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Electrical transport properties of semiconducting chromium molybdenum diselenide single crystals

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ABSTRACT

Mixed chromium–molybdenum diselenides ($Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75)) have been grown in single crystalline forms by the chemical vapor transport technique. Electrical transport properties like electrical resistivity (perpendicular and parallel to the *c*-axis), thermoelectric power measurements at high temperature and Hall effect measurements at room temperature were performed on these single crystals. Preliminary study of electrical measurements suggest a semiconducting behavior of $Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75) single crystals. Data of Hall coefficient and thermoelectric power have good agreement with each other and confirms the p-type nature of these crystals. Our findings should motivate an in-depth investigation of the underlying mechanisms.

1. Introduction

Recently, Transition Metal Dichalcogenides (TMDCs) have attracted to a large extent because of their possible applications as lubricants, switching devices and photo-electrochemical solar energy converters and also marked anisotropy in many of their physical properties. They form a wide range of solid solutions [1,2] with either mixed metals or mixed chalcogenide compositions. The crystals of TMDCs are layered type, each layer being a sandwich 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. This crystalline anisotropy leads to anisotropy in their electrical properties. The VIB–VIA group of compounds have been studied extensively for their electrical properties [3–5]. Also, studies have been made so far on mixed systems such as $(Mo/W)Te_2$, $(Mo/W)Se_2$ [6] and $(Mo/W)(Se/Te)_2$ [7]. It appears from the literature that no attempt has been made to investigate the variation of properties like resistivity, Hall coefficient and thermoelectric power with the composition of $(Cr/Mo)Se_2$ solid solution in a single crystalline form. Recently we have reported the growth of single crystals of $Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75) by the chemical vapor transport technique using dual zone horizontal furnace [8]. In this paper [8] we have studied structural parameters by mean of powder X-ray diffraction, SAED pattern, surface topography and optical response of $Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75) single crystals. It is evident that the electrical resistivity is a physical property of enormous importance, both for the understanding of the solids and their actual applications. The temperature dependence of the electrical resistivity changes in a quite irregular manner because of various mechanisms, including the phonon scattering, mutual scattering of electrons and so forth, are involved in the electrical transport in different temperature ranges [9,10]. The thermoelectric effect proposes a distinct advantage over other methods because the measured thermoelectric voltage is directly related to the carrier concentration which makes the thermoelectric measurements simpler even for high mobility materials [4]. The study of thermoelectric power provides an independent way to determine carrier sign, density and position of Fermi level in semiconductors [11,12]. The materials with high electrical conductivity and large thermoelectric power possess outstanding thermoelectric properties. The temperature dependence of the electrical

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conductivity is inclined to many influencing factors. For a semiconductor, both the carrier mobility and carrier density are temperature dependent [13]. The objective of this study was to evaluate electrical resistivity (perpendicular and parallel to the *c*-axis), thermoelectric power and Hall coefficient of $Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75) single crystals.

2. Experimental

Single crystals of $Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75) were grown by the chemical vapor transport technique using iodine as a transporting agent. The growth parameters are shown in Table 1. The stoichiometric compositions of all the samples were confirmed through EDAX.

The high temperature resistivity measurements parallel and perpendicular to the *c*-axis were carried out in the temperature range 303–423 K for all the samples using four probe setup (Model:DFP-02), SES instruments Pvt. Ltd., Roorkee. Several readings were taken over different regions of specimen and consistent results were obtained in each case. The anisotropy ratio was calculated using the values of resistivity parallel and perpendicular to the *c*-axis. In order to evaluate the semiconducting nature of samples, Hall effect measurements were done by using the instrument Lakshore 7504 Hall measurement system at room temperature. For the confirmation of ohmic nature of the contacts, *I–V* characteristics for each contact were verified. The variations of thermoelectric power (TEP) with temperature were performed in the temperature range 308–423 K with the use of thermo power setup TPSS-200, scientific solutions, Mumbai, India. This experimental setup consists of two assemblies: one is the sample chamber with two heaters and pickup probes and the other is electronic circuits to control the temperature and also the temperature gradient across the sample. The temperature is measured by the thermocouple and the gradient is measured by the deferential temperature sensor. The sample is directly mounted on the two heaters and by applying the temperature gradient (5 K) between two ends of the sample, the thermoelectric power is generated which is measured by digital voltmeter of Keithly.

3. Results and discussion

3.1. Resistivity measurements

The resistivity variations of $Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75) single crystals with temperature (both perpendicular and parallel to the *c*-axis) were studied from 303 K to 423 K. The results plotted as log ρ vs. 1000/T for parallel and perpendicular to the *c*-axis are shown in Figs. 1 and 2 respectively. It is seen from Figs. 1 and 2 that there is a linear decrease in resistivity with increasing temperature, which is a characteristic of semiconducting materials. Also, the values of resistivity are higher in parallel direction than the perpendicular direction which suggests the conduction of electrons is very low in parallel direction. The conductivity curves seen to be in good agreement with the models related to the thermal carrier emission across

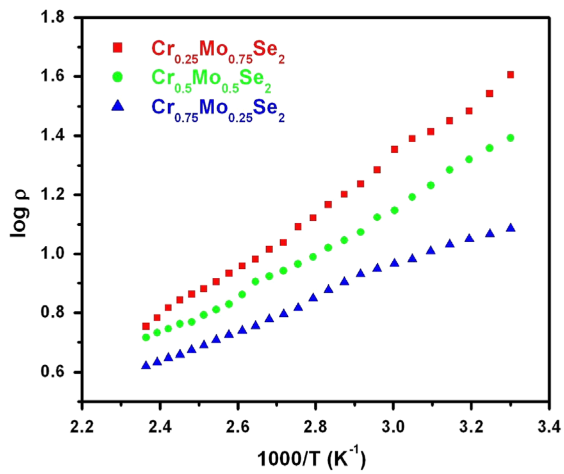

Fig. 1. Log ρ vs. 1000/T for parallel to the *c*-axis.

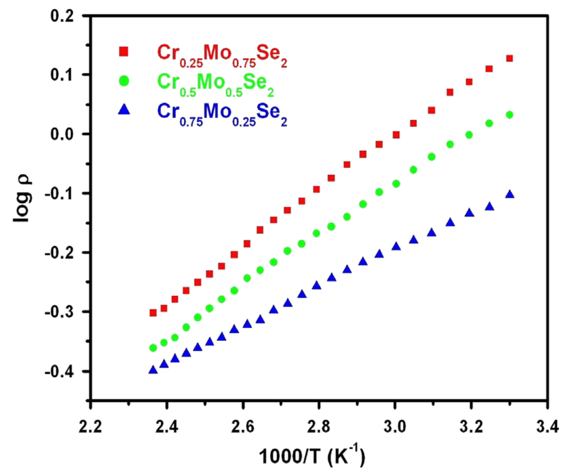

Fig. 2. Log ρ vs. 1000/T for perpendicular to the *c*-axis.

Table 1
Growth parameters of $Cr_xMo_{1-x}Se_2$ (x=0.25, 0.50, 0.75) single crystals.

Compound	Compound preparation		Single crystal growth			
			Temperature distribution		Growth time (h)	Dimensions (of largest crystal) (mm^3)
	Temperature (°C)	Time (h)	Cold zone (°C)	Hot zone (°C)		
$Cr_{0.25}Mo_{0.75}Se_2$	1000	100	900	1050	246	11 × 6 × 0.3
$Cr_{0.5}Mo_{0.5}Se_2$	1000	95	920	1050	240	13 × 7 × 0.3
$Cr_{0.75}Mo_{0.25}Se_2$	1000	90	950	1050	220	10 × 6 × 0.4