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Transport properties of $MoSe_xTe_{2-x}$ $(0 \leqslant x \leqslant 2)$ single crystals

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Abstract. The layer type $MoSe_xTe_{2-x}$ $(0 \leqslant x \leqslant 2)$ have been grown in single crystalline form by chemical vapour transport technique using bromine as the transporting agent. The electrical resistivity and Hall mobility perpendicular to the *c*-axis of the crystals were measured at room temperature. The variation of the Seeback coefficient with temperature was also investigated.

Keywords. Electrical resistivity; Hall mobility; thermoelectric power; $MoSe_xTe_{2-x}$ $(0 \leqslant x \leqslant 2)$ single crystals.

1. Introduction

Recently, transition metal dichalcogenides have attracted much attention because of their possible applications as lubricants, switching devices and photoelectrochemical solar energy converters. They form a wide range of solid solutions (Schneemeyer and Sienko 1980; Mentzen and Sienko 1976) either with mixed metals or with mixed chalcogenide compositions. The crystals of transition metal dichalcogenide are of layered type, each layer being a sandwitch of chalcogen-metal-chalcogen sheets. The metal-chalcogen bonding is partly ionic and partly covalent whereas the interlayer bonds are of van der Waal's type. These VIB–VIA group of compounds have been studied extensively for their electrical properties (Wilson and Yoffe 1969; Brixner 1963; Mansfield and Salam 1953). Studies have also been made on mixed systems such as $(Mo/W)Te_2$, $(Mo/W)Se_2$ (Revolinsky and Beerntsen 1964), $(W/Mo/Te)Se_2$ (Brixner and Teufer 1963) and $Mo(S/Se)_2$ (Agarwal and Talele 1986). However, no attempt has been made to investigate the variation of the properties like resistivity, Hall coefficient and thermoelectric power with composition for $Mo(Se/Te)_2$ solid solutions in the single crystalline form. The present paper reports a study of these properties for $Mo(Se/Te)_2$ single crystals grown by chemical vapour transport technique.

2. Experimental

Single crystals of $MoSe_xTe_{2-x}$ $(0 \leqslant x \leqslant 2)$ were prepared from 99·999% pure molybdenum, selenium and tellurium. Powdered starting material in the required composition was taken in a quartz ampoule and vacuum-sealed with a residual air of 10^{-5} torr. The powder was thoroughly mixed and distributed along the length of horizontally held ampoule. The charge was slowly heated over 72 hr to 700°C. At this stage a reaction product was obtained in the form of free flowing shining polycrystalline material. The ampoule and the product were thoroughly mixed by shaking. Large single crystals were found to grow after heating the ampoule at appropriate temperatures for about 2–7 days (table 1). These crystals were characterized for their structure and composition.

The electrical resistivity and Hall coefficients of the crystals were determined using the standard method of Van der Pauw (1958). Electrical contacts were provided by conducting silver paste and thin copper wires attached to the periphery of a thin flat crystal. Seeback coefficient was measured using an integral method. The specimen holder used for the measurement is shown in figure 1.

3. Results and discussion

A detailed study of the variation of d.c. resistivity, ρ (ohm cm) as a function of the crystal composition reveals that the resistivity increases non-linearly with the increasing selenium content in the solid solution $MoSe_xTe_{2-x}$ $(0 \leqslant x \leqslant 2)$ as shown in figure 2. The room temperature (30°C) resistivities of $MoSe_2$ and $MoTe_2$ have been obtained as 9·5 and 0·25 Ω cm respectively. These results agree with those reported earlier (Revolinsky and Beerntsen 1964; Lepetit 1965). The resistivity value is found to increase as the selenium content increases in the solid solution. Analogus behaviour is observed in the case of WSe_xTe_{2-x} system (Champion 1965).

In order to judge the semiconducting nature of $MoSe_xTe_{2-x}$ $(0 \leqslant x \leqslant 2)$, the Hall effect was measured. The Hall mobility, μ_H was determined using Van der Pauw's method for various compositions at room temperature. The Hall coefficient R_H and

Table 1.

Nominal composition (X)	Reaction temperature (°C)	Growth temperature (°C)	Growth time (hr)
$MoTe_2$ 0·0	700	650	72
0·5	900	800	48
1·0	800	670	96
1·5	880	720	168
$MoSe_2$ 2·0	900	800	120

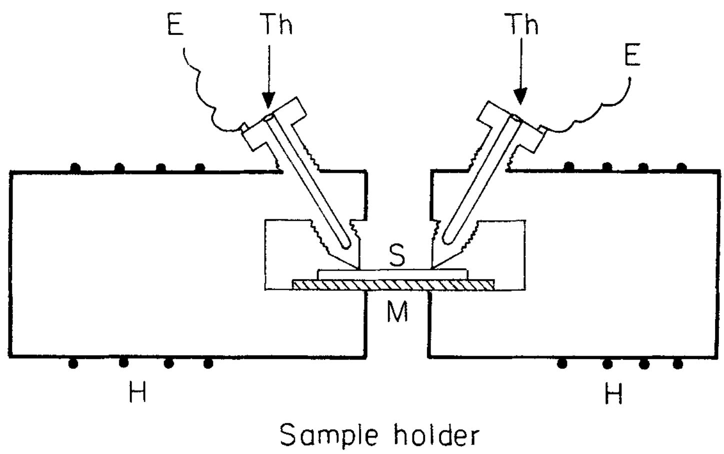

Figure 1. Schematic diagram of the sample holder for Seeback coefficient measurements. H, Heater, Th, Thermocouples E, Electrodes, S, Sample M, Mica sheet.

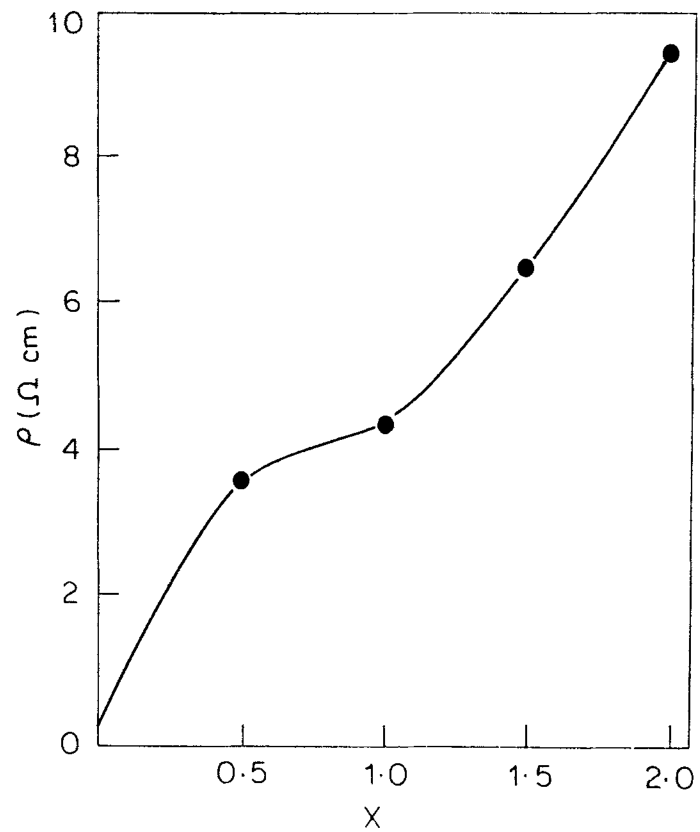

Figure 2. Variation of resistivity (ρ) as a function of composition X at $T = 30°C$.

the carrier concentration n were also calculated assuming the single carrier conduction model using the relations

$$\mu_H = R_H/\rho \text{ and } n = -1/eR_H,$$

where e is the electronic charge. The variation of μ_H, R_H and n with the composition of $MoSe_xTe_{2-x}$ is shown in figure 3. It is observed that Hall mobility increases with increasing selenium content. As resistivity also increases with increasing selenium content in the crystal, it is concluded that the Hall coefficient increases and hence carrier concentration decreases as we go from $MoTe_2$ to $MoSe_2$.

It is interesting to note that the optical band gap determined from the spectral response of the crystals increases with increasing selenium content in the $MoSe_xTe_{2-x}$ system (Agarwal *et al* 1987). The atomic radius decreases as we go from Te (1·37 Å) to Se (1·17 Å) leading to changes in the band strengths and hence in the structure. Further the electro-negativity of the atoms increases from Te (2·1) to Se (2·4) thereby indicating an increase in the ionic nature of the bonding. As a result, an increase in the resistivity and a decrease in the effective carrier concentration should be expected which agree with the experimental observations.

Thermoelectric measurements were made in the temperature range 40 to 200°C. The variation in the Seeback coefficient S with temperature for $MoSe_xTe_{2-x}$ system

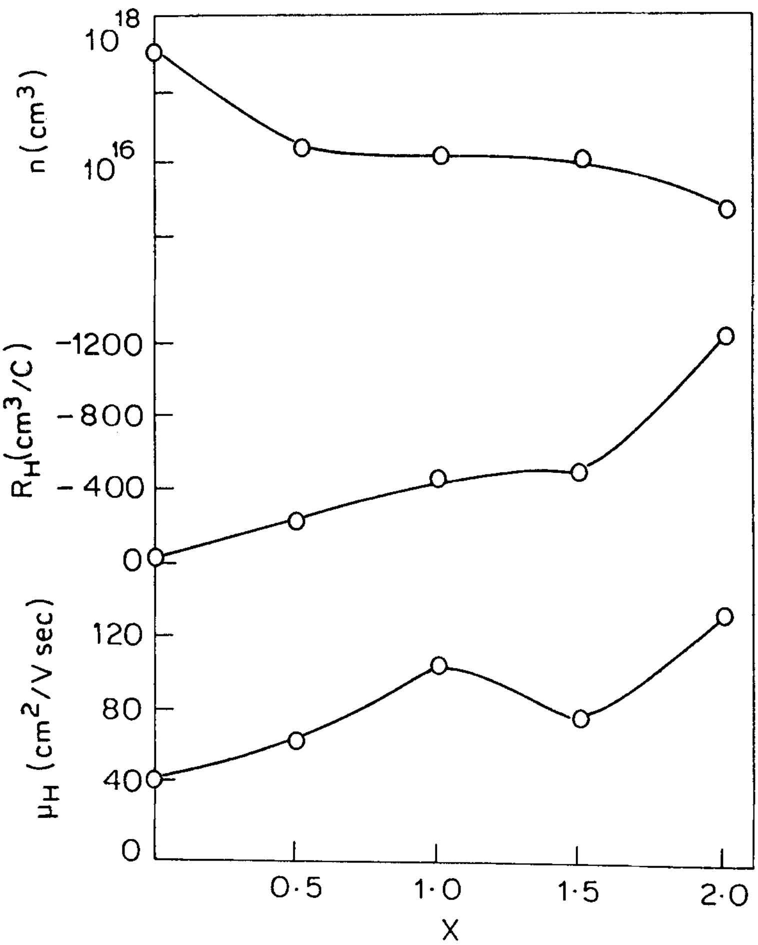

Figure 3. Variation of Hall mobility (μ_H), Hall coefficient (R_H) and carrier concentration (n) as a function of composition X at $T = 30°C$.

is shown in figure 4. The value of S increases initially with temperature and then decreases to a nearly constant value. The nature of variation is identical for all compositions in the $MoSe_xTe_{2-x}$ system except that the peak value of Seeback coefficient occurs at different temperature. The existence of a peak in S vs temperature plot and its relation to the variation in concentration and mobility of charge carriers needs to be investigated. However, it is worth noting that S showed a negative value for all compositions of the solid solution throughout the temperature range in the present study indicating the crystals to be n-type semiconductors.

Acknowledgement

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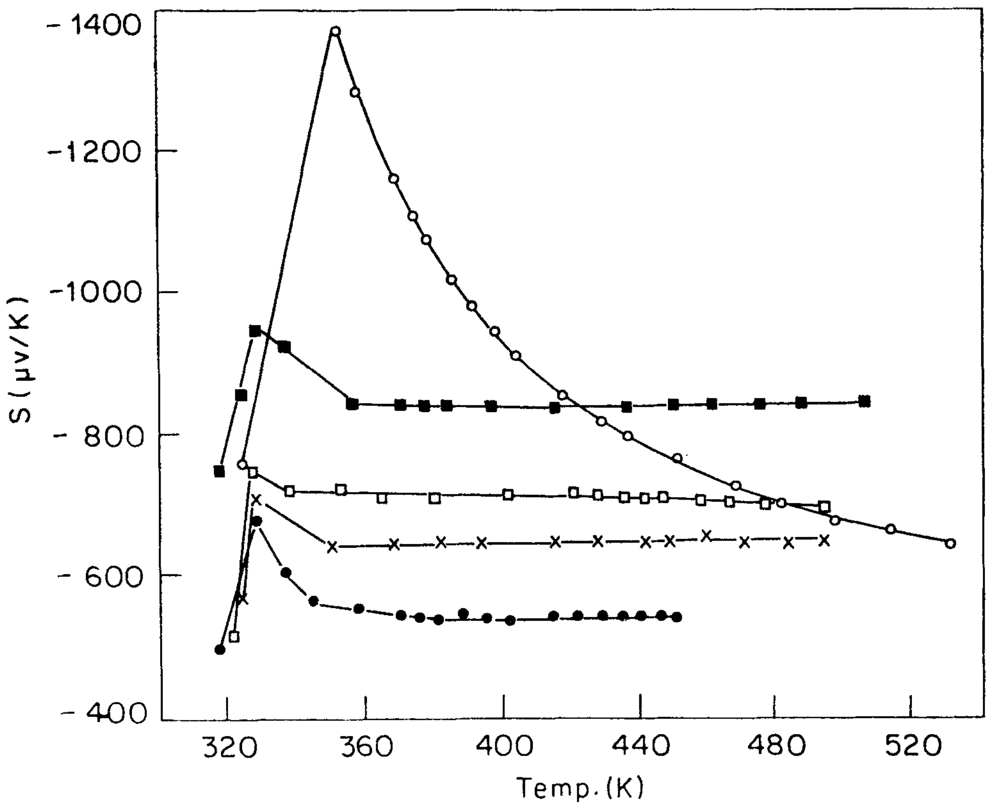

Figure 4. Seeback coefficient as a function of temperature for $MoSe_xTe_{2-x}$ system.

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