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The Electrical Resistance of $Mo_{0.5}W_{0.5}S_2$ Single Crystal Under Pressure

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Abstract

Single crystals of $Mo_{0.5}W_{0.5}S_2$ were grown by chemical vapour transport and direct vapour transport techniques. The crystals have been characterized by X-ray energy dispersive analysis and X-ray powder diffraction. The dc electrical resistance of the grown single crystals of $Mo_{0.5}W_{0.5}S_2$ was measured in Bridgman anvil set-up to 8 GPa to identify occurrence of structural phase transitions. The drastic changes in electrical resistance were observed at ~2.5 GPa and ~4.6 GPa, and are similar to the structural phase transitions in WS_2 single crystals.

Key Words: Electrical resistance, transition metal dichalcogenides, single crystal, structural phase transition.

PACS: 62.50+p; 73.0+f; 73.61Ga

1. Introduction

Lamellar solid of transition metal dichalcogenides of MX_2 (M=Mo, W, Nb, Ta and X = S, Se, Te) type have been extensively studied because of their excellent self-lubricating and photovoltaic properties [1]. Among the above MX_2, MoS_2 occurs naturally while other dichalcogenides are produced synthetically by direct combination of the constituent elements at elevated temperature. The use of MoS_2 is limited because of its relatively poor oxidation resistance above 400 °C, which results in formation of MoO_3 whose dynamic coefficient of friction is 0.5–0.6, and electrical resistivity is relatively high. A comparison between physical properties of MoS_2 and WS_2 suggests that WS_2 may have better high temperature, high pressure electrical conduction than MoS_2. Also, a low friction coefficient of WS_2 [2] makes them more promising for use in sliding electrical contacts. In our literature survey, a number of reports on high-pressure studies of MoS_2 are found [2–7], while single report is found for WS_2 [1]. In all these reports structural phase transition of MoS_2 is not reported until 8 GPa, while it is pointed out that WS_2 has phase transition at 4.1 to 4.35 GPa. This distinct character of structural transition of WS_2 in contrast to MoS_2 have motivated us to grow $Mo_{0.5}W_{0.5}S_2$ single crystals and to monitor dc electrical resistance against pressure to identify occurrence of any structural phase transition. To fulfil above objective, single crystal of $Mo_{0.5}W_{0.5}S_2$ have been grown using chemical vapour transport (CVT) technique with iodine as transporting agent and direct vapour transport (DVT) technique. The X-ray energy dispersive analysis confirmed the composition and X-ray diffraction studies supplied information about structural properties [8]. The temperature dependency of electrical resistivity, in the range of 70–443 K, and optical absorption study in tungsten-substituted molybdenum disulphide single crystals, have been reported elsewhere [8, 9]. Srivastava et al [10] reported micro structural parameters and other properties on $Mo_{1-x}W_xS_2$. Thus the present report is aimed on the measurement of dc electrical resistance of grown crystals of $Mo_{0.5}W_{0.5}S_2$ up to 8 GPa to observe the effect of structural phase transition.

2. Experimental Procedure

$Mo_{0.5}W_{0.5}S_2$ was synthesized in the form of single crystals. The materials for growth were thoroughly mixed in a quartz ampoule which was then evacuated at a pressure of 10^{-5} torr. The total amount of powder was 10 grams, consisting of 99.999% pure molybdenum, tungsten and sulphur powder taken in stoichiometric proportions. The sealed ampoule was placed into two-zone furnace at constant temperature 850 °C and the duration of charge preparation was five days. The thus-prepared charge was rigorously shaken to ensure proper mixing of constituents. The ampoule was finally placed coaxially in a two-zone furnace with reaction zone at 1200 °C and growth zone at 1100 °C for six days, and then allowed the ampoule to cool down slowly. Shining black opaque crystals were obtained. The average size of the crystals varied in the range 0.55–7 mm × 0.6–4 mm × 0.002–0.006 mm. The energy dispersive X-ray analysis confirmed the composition of grown crystal $Mo_{0.5}W_{0.5}S_2$ and X-ray diffraction study had confirmed the structural properties [11]. The room temperature measurement of resistance was carried out under pressure limiting up to 8 GPa. The pressure was generated using Bridgman anvil apparatus with tungsten carbide anvils. The cell assembly consisted of two pirophyllite gaskets, 12.7 mm outside diameter, 3 mm inside diameter and 0.20 mm thick and the specimen was located between two talc disks, 3 mm diameter and 0.20 mm thick, at the centre of the gasket ring. The pressure was calibrated with bismuth transitions at 2.5, 2.69 and 7.67 GPa. The reproducibility in the pressure measurement was ±0.1 GPa. A two-probe technique was used to evaluate the dc electrical resistance of $Mo_{0.5}W_{0.5}S_2$ single crystals.

3. Results and Discussion

Two different independent sets of data on two different samples of $Mo_{0.5}W_{0.5}S_2$ single crystal were taken: one grown via DVT, the second grown via CVT. Both sets of data showed the same nature of resistance variation as a function of pressure at room temperature. The obtained variations of dc electrical resistance of $Mo_{0.5}W_{0.5}S_2$ are shown in Figure.

From Figure it is observed that, at very low pressure, there was an initial decrease in resistivity with increase in pressure. This is indicative of a reduction in energy gap of two materials which then stabilized. As pressure is increased further, it is seen that resistance remains almost constant up to pressure of nearly 2.5 GPa. At ∼2.5 GPa, there is a sharp decrease in the resistance by two orders of magnitude, from $10^6\Omega$ to $10^4\Omega$. After the drop, the resistance of the sample remains constant up to a pressure of nearly 4.6 GPa. Then at ∼4.6 GPa the resistance of the sample sharply increases again, from $\sim10^4$ Ω to $\sim10^7\Omega$. Further increase in the pressure up to 8 GPa shows stability of the resistance of the sample.

These two drastic changes in the resistance seen in $Mo_{0.5}W_{0.5}S_2$single crystal around pressures of 2.5 GPa and 4.6 GPa confirm two-phase transitions at these pressures. In p-type WS_2, such two phase transitions were reported at 4.35 GPa and 5.5 GPa [1]. While in n-type WS_2, one phase transition was observed at 4.1 GPa. On the other hand, Dave et al [7] have reported initial decrease in resistance of MoS_2 at low pressure. Thus from the dc electrical resistance against pressure studies we conclude that at initial low pressure the grown $Mo_{0.5}W_{0.5}S_2$ single crystals may have structural characteristics of MoS_2 and than transforms to structure similar to that of the WS_2 crystals.

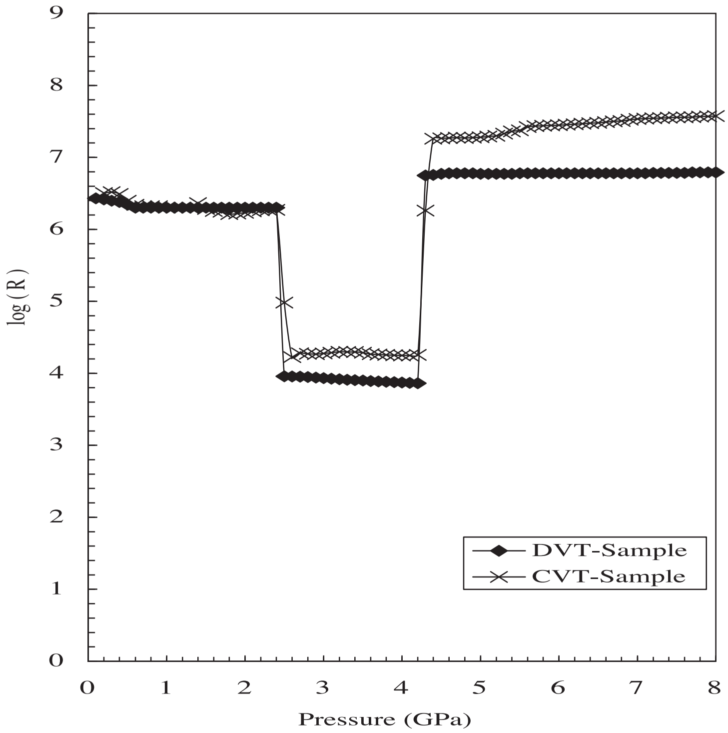

Figure. The dc electrical resistance of $Mo_{0.5}W_{0.5}S_2$ as a function of pressure at room temperature.

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