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ELECTRICAL PROPERTIES MEASUREMENTS OF In_xMoSe_2 ($0 \leq x \leq 1$) SINGLE CRYSTALS

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The crystals of In_xMoSe_2 $(0 \leq x \leq 1)$ have been grown by a direct vapour transport technique in the laboratory. The crystals were found to be exhibiting semiconducting behaviour in the temperature region 308K-423K range. The measurement of the thermoelectric power and conductivity enabled the determination of both carrier mobility and carrier concentration. The variation of both i.e. carrier concentration and carrier mobility indicates the presence of deep trapping centres and their reduction with temperature in these crystals.

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Keywords: In_xMoSe_2 $(0 \leq x \leq 1)$ single crystals, electrical conductivity, thermoelectric power, trapping centres, transition metal dichalcogenides.

1. Introduction

During recent years, transition metal dichalcogenides (TMDC) of group IV-b,V-b and VI-b have received considerable attention because of their uses particularly as electrodes in photoelectrochamical (PEC) solar ce1l for conversion of solar energy into electrical energy as well as photonic devices in various electronic applications [1-10]. The compounds crystallize in quasi-two-dimensional layer structure consisting of chalcogenes, which are held together by relatively weak Van der Waal's forces. Because of these weak Van der Waal's forces between the layers, facilitates to intercalate foreign atoms, ions or neutral molecules to form new compounds [1-10]. Intercalated compounds of disulphide and diselenide of molybdenum and tungsten have been extensively studied by various researchers. These crystals become superconducting when intercalated with alkali and alkaline earth metals [1-10]. The study of stacking fault is very important one, because it plays an important role in the description of defects. The conversion behaviour of a solar cell is closely related to the perfection of the electrode material and since stacking fault play a fundamental role in the description of defects structure, therefore their study is of both practical and theoretical interest [2]. The enhanced conduction of the stacking fault along the c-axis is difficult to understand because of the extreme two-dimensional characters of the layered compounds of $MoSe_2$ and its intercalated compounds of i.e. $In_xMoSe_2(0 \leq x \leq 1)$. The only way to understand this conduction is by supposing the presence of stacking faults in these crystals. It is clear from the literature survey that, the research work on intercalated compounds of $MoSe_2$ is almost negligible. Hence, it was decided to work on In_xMoSe_2 $(0 \leq x \leq 1)$ single crystals [1-6]. These crystals have interesting electrical and semiconducting properties. They also have exhibits some interesting switching and memory effects. The great advantages of these in fabrication of solar cells have also been predicted [1-10]. In this paper we, therefore, report the measurements of d.c. resistivity, thermoelectric power, mobility and anisotropy in electrical resistivity in the different temperature range.

2. Experimental methodology

The d.c. resistivity ($\rho_\perp$) of In_xMoSe_2 $(0 \le x \le 1)$ single crystals perpendicular to c-axis was investigated by using d.c. resistivity apparatus [2]. While, the high temperature d.c. resistivity (ρ_{ll}) measurements performed on the basal plane in the direction parallel to c-axis in the temperature range 308K-423K is made by resistivity apparatus. Starting from the room temperature (303K), the temperature of the sample was increased slowly in the steps of 10K until a temperature of 420K was reached. At each step the corresponding value of the resistivity was evaluated. Results of the d.c. resistivity ($\rho_\perp$) and high temperature (308K-420K) resistivity (ρ_{ll}) measurements on a representative sample are shown in Figures 1-2. It is seen that resistivity decrease with increase in the temperature. The graph of $\log(\rho_{ll})$ verses $1000/T$ shows almost a flattened region similar to observe by Mahalway [11] for $MoSe_2$. The activation energies obtained from the graph are 0.3895 eV, 0.06207 eV, 0.04979 eV, 0.04831 eV for In_xMoSe_2 $(0 \le x \le 1)$ single crystals respectively, in the temperature range 308K-423K. In our investigation anisotropy measurements have been carried out in the temperature range 308K-423K. It is seen in Fig. 3 that the anisotropy $(\rho_\perp / \rho_{//})$ ratio increases with increase in the temperature. This variation of anisotropy with temperature shows an identical behaviour to that reported by Zheng et al [12].

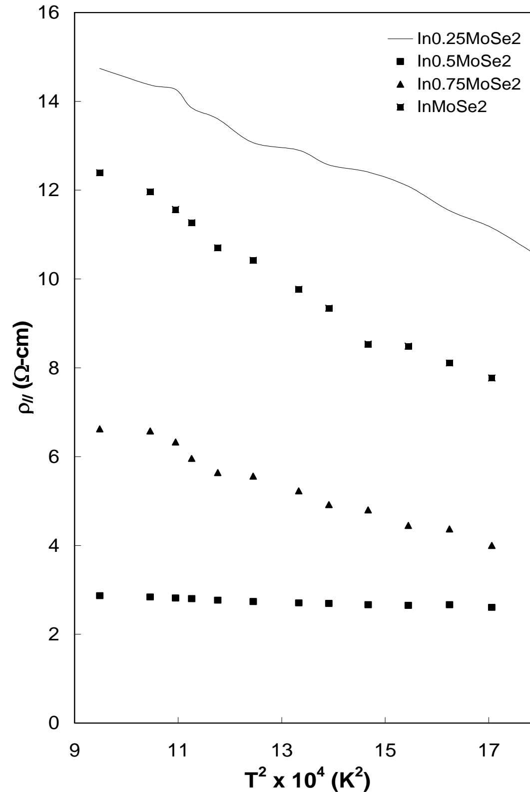

Fig. 1. Variation of resistivity with reciprocal of temperature of In_xMoSe_2 $(0 \le x \le 1)$.

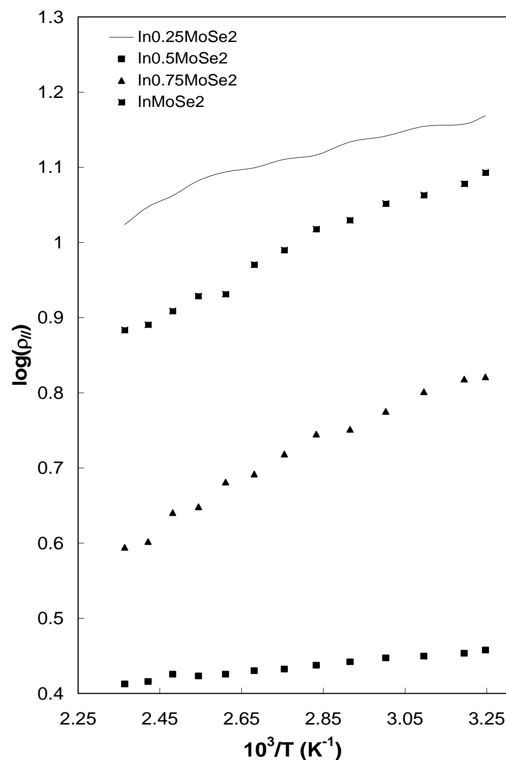

Fig. 2. Variation of resistivity with reciprocal of temperature of In_xMoSe_2 ($0 \le x \le 1$).

The thermoelectric power (TEP) measurements were carried out using the thermoelectric measurements setup apparatus. In all the measurements ΔT was kept as 5K and TEP ($S_{//}$) measurements were carried out in the temperature range 308K–423K. Due to experimental limitations, TEP ($S_{\perp}$) measurements normal to the basal plane i.e. parallel to c-axis could not be made. The polarity of the thermally generated voltage at the hot end was negative indicating that the crystals are p-type in nature. The TEP was found to increase linearly with temperature. The graphical behaviours of the Seeback coefficient (S) are displayed in Fig. 4. The TEP $(S = S_{ll})$ has been used to evaluate the carrier mobility using relation given by [13-15]

$$TEP = S = -\frac{k}{e}\left(\frac{E_a}{kT} + A\right), \quad (1)$$

or

$$S = -\frac{k}{e}\left\{A + \ln\left[2\left(2m_e^* kT\right)^{3/2} / nh^3\right]\right\}. \quad (2)$$

where A is the thermoelectric factor, n the electron density, h the plank constant and m_e^* the effective mass of the electron. The above equation (1 or 2) after the substitution of various constant and taking $A = 1.5$ for ionized impurity scattering simplifies to [15]

$$\log n = (3/2)\log T - 0.005S + 15.719\,. \quad (3)$$

The electron density has been evaluated by using the above relation. The mobility μ of the charge carrier is determined from the relation

$$\mu = \sigma / ne \,, \tag{4}$$

where n is the carrier concentration, e is the charge of the electron and σ the electrical conductivity.

4. Results and discussion

The T^2 dependence of the high temperature (308K-423K) resistivity (ρ_{ll}) can be attributed to carrier scattering rather than carrier activation. However due to experimental limitations the scattering and degeneracy could not be studied in detail in the range 308K-423K of the temperature. The high value of the resistivity in the perpendicular direction suggests that conduction of the electron in the direction normal to the layer is very little. Further, the anisotropic behaviour and its variation with the temperature clearly shows that electronic conduction in In_xMoSe_2 $(0 \le x \le 1)$ single crystals is highly anisotropic, which may be attributed to the sufficiently larger effective mass anisotropy [15]. The high values of the resistivity and large anisotropy further suggest that electron states in In_xMoSe_2 $(0 \le x \le 1)$ single crystals is two dimensional in contrast to a three dimensional behaviour seen in GaSe and SnSe crystals [15].

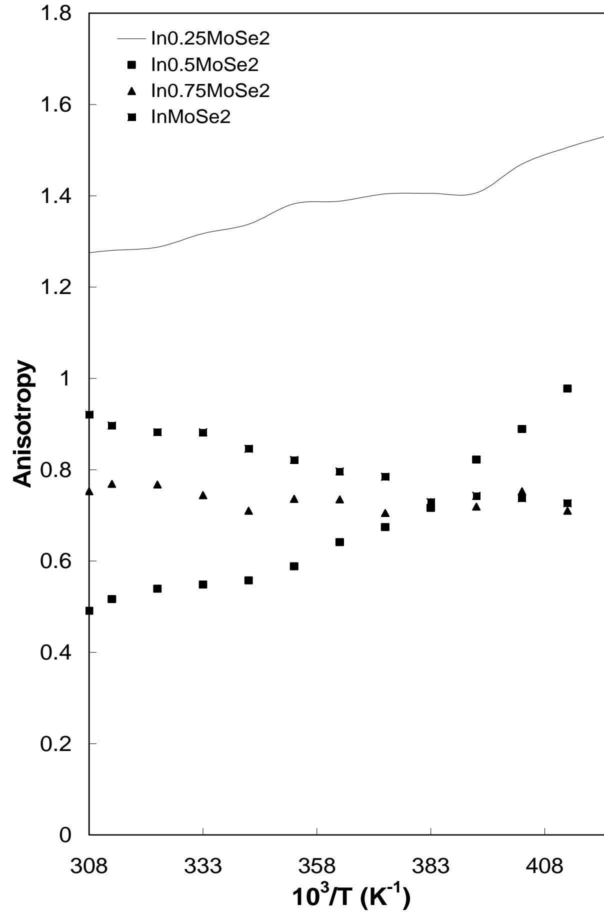

Fig. 3.Variation of anisotropy temperature of In_xMoSe_2 $(0 \le x \le 1)$.

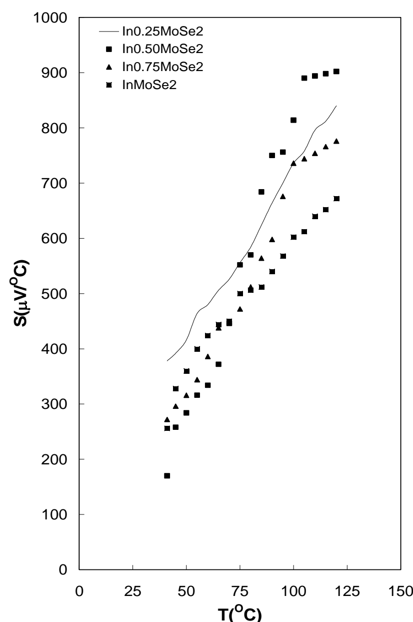

Fig. 4. Variation of Seeback Coefficient of In_xMoSe_2 ($0 \leq x \leq 1$).

The low value of the activation energy obtained from Fig. 2 in the temperature region 308K-423K suggests that the measured conductivities are the results of intrinsic process in the crystals; this can be attributed to the high carrier concentration density, which gives rise to energy levels very close to the conduction band. These carriers will also be scattered by various centres by regions such as grain boundaries, dislocations, surface states etc. in addition to the normally observed scattering modes, viz. ionized impurity, lattice or phonon piezoelectric etc. The positive temperature dependence of mobility suggests that ionized impurity scattering might be the dominant scattering mechanism in these crystals in the observed temperature range.

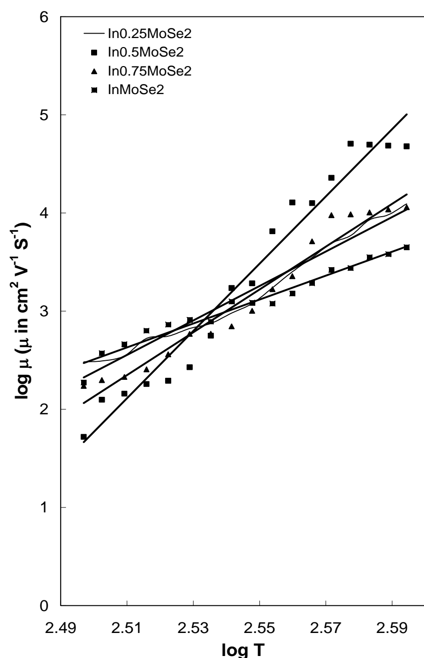

Fig. 5. Variation of mobility with temperature of In_xMoSe_2 ($0 \leq x \leq 1$)

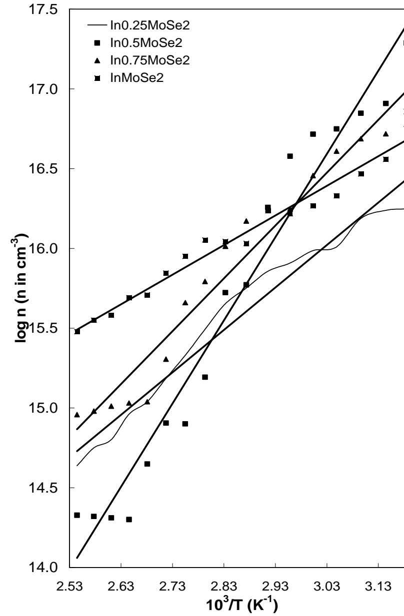

Fig. 6. Variation of carrier concentration with reciprocal of temperature of In_xMoSe_2 ($0 \le x \le 1$)

From the slope of temperature dependent mobility graph (Fig. 5), it is possible to obtain some qualitative idea about the scattering mode. Since, all scattering processes are likely to follow the relation $\mu \propto T^x$, the magnitude and sign of x will determine the scattering mode. In the present case the value of x from Figure 5 comes to about 17.56, 34.27, 21.81 and 12.18, which is found positive. The theoretical value of x for ionized impurity acting, as a single mode of scattering is $3/2$. The deviation in the observed value seems to be due to the superimposition of the ionized impurity scattering with some of the above mentioned scattering process. The observed range of temperature i.e. 308K-423K corresponds to the extrinsic / impurity range only as seen from the low values of conductivity activation energy. Also, the carrier concentration can be expressed as [15]

$$n \approx \exp\left(\frac{E_n}{kT}\right), \tag{5}$$

where E_n is the carrier activation energy of the p-type In_xMoSe_2 $(0 \le x \le 1)$ single crystal. The above equation predicts a linear relation between $\log n$ and $1/T$ as observed in Figure 6. The carrier activation energy estimated from the slope was found to be 2.66 eV, 5.22 eV, 3.31 eV, 1.86 eV. Since, this value is much higher than the reported values of electrical band gap of $MoSe_2$ i.e. 1.1 eV [16], the presence of deep donor like levels is possible in this material. Hence, heating the higher temperature range increases the number of deep trapping centres, and thereby decreasing the number of free carriers and carrier mobility. The mobility may reduce only at still higher temperatures where the scattering due to lattice thermal vibration dominates.

5. Conclusion

The single crystals of In_xMoSe_2 $(0 \le x \le 1)$ exhibit semiconducting behaviour in the temperature range 308K-423K. The positive temperature dependent of carrier mobility suggested that ionized impurity scattering might be dominant scattering mechanism in these crystals. The variation of carrier mobility and carrier concentration with temperature in the semiconducting range indicates that the presence of deep centres.

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