials, which is dependent on the material's band gap. To provide perspective, the pressure-dependent band gap for multilayered MoS_2 can be understood from theoretical analysis using the PBE functional under the generalized gradient approximation (GGA). We note that the calculated unstrained Eg of 1.03 eV is B16% less than the experimental value [25]. This underestimation of the bandgap is a well-known problem due to the presence of artificial self-interaction and the absence of the derivative discontinuity in the exchange-correlation potential with the PBE/GGA methods[26]. Hybrid Heyd–Scuseria–Ernzerhof [27] functional and DFT with many body perturbation theory in the GW approximation [28] are among the few methods to correctly predict the band gap of TMDs; however, these methods are computationally very expensive.

III. Results

A. Single crystal of M_OS_2 and M_OSe_2 has been grown by chemical vapour transport (CVT) technique.
B. From the figure 1 and 2, decrease in resistivity with increase in temperature confirms the semiconducting nature of MoS_2 and $MoSe_2$ single crystals.
C. The variation of the Seeback coefficient with temperature in figure 4 reveals that in both the crystals the sign of thermoelectric power is positive and remains positive over the entire range, thus confirming typical semiconducting behavior of the crystals.
D. With increasing pressure, our theoretical calculations show that the electronic charge moves away from the S atoms and accumulates onto the Mo atoms.
E. Near the critical transition pressure, the maximum charge redistribution is predicted to occur in between the MoS_2 layers across the vdW gap, indicating enhanced S–S interaction.

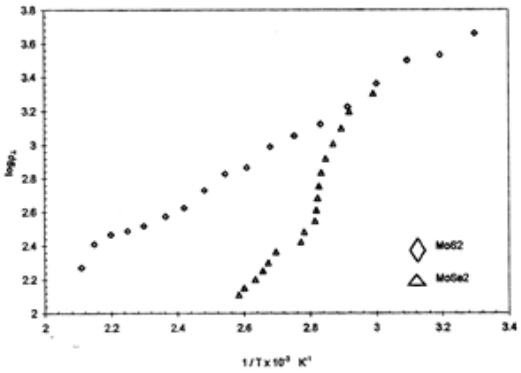


Figure 1: Variation of resistivity (log$\rho_{\perp}$) with temperature ($1/T \times 10^{-3}$) in the range 303-473 K obtained from four probe method.

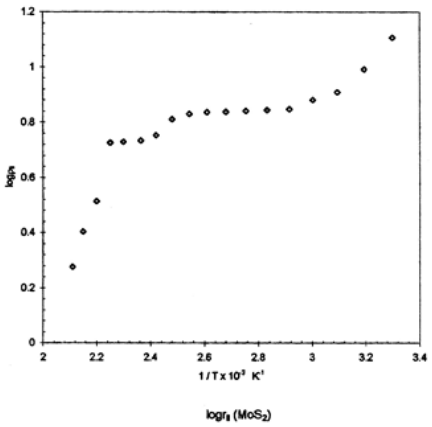
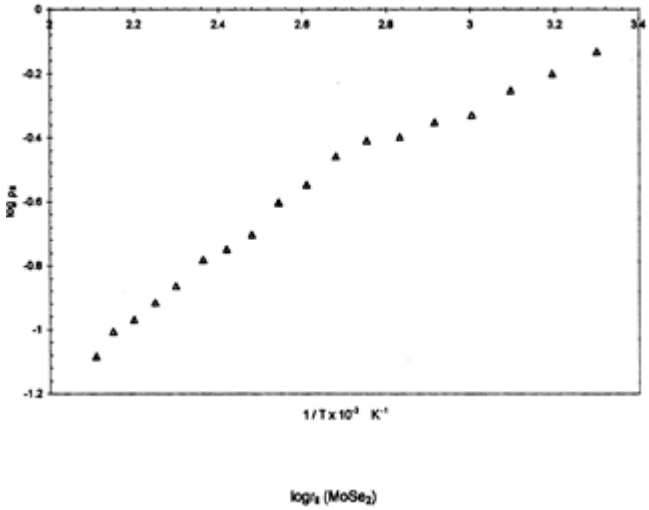


Figure 2(a): Variation of resistivity ($\log\rho_n$) with temp.in the range 303- 473 Kobtained From high temperature for M_OS_2 single crystal.



: Variation resistivity ($\log\rho_n$) with temp.in the range 303-473K obtained from high temp.for$MoSe_2$ single crystal.

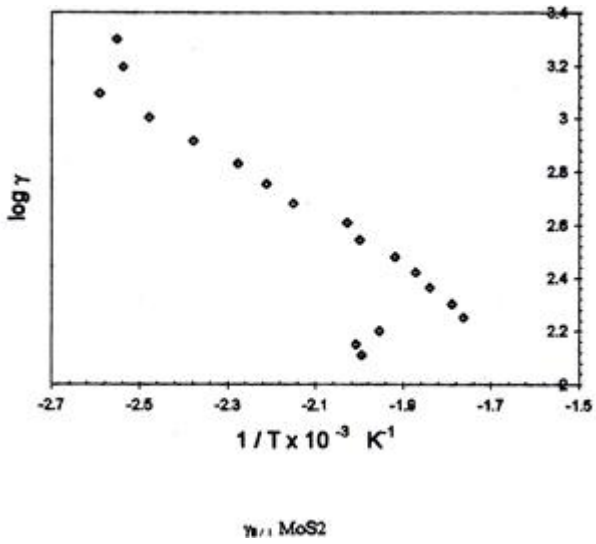
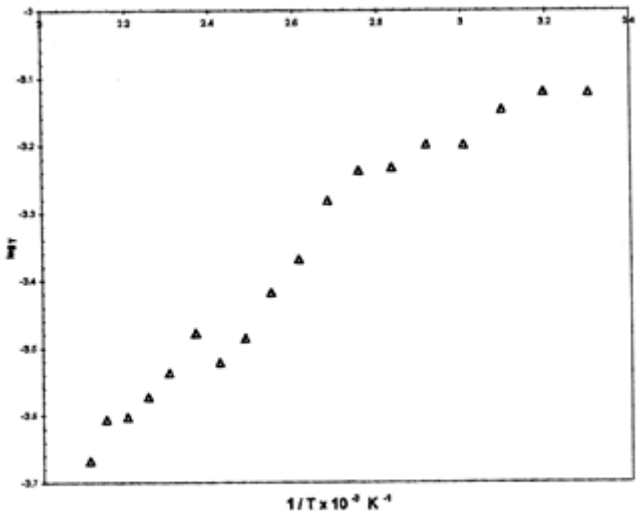


Figure 3(a): Variation of γ versus 1/T for MoS_2 Single crystal.



$\gamma_{\parallel,\perp}$ ($MoSe_2$)

Figure 3(b): Variation of γ versus 1/T for $MoSe_2$ single crystal.

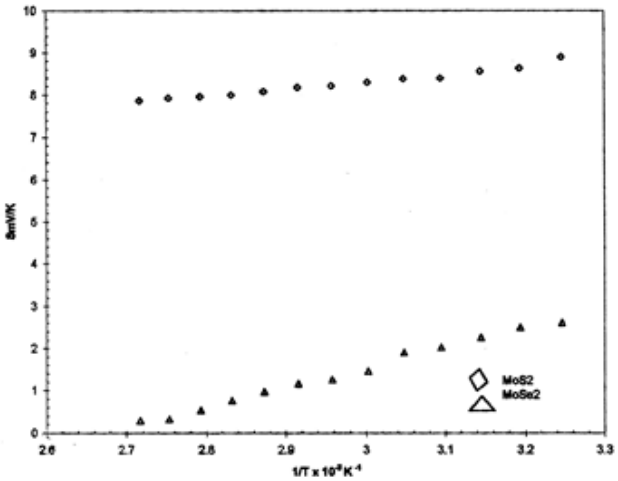


Figure 4a: Variation of TEP with temperature for MoS_2 and $MoSe_2$ single crystal.

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