

## EFFECT OF RHENIUM DOPING ON VARIOUS PROPERTIES OF $\text{MoRe}_{0.001}\text{Se}_{1.999}$ SINGLE CRYSTAL

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Rhenium doped  $\text{MoSe}_2$  single crystal viz.  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  is grown by direct vapour transport (DVT) technique in the laboratory. This crystal is structurally characterized by X-ray diffraction, by determining their lattice parameters 'a' and 'c' and X-ray density. The Hall Effect and thermoelectric power measurements shows that  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  is p-type in nature. The direct and indirect band gap measurements are also undertaken on this semiconducting material.

*Keywords:* Structural properties, Electrical properties and Optical properties,  
 $\text{MoRe}_{0.001}\text{Se}_{1.999}$  single crystal

### 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 photoelectrochemical (PEC) solar cell for conversion of solar energy into electrical energy as well as photonic devices in various electronic applications. 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 [7-14]. These crystals become superconducting when intercalated with alkali and alkaline earth metals [15]. It is clear from that the literature survey that a lot of research work has been done on  $\text{MoSe}_2$  single crystal, however, the work on doping compounds of  $\text{MoSe}_2$  by metals is almost negligible. Hence, it was decided to work on Rhenium doped single crystal of  $\text{MoRe}_{0.001}\text{Se}_{1.999}$ . The results obtained in detail are described in the paper.

### 2. Experimental details

$\text{MoRe}_{0.001}\text{Se}_{1.999}$  single crystal is grown by direct vapour transport technique. The X-ray powder diffractograms recorded with the help of X-ray diffractometer using  $\text{CuK}\alpha$  radiation. For this purpose, many small crystals from each group were finely ground with the help of agate mortar and filtered through 106 micron sieve to obtain grains of nearly equal size. The values of lattice parameter 'a' and 'c', volume, X-ray density obtained from the diffractograms of the sample of the  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  single crystal are shown in Table 1.

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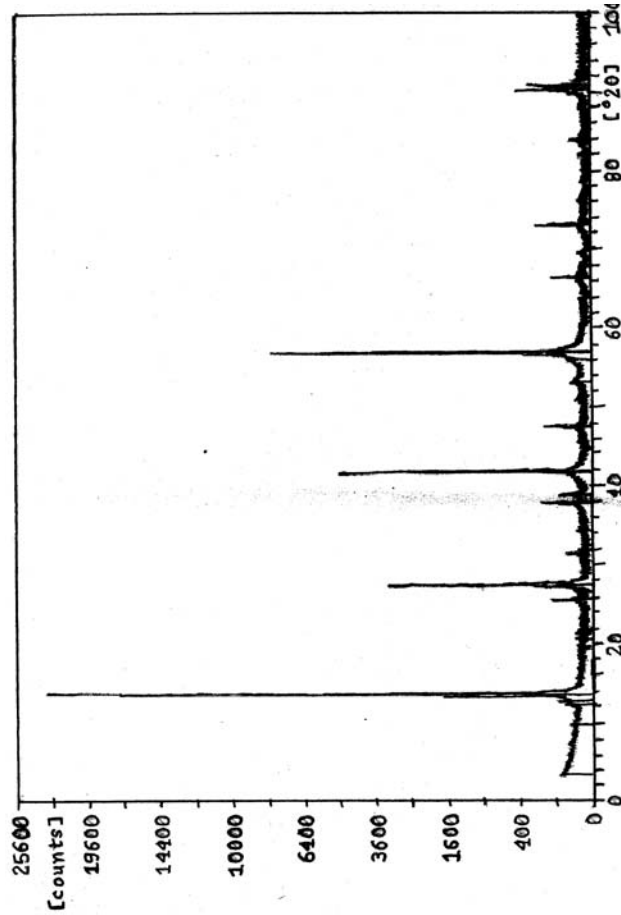


Fig. 1. X-ray diffractograms of  $\text{MoRe}_{0.001}\text{Se}_{1.999}$ .

Table 1. Structural, electrical and optical data of  $\text{MoRe}_{0.001}\text{Se}_{1.999}$ .

Parameters	$\text{MoSe}_2$	$\text{MoRe}_{0.001}\text{Se}_{1.999}$
$a$ (Å)	3.287	3.776
$c$ (Å)	12.921	13.140
Volume (Å) <sup>3</sup>	120.90	121.88
X-ray density (gm/cm <sup>3</sup> )	6.972	6.8344
Room Temperature Resistivity (Ω- cm)	5.4577	1.3590
Hall Coefficient (cm <sup>3</sup> /coul.)	638.22	2594.47
Mobility (cm <sup>2</sup> /V-Sec)	117.02	1909.08
Carrier concentration (cm <sup>-3</sup> )	$0.97 \times 10^{16}$	$2.41 \times 10^{16}$
Direct band gap (eV)	1.47	1.425
Indirect band gap (eV)	1.195	1.125

From Hall Effect measurements on each sample, the resistivity, mobility and carrier concentration were determined whose values are also shown in the Table 1. Thermo power measurements were carried out on TEP apparatus in the temperature range room temperature to 122 °C which is shown in Fig. 2. Since these crystals are semiconducting in nature, the optical

characterization for determining the direct and indirect band gap is carried out on UV-VIS-NIR spectrophotometer in the range 700 nm to 1450 nm.

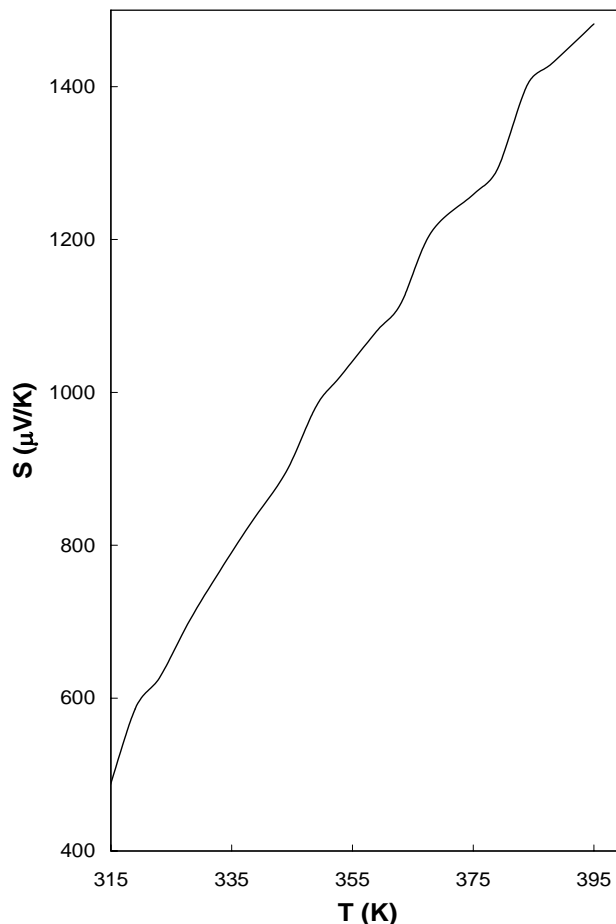


Fig. 2. Temperature dependent Seeback coefficient (S) (in  $\mu\text{V/K}$ ) of  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  single crystal.

### 3. Results and discussion

The X-ray diffractograms of  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  in Fig. 1 clearly shows that (002) reflection is of the maximum intensity and thereby indicates strong orientation along the c-axis. The diffractograms for  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  is similar to those of  $\text{MoSe}_2$ . The lattice parameter 'a' remains constants for all the samples while there is a slight amount of increase in 'c' parameter indicates that rhenium has been doping in between the layers thereby expanding the 'c' parameter. This increase is very small because the amount of rhenium doped with  $\text{MoSe}_2$  is also lesser in proportion. As proportion of rhenium addition is increased in  $\text{MoSe}_2$ , its X-ray density also increases which can be seen from the Table 1. This may be because of rhenium atoms added to the lattice of  $\text{MoSe}_2$ . Room temperature resistivity obtained from Hall Effect decreases by addition of rhenium, which can be correlated to the decrease in band gap. Mobility and carrier concentration also increases as the proportion of rhenium increases in  $\text{MoSe}_2$  crystal, which indicates the increase in the charge carriers.

The variation of Seeback coefficient with temperature for  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  is shown in Fig. 2. It is observed from the Fig. 2 that, the sample is semiconducting in behavior and p-type in nature, which is also confirmed from Hall measurements. The optical absorption spectra have been obtained in the range 700 nm to 1400 nm because the absorption edge is obtained in this region. The direct and indirect band gap for  $\text{MoRe}_{0.001}\text{Se}_{1.999}$  are obtained from the graph of  $(\alpha h\nu)^2$  Vs.

$h\nu$  and  $(\alpha h\nu)^{1/2}$  Vs.  $h\nu$ . The values obtained are shown in Table 1, which shows that there is no change in the indirect band gap of MoSe<sub>2</sub> after doping of rhenium while small variation in the direct band gap has been observed. The decrease in the band gap may be because of the impurity levels introduced due to the addition of rhenium in MoSe<sub>2</sub> [1-8]. One of a possible mechanism determining the features of the energy bands may be caused by inter-layer low-energy membrane rigid phonon modes, which was demonstrated by Rybak *et al.* [16].

#### 4. Conclusion

The analysis of accurate measurements of the structural, electrical and optical properties of MoRe<sub>0.001</sub>Se<sub>1.999</sub> single crystals has shown that rhenium doping affects the properties of MoSe<sub>2</sub> single crystals. Also the Hall Effect and thermoelectric power measurements shows that MoRe<sub>0.001</sub>Se<sub>1.999</sub> is p-type in nature. There is no change in the indirect band gap of MoSe<sub>2</sub> after doping of rhenium while small variation in the direct band gap has been observed.

#### References

- [1] A. M. Vora, P. K. Garg, Indian J. Phys. **74A**, 563 (2000).
- [2] A. M. Vora, M. Phil. Dissertation, Sardar Patel University, Vallabh Vidyanagar, India (1998).
- [3] Mihir M. Vora, Aditya M. Vora, Cryst. Res. Tech. **41**, 803 (2006).
- [4] Mihir M. Vora, Aditya M. Vora, Cryst. Res. Tech. **42**, 50 (2007).
- [5] Mihir M. Vora, Aditya M. Vora, Cryst. Res. Tech. **42**, 186 (2007).
- [6] Aditya M. Vora, Cryst. Res. Tech. **42**, 286 (2007).
- [7] Mihir M. Vora, Aditya M. Vora, Chalcogenide Lett. **4**, 77 (2007).
- [8] Mihir M. Vora, Aditya M. Vora, Chalcogenide Lett. **4**, 85 (2007).
- [9] Mihir M. Vora, Aditya M. Vora, Chalcogenide Lett. **4**, 85 (2007).
- [10] G. V. Subba Rao, M. W. Schafer, Physics and Chemistry of Materials with Layered Structures, Vol.-VI, D. Reidal, Holland (1976).
- [11] G. V. Subba Rao, C. S. Sunandana, in Preparation and Characterization of Materials, Eds. J. M. Honing and C. N. R. Rao (Eds) Academic Press, London (1981) p. 269.
- [12] E. Bayer, W. Rudorff, Z. Natureforsch **71**, 128 (1959).
- [13] W. Rudorff, M. H. Sicks, Angew. Chem. **71**, 128 (1959).
- [14] W. Rudorff, Chimia **19**, 128 (1965).
- [15] J. A. Woolam, R. B. Somoano, Phy. Rec. **13**, 3483 (1976)
- [16] R. B. Somoano, J. A. Woolam, in Intercalated Materials, Eds. F. Levy and Reidal, Dordrecht (1979) p. 307.