Chapter 6

Temperature dependent electrical properties of
MoSe$_{2-x}$Te$_x$ ($x = 0.25, 0.5, 1, 1.5, 1.75$) single crystals

Discovery of electric current have provided an accelerating force in the development of human life. A desire to get the improved functionality of existing systems and to find something superior resulted in the development of electronic technology. Currently this development is hastening mainly due to the researches going in the direction of finding new materials having different electronic transport properties. Knowledge of such properties of different materials can be used to design or improve any electrical or electronic device. This chapter provides the results obtained by measurement of electrical properties of 2H-Mo Se$_{2-x}$Te$_x$ single crystals grown by chemical vapor transport technique.
6.1 INTRODUCTION

The study of structural, optical and electrical properties of the layered compounds of the group VIA-VIB have aroused a wide spread interest and attention of the material scientists all over the world during the last few decades [1-4].

Most of the semiconductor applications are governed by the electrical properties of the materials. The electrical properties of the VIA-VIB compounds have been carried out by different investigators [5-8]. Most of these studies are nearly confined to investigations of electrical properties along the cleavage plane and very few of them report the interesting question of electrical transport normal to the cleavage plane [6-7]. Transition metal dichalcogenides (TMDCs) are one kind of important two-dimensional materials with thickness of the order of two or three atomic layers, is of particular interest due to their remarkable electronic, optical and electrical properties. In general, the 2D layered TMDCs (with few layers to monolayer) have attracted wide interest both experimentally and theoretically during recent years [8-15]. The material MoSe$_{2-x}$Te$_x$ (x = 0.25, 0.5, 1, 1.5, 1.75) is a diamagnetic semiconductor belong to the family of groups VIA-VIB layered type TMDCs [16-20], with formula MX$_2$, where M is the transition metal atom (i.e. Mo, W, etc.) and X being the chalcogen atom (i.e. S, Se and Te). The material exhibits high anisotropy in both electrical and optical properties along and perpendicular to the van-der Waals planes. The reason of this extreme anisotropy is the sandwich structure X-M-X atomic layers, loosely bonded by weak van-der Waals forces interacting with each other [20-25].

In the present work, we report the electrical transport properties measurements of MoSe$_{2-x}$Te$_x$ (x = 0.25, 0.5, 1, 1.5, 1.75) single crystals. The electrical resistivity (parallel and perpendicular to c-axis), thermoelectric power, and Hall effect measurements have been carried
out using standard methods to study the electrical transport phenomena of MoSe$_{2-x}$Te$_{x}$ ($x = 0.25, 0.5, 1, 1.5, 1.75$) single crystals.

**6.2 METHODS FOR ELECTRICAL RESISTIVITY MEASUREMENT**

The resistivity of a conducting material is determined by measuring the resistance of a sample of known geometry by forcing a current through the sample with one pair of leads while measuring the voltage drop with a second pair of leads. Different methods can be used to determine the resistivity of a sample depending on the size and shape of the sample. All the methods require a sensitive voltmeter with a current source or a micro-ohmmeter because the resistance to be measured is very low.

**6.2.1 Bulk Resistivity Measurement**

Figure 6.1 shows a resistivity measurement scheme for a bulk sample. The current source is connected to both ends of the sample. The voltmeter leads are placed at known distance apart. The resistivity is calculated from the cross-sectional area of sample and distance between voltmeter leads as

$$\rho = \frac{V}{I} \left( \frac{A}{L} \right)$$  \hfill (6.1)

Where $\rho$ = resistivity  
$V$ = voltage measured by voltmeter  
$I$ = source current  
$A$ = cross section area of sample ($w \times t$)  
$L$ = distance between voltmeter leads

![Resistivity measurement scheme for bulk samples.](image)

**Figure 6.1** Resistivity measurement scheme for bulk samples.
To compensate for thermoelectric voltages, one voltage reading is taken with positive test current and other is taken with negative test current. The absolute values of these two readings are then averaged and used in the equation (6.1).

### 6.2.2 Four probe method

The four probe method is used when the sample to be tested is very thin such as epitaxial wafers and conductive coatings. Figure 6.2 is a diagram of four collinear probe set-up for resistivity measurements. The current is sourced through the two outer probes and the voltage drop is measured between two inner probes. The surface or sheet resistivity is calculated as

$$\rho_s = \left( \frac{\pi}{\ln 2} \right) \left( \frac{V}{I} \right)$$

Where $\rho_s$ = sheet resistivity

$V$ = measured voltage

$I$ = source current

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**Figure 6.2** Resistivity measurement scheme in four probe method.
If the thickness of the sample is known, the bulk or volume resistivity can be calculated as

\[ \rho = \left( \frac{\pi}{\ln 2} \right) \left( \frac{V}{I} \right) t \]  

(6.3)

Where \( \rho \) = bulk resistivity

\( t \) = thickness

### 6.2.3 Van der Pauw method

The van der Pauw method is used for the samples that are flat, homogeneous in thickness and arbitrarily shaped. As shown in the figure 6.3, contacts should be small and placed on the periphery of the sample.

![Resistivity measurement scheme in van der Pauw method](image)

**Figure 6.3** Resistivity measurement scheme in van der Pauw method.

To make a measurement, current is caused to flow along one edge of the sample (for instance, \( I_{12} \)) and the voltage across the opposite edge (for instance, \( V_{34} \)) is measured. Then the resistance can be calculated as

\[ R_{12,34} = \frac{V_{34}}{I_{12}} \]  

(6.4)

Van der Pauw discovered that the sheet resistance of an arbitrarily shaped sample can be determined from such resistances. The actual sheet resistance is related to these resistances by van der Pauw formula

\[ e^{\left( -\frac{\pi R_{2,34}}{R_s} \right)} + e^{\left( -\frac{\pi R_{3,41}}{R_s} \right)} = 1 \]  

(6.5)
6.3 MEASUREMENT OF TEMPERATURE DEPENDENT ELECTRICAL RESISTIVITY OF 2H-MoSe$_{2-x}$Te$_x$ SINGLE CRYSTALS

6.3.1 Experimental arrangement

In order to measure the temperature dependent resistivity, a high temperature resistivity measurement set-up was designed at the Department of Physics, Sardar Patel University. Using this set-up a temperature dependent resistivity can be measured from room temperature to 778K. Photograph of the sample holder and schematic arrangement of sample in it are shown in figure 6.4. The sample under test is pressed on the ceramic base containing horizontal electrical leads. Then the sample holder is inserted in a vertical tubular furnace. Source current is applied by a constant current source and voltage is measured by Keithley-2700 digital multimeter.
6.3.2 Temperature dependent electrical resistivity parallel to c-axis

Single crystals of 2H-MoSe$_{2-x}$Te$_x$ always grow in the form of platelets having thickness along c-axis. This immediately allows any electrical measurement for both parallel and perpendicular to c-axis. In present case single crystals were cut in rectangular shape and the temperature dependent resistivity (parallel and perpendicular to c-axis) was measured by four probe method from room temperature to 778K. Obtained results are plotted in figures 6.5-6.14. A detailed study of the variation of dc electrical resistivity as a function of the crystal composition reveals that the resistivity increases non-linearly with the increasing selenium content in the solid solution of 2H-MoSe$_{2-x}$Te$_x$ (x = 0.25, 0.5, 1, 1.5, 1.75) as shown in figures 6.5-6.14. This analogous behavior is also observed in the WSe$_{2-x}$Te$_x$ [5]. The room temperature in-plane resistivity of 2H-MoSe$_{2-x}$Te$_x$ is ranging from 1.56 Ω-cm to 4.5 Ω-cm (with increasing proportion of selenium) which is in good agreement with the earlier reported values [5].

![Figure 6.5](image)

**Figure 6.5** Temperature dependent electrical resistivity parallel to c-axis of 2H-MoSe$_{1.75}$Te$_{0.25}$ single crystals.
Figure 6.6 Temperature dependent electrical resistivity parallel to c-axis of 2H-MoSe\textsubscript{1.5}Te\textsubscript{0.5} single crystals.

Figure 6.7 Temperature dependent electrical resistivity parallel to c-axis of 2H-MoSeTe single crystals.
Figure 6.8 Temperature dependent electrical resistivity parallel to c-axis of $2H$-MoSe$_{0.5}$Te$_{1.5}$ single crystals.

Figure 6.9 Temperature dependent electrical resistivity parallel to c-axis of $2H$-MoSe$_{0.25}$Te$_{1.75}$ single crystals.
Figures 6.5-6.9 reveal that the temperature dependence of resistivity parallel to c-axis for all materials shows decreasing trend with increasing temperature. This can be attributed to the high carrier concentration which gives rise to energy levels very close to the conduction band. These carriers will also be scattered by various centers or regions such as grain boundaries, dislocations, surface states etc. The loosely coupled X-M-X atom sheet sandwiches make such material extremely anisotropic both mechanically and electrically. The carriers move by hopping rather than a band mechanism in the former direction [14].

### 6.3.3 Temperature dependent electrical resistivity perpendicular to c-axis

Measurements of electrical resistivity perpendicular to c-axis of the grown crystals were also performed by four probe resistivity measurement technique. Obtained results are plotted in figure 6.10-6.14. Here the value of resistivity perpendicular to c-axis of single crystals of 2H-MoSe$_{2-x}$Te$_x$ is found to be ~10 times smaller than the resistivity parallel to c-axis. It is quite obvious because the inlayer bonding in the grown crystals is short ranged covalent type while the interlayer bonding is relatively long ranged van der Waals type.
Figure 6.10 Temperature dependent electrical resistivity perpendicular to c-axis of 2H-MoSe$_{1.75}$Te$_{0.25}$ single crystals.

Figure 6.11 Temperature dependent electrical resistivity perpendicular to c-axis of 2H-MoSe$_{1.5}$Te$_{0.5}$ single crystals.
Figure 6.12 Temperature dependent electrical resistivity perpendicular to c-axis of 2H-MoSeTe single crystals.

Figure 6.13 Temperature dependent electrical resistivity perpendicular to c-axis of 2H-MoSe_{0.5}Te_{1.5} single crystals.
Figure 6.14 Temperature dependent electrical resistivity perpendicular to c-axis of 2H-MoSe$_{0.25}$Te$_{1.75}$ single crystals.

Obtained results of the temperature dependent electrical resistivity perpendicular to c-axis of 2H-MoSe$_{2-x}$Te$_{x}$ single crystals show some remarkable features as beneath.

- The electrical measurements on 2H-MoSe$_{2-x}$Te$_{x}$ single crystals have proved very difficult to obtain satisfactorily, due to the layered structure of these materials. The crystal edges are exceedingly soft and any damage on a microscopic level lead to extensive ‘shorting out’ of the high crystalline anisotropy of the sandwiches.

- Temperature dependent electrical resistivities of 2H-MoSe$_{2-x}$Te$_{x}$ except 2H-MoSe$_{0.25}$Te$_{1.75}$ vary smoothly within the entire temperature range. Like resistivity parallel to c-axis, here the resistivity perpendicular to c-axis of 2H-MoSe$_{2-x}$Te$_{x}$ does not show any transition corresponding to structural changes.
• The temperature dependent electrical resistivity of 2H-MoSe$_{0.25}$Te$_{1.75}$ shows the hump at 475K that may due to the rapid increment in the temperature cause the sudden decrement in resistivity.

6.3.4 Anisotropy

For the single crystals belonging to the layered structure family, the anisotropy of the transport properties is an interesting phenomenon. These types of materials behave extremely two-dimensionally as far as their mechanism is concerned. They are very difficult to handle because planes slide easily along the layers held together by the very weak van der Waals bonding. Intuitively and inquisitively enough; one might also expect similar anisotropies in the electrical properties i.e. the conductivities.

Although layered compounds are indeed anisotropic, there is a great variation in the anisotropy ratio among them. In some cases, anisotropy factors up to $10^6$ have been reported [22]. Here the measurements of resistivity perpendicular to c-axis $\rho_\perp$ and parallel to c-axis $\rho_{\parallel}$ in the temperature range 295K to 778K were used to determine the anisotropy ratio for the single crystals of 2H-MoSe$_{2-x}$Te$_x$ ($x = 0.25, 0.5, 1, 1.5, 1.75$).

The anisotropy ratio $\gamma$ can be defined as,

$$\gamma = \frac{\rho_{\parallel}}{\rho_\perp}$$  (6.6)

Dependence of $\gamma$ on the temperature is shown in figures 6.15-6.19.
Figure 6.15 Temperature dependence of anisotropy for electrical resistivity of 2H-MoSe$_{1.75}$Te$_{0.25}$ single crystals.

Figure 6.16 Temperature dependence of anisotropy for electrical resistivity of 2H-MoSe$_{1.5}$Te$_{0.5}$ single crystals.
**Figure 6.17** Temperature dependence of anisotropy for electrical resistivity of 2H-MoSeTe single crystals.

**Figure 6.18** Temperature dependence of anisotropy for electrical resistivity of 2H-MoSe$_{0.5}$Te$_{1.5}$ single crystals.
Figure 6.19 Temperature dependence of anisotropy for electrical resistivity of 2H-MoSe$_{0.25}$Te$_{1.75}$ single crystals.

It is seen from figures 6.15-6.19 that the dependence of anisotropy ratio on temperature is quite random for all the materials. It is obvious because the temperature dependence of electrical resistivity parallel and perpendicular to c-axis of these materials are completely different [23].

6.3.5 Activation energy measurement

Thermal activation energies were calculated from the different slopes of figure 6.20-6.24 using the Arrhenius type relation:

$$\rho = \rho_0 \exp\left(\frac{E_a}{k_B T}\right)$$  \hspace{1cm} (6.7)

Where $k_B$ is Boltzmann’s constant, $E_a$ is the activation energy and $T$ is the absolute temperature.
Figure 6.20 Variation of $\ln \rho$ with inverse of temperature for $2\text{H-MoSe}_{1.75}\text{Te}_{0.25}$ single crystals.

Figure 6.21 Variation of $\ln \rho$ with inverse of temperature for $2\text{H-MoSe}_{1.5}\text{Te}_{0.5}$ single crystals.
Figure 6.22 Variation of $\ln \rho$ with inverse of temperature for 2H-MoSeTe single crystals.

Figure 6.23 Variation of $\ln \rho$ with inverse of temperature for 2H-MoSe$_{0.5}$Te$_{1.5}$ single crystals.
Figure 6.24 Variation of $\ln \rho$ with inverse of temperature for $2H$-MoSe$_{0.25}$Te$_{1.75}$ single crystals.

Table 6.1 Activation energies for different temperature ranges for $2H$-MoSe$_{2x}$Te$_x$ single crystals.

<table>
<thead>
<tr>
<th>Temperature range</th>
<th>Activation energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$2H$-MoSe$_{2-x}$Te$_x$</td>
</tr>
<tr>
<td></td>
<td>x = 0.25</td>
</tr>
<tr>
<td>298-563 (K)</td>
<td>0.2814</td>
</tr>
<tr>
<td>568-778 (K)</td>
<td>0.7060</td>
</tr>
</tbody>
</table>

The activation energies for high temperature region 568-778 K from the slope of the linear regions of figures 6.20-6.24 varies from 0.41-0.70 eV (as the selenium concentration is increase) which is almost of the half of the electrical band gap. The low value of activation energies ranging from 0.28-0.12 eV is obtained for low temperature range 298-563 K. Our measurements for activation energies in high temperature region are similar to those of the earlier investigators [20]. Above 568K, the $\ln \rho$ vs. 1000/T curves for MoSe$_{2-x}$Te$_x$ yield thermal energies ranging from 0.70-0.41 eV. Evans and Hazelwood [20] reported observations on n type
MoSe$_2$ single crystals grown by direct vapor transport technique of $E_g = 1.1\text{eV}$ in the temperature range above 700K.

### 6.4 MEASUREMENT OF HALL-EFFECT

Measurements of Hall-effect were performed on the grown single crystals for the determination of carrier concentration. Schematic arrangement for the measurement is shown in Figure 6.25.

![Schematic arrangement for the Hall-effect measurement.](image)

**Figure 6.25** Schematic arrangement for the Hall-effect measurement.

Charge carriers in a magnetic field $B_z$ are subject to the Lorentz force $F_{\text{Lorentz}}$, given by

$$F_{\text{Lorentz}} = e(v_x \times B_z)$$  \hspace{1cm} (6.8)

Where $e$ is the charge of a carrier, and $v_x$ is the velocity of carriers. Due to the Lorentz force, charge carriers deflect to one side of the sample (x-z plane), forming a transverse electric field $E_y$ which opposes further deflection and accumulation. At the steady state condition, the electric force $F_{\text{electric}} = eE_y$ counter balances the Lorentz force $F_{\text{Lorentz}}$, so enabling the continuous current flow as before. The required electric field $E_y$ is

$$E_y = (v_x \times B_z)$$  \hspace{1cm} (6.9)
Figure 6.26 Carrier concentrations in 2H-MoSe$_{2-x}$Te$_x$ single crystals.

The relationship between current density $j_x$ and velocity $v_x$ is given by

$$j_x = nev_x$$  \hspace{1cm} (6.10)

Where $n$ is the carrier concentration. Hence, we obtain

$$E_y = \frac{j_x}{ne} B_z$$  \hspace{1cm} (6.11)

The Hall coefficient $R_H$ is defined by the equation

$$E_y = R_H j_x B_z$$  \hspace{1cm} (6.12)

Thus the Hall coefficient is given by

$$R_H = -\frac{1}{ne}$$  \hspace{1cm} (6.13)

Equation obtained here is valid for metals and strongly degenerate semiconductors because the carriers occupy a narrow energy range in the order of $k_B T$ around the Fermi level. Therefore, all carriers have nearly the same velocity and they will be deflected in a given magnetic field by approximately the same amount. Obtained values of carrier concentration for the grown single crystals are plotted in figure 6.26 which lies in the semiconducting range of carrier concentration.
6.5 THERMO-ELECTRIC POWER

Thermoelectric power concerns the generation of an EMF (Electro Motive Force) due to thermal gradient. Physically in a metal this phenomenon arises because electrons at the hot end find state of lower energy at the cold end and try to diffuse towards cold end. Electrons at the hot end become more energetic and therefore get greater velocities than those in the cold end. Consequently there is a net diffusion of electrons from hot end towards cold end which leaves behind exposed positive ions in the hot end and accumulates electrons in the cold end. This situation prevails until the electric field developed between the two ends prevents further electron motion from hot end to cold end. A potential difference is therefore developed between two ends of the sample, which is known as Seebeck effect. This phenomenon is expressed in figure 6.27.

![Figure 6.27](image)

**Figure 6.27** Generation of potential difference due to a temperature gradient: The Seebeck effect.

The potential difference developed per unit temperature difference is denoted as Seebeck coefficient ‘S’ and it is expressed in terms of equations as

\[ S = \frac{\Delta V}{\Delta T} \]  \hspace{1cm} (6.14)

and

\[ \Delta V = \int_{T_i}^{T_f} S \, dT \]  \hspace{1cm} (6.15)
6.5.1 **Experimental arrangement**

To measure the Seebeck coefficient as a function of temperature for the samples used in the present investigations, “*Thermoelectric power set-up TPSS-200*” was used [23]. The experimental set-up is shown in figure 6.28. It consists of two blocks:

1. Sample holder with heaters and pick up probes
2. Electronic circuit controlling temperature and temperature gradient across the sample.

The sample holder consists of two low power heaters A and B (25 W each). The temperature $T$ of the heater A is measured by thermocouple $(TC_1)$ and the temperature gradient $\Delta T$ between A and B is measured by differential temperature sensor $(TC_2)$. Both the thermocouples are of $K$ type. The sample under investigation is mounted directly on the heaters, and is held by two pick up probes, which are of brass. These probes also measure the Seebeck voltage developed across the two ends of the sample.

![Figure 6.28](image)

**Figure 6.28** The thermoelectric power measurements system(TPSS-200).
The second block consists of temperature indicator, proportional controller and two-heater control circuit which drive the two heaters A and B. With the help of this electronic control circuit it is possible to generate a stable temperature gradient between the two heaters. It is possible to control the temperature from 298K to 573K and $\Delta T$ of $\pm 1$ to $\pm 10$K simultaneously with better than $\pm 1$ K stability. The problem usually encountered in making thermoelectric power measurements are stray thermal emfs. In the present instrument these have been eliminated by providing choice of selection of temperature gradient in the range of 1K to 10K. The sample and the electronic circuit have been incorporated into one unit. Use of low power heaters and electronic controllers makes the operation very easy and Seebeck coefficient of the sample can be measured conveniently.

### 6.5.2 Measurement of thermoelectric power in 2H-MoSe$_{2-x}$Te$_x$ single crystals

Thermoelectric power in 2H-MoSe$_{2-x}$Te$_x$ single crystals was measured in the temperature range from room temperature to 573K with a temperature gradient of 5K. Obtained results are plotted in figure 6.29-6.38.

![Figure 6.29](image)

Figure 6.29 Temperature dependence of Seebeck coefficient for 2H-MoSe$_{1.75}$Te$_{0.25}$ single crystals.
Figure 6.30 Temperature dependence of Seebeck coefficient for 2H-MoSe$_{1.5}$Te$_{0.5}$ single crystals.

Figure 6.31 Temperature dependence of Seebeck coefficient for 2H-MoSeTe single crystals.
Figure 6.32 Temperature dependence of Seebeck coefficient for 2H-MoSe$_{0.5}$Te$_{1.5}$ single crystals.

Figure 6.33 Temperature dependence of Seebeck coefficient for 2H-MoSe$_{0.25}$Te$_{1.75}$ single crystals.
Figures 6.29-6.33 show the variation of the thermoelectric power with temperature for 2H-MoSe$_{2-x}$Te$_x$ crystal. The thermoelectric power rapidly increases with increasing the temperature up to 523K. Then it slowly increases up to the values ≈ -1.5 to -0.78 mV/K till the temperature 573K is reached. Any transition is not found in the variation of thermoelectric power with temperature. The high Seebeck coefficient of 2H-MoSe$_{2-x}$Te$_x$ is due to the selenium incorporated into the compound. The thermoelectric power for transition metal selenides compounds is high compared to the transition metal tellurides due to the fact that selenium is more semiconducting than tellurium. There is no any peak observed in the variation of thermoelectric power with temperature which is not similar with data reported by Agarwal et al [26]. However, the resistivity data are similar to those reported by Agarwal et al [26]. It is also noticed from the variation of thermoelectric power that little addition of tellurium in the system of 2H-MoSe$_{2-x}$Te$_x$ up-to several atomic percent cause only moderate lowering of the Seebeck co-efficient. Larger additions of tellurium in this system cause a rapid decrease in the Seebeck co-efficient in the whole temperature range. This may be due to the appearance of the metallic nature of the tellurium.

From the study of thermoelectric power, the polarity of the thermally generated voltage at the hot end is positive indicating that the crystal is n-type in nature. The effective mass of the charge carriers, i.e. electrons and scattering constants have been obtained from the analysis of the data of TEP (thermoelectric power) measurement. The information which is obtained from TEP measurement is used to understand the scattering mechanism. The systematic study of TEP with temperature variation provides carrier sign, density of charge carriers and position of Fermi level in the semiconductor.

For the study of temperature dependent TEP for non-degenerate n-type semiconductor, the expression given by Mohanchandra & Uchil [27] is used as,
\[ S = \frac{k_B}{e} \left[ A + \left( \frac{E_F}{k_B T} \right) \right] \]  

(6.16)

From the above equation one can plot \( S \) versus inverse of temperature and get the values of scattering parameters and Fermi energy which are plotted in figures 6.34-6.38.

**Figure 6.34** The variation of the thermoelectric power with inverse of temperature for 2H-MoSe\(_{1.75}\)Te\(_{0.25}\) single crystals.
Figure 6.35 The variation of the thermoelectric power with inverse of temperature for 2H-MoSe$_{1.5}$Te$_{0.5}$ single crystals.

Figure 6.36 The variation of the thermoelectric power with inverse of temperature for 2H-MoSeTe single crystals.
Figure 6.37 The variation of the thermoelectric power with inverse of temperature for $2\text{H-MoSe}_{0.5}\text{Te}_{1.5}$ single crystals.

Figure 6.38 The variation of the thermoelectric power with inverse of temperature for $2\text{H-MoSe}_{0.25}\text{Te}_{1.75}$ single crystals.
From the slopes and intercepts of figures 6.34-6.38, we can get the values of $E_F$ (Fermi energy) and $A$ (scattering constant) respectively for 2H-MoSe$_{2-x}$Te$_x$. The dominant scattering mechanism in the n-type non degenerate semiconductor is understood by the value of $A$. The value of $A$ is given by,

$$ A = \frac{5}{2} - s $$  \hspace{1cm} (6.17)

Where, $s$ is the scattering parameter.

The value of $A$ varies from 0 to 4. From the graphs of $S$ versus 1000/T the obtained values of $A$ vary in the range 3.26-1.33. Using this value of $A$, the values of $s$ were found to be -0.76 to 1.17 using equation (6.17).

The constant value of $E_F$ for the whole temperature range implies that the carrier concentration $n$ does not change with the temperature. Therefore the equation (6.16) for thermoelectric power is written as,

$$ S = -\frac{k_B}{e} \left[ A + \ln \left( \frac{N_A}{n} \right) \right] $$ \hspace{1cm} (6.18)

Where $N_A$ is the density of the states and it is given by the equation,

$$ N_A = 2(2\pi m^*_n k_B T)^{\frac{3}{2}} $$ \hspace{1cm} (6.19)

$m^*_n$ is the band effective mass of the electrons. The effective density of the states can be calculated using the obtained value of carrier concentration from Hall Effect measurement. $N_A$ is calculated from the formula,

$$ n = N_A \exp \left( \frac{E_F - k_B T}{k_B T} \right) $$ \hspace{1cm} (6.20)

Where $E_F$ is the Fermi energy, $k_B$ is the Boltzmann constant and $T$ is the temperature. By using the value of effective density of states, the band effective mass of the electrons can be evaluated from the equation (6.19). The aforesaid parameters are tabulated in table 6.2.
### TABLE 6.2

Calculated values of Fermi energy ($E_F$), Density of states ($N_A$), Band effective mass ($m^*_{n}$), Scattering constant ($A$), Scattering parameter ($s$) and Hall co-efficient.

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$E_F$ (eV)</th>
<th>$N_A$/cm$^3$</th>
<th>$m^*_{n}$ (gm)</th>
<th>$A$</th>
<th>$s$</th>
<th>$R_H$ cm$^3$/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>2H-MoSe$<em>{1.75}$Te$</em>{0.25}$</td>
<td>0.9469</td>
<td>-3.84×10$^{19}$</td>
<td>0.06$m_e$</td>
<td>3.26</td>
<td>-0.76</td>
<td>-193.50</td>
</tr>
<tr>
<td>2H-MoSe$<em>{1.5}$Te$</em>{0.5}$</td>
<td>0.8792</td>
<td>-3.37×10$^{20}$</td>
<td>0.12$m_e$</td>
<td>2.99</td>
<td>-0.49</td>
<td>-131.86</td>
</tr>
<tr>
<td>2H-MoSeTe</td>
<td>0.8140</td>
<td>-1.01×10$^{21}$</td>
<td>0.17$m_e$</td>
<td>2.65</td>
<td>-0.15</td>
<td>-76.40</td>
</tr>
<tr>
<td>2H-MoSe$<em>{0.5}$Te$</em>{1.5}$</td>
<td>0.6800</td>
<td>-1.64×10$^{21}$</td>
<td>0.25$m_e$</td>
<td>2.15</td>
<td>0.35</td>
<td>-60.96</td>
</tr>
<tr>
<td>2H-MoSe$<em>{0.25}$Te$</em>{1.75}$</td>
<td>0.4334</td>
<td>-3.19×10$^{21}$</td>
<td>0.29$m_e$</td>
<td>1.33</td>
<td>1.17</td>
<td>-26.70</td>
</tr>
</tbody>
</table>

**Figure 6.39** The variation of constant A with concentration of selenium for 2H-MoSe$_{2-x}$Te$_x$ single crystals.
Figure 6.40 The variation of Fermi energy ($E_F$) with concentration of selenium for 2H-MoSe$_{2-x}$Te$_x$ single crystals.

Figure 6.41 The variation of scattering parameter $s$ with concentration of selenium for 2H-MoSe$_{2-x}$Te$_x$ single crystals.
Figures 6.39-41 show the variation of A (Scattering Constant), Fermi Energy (E_F) and s (scattering parameter) with increasing concentration of selenium in 2H-MoSe_{2-x}Te_x single crystals respectively. The value of A (Scattering Constant) varies from 0 to 4. A = 3.0 for piezoelectric scattering and A = 4.0 for charged impurity scattering. For optical mode scattering, the value of A varying between 1.8 to 2.4. From S vs. 1000/T the value of A varies from 3.26 -1.33. From the obtained values of scattering constant for MoSe_{1.75}Te_{0.25} and MoSe_{1.5}Te_{0.5} single crystals it is confirmed that the piezoelectric scattering is dominant in these single crystals. While in case of MoSeTe, MoSe_{0.5}Te_{1.5} and MoSe_{0.25}Te_{1.75} optical mode lattice scattering is dominant which is in good agreement with the data reported earlier by Harry and Kwok for scattering constant [28].

Some remarks drawn from the temperature dependence of Seebeck coefficient of grown crystals are summarized below.

- TEP of 2H-MoSe_{2-x}Te_x increases steadily with temperature in the entire range of measurements.
- Thermoelectric power of all the materials shows the negative value which indicates the n-type nature of these materials also confirmed by the Hall Effect measurement.

6.6 CONCLUSIONS

On the basis of obtained results of the measurements performed and presented in this chapter, some conclusions are drawn as below.

- Single crystals of 2H-MoSe_{2-x}Te_x exhibit the resistivity in the range from ~0.1-10 Ω-cm for 2H-MoSe_{2-x}Te_x at room temperature. Also the resistivity is found to increase non-linearly with selenium proportion in 2H-MoSe_{2-x}Te_x single crystals.
- Behavior of temperature dependent in-plane resistivity of these materials reveals that all the materials are semiconducting in nature.
- Resistivity parallel to c-axis of these materials is found to be higher than the perpendicular to c-axis, which proves the highly
anisotropic electrical nature of these materials. This type of anisotropy is obvious because of the structural difference along these two directions.

- Resistivities parallel c-axis in all the materials are found to behave differently than those perpendicular to c-axis. Resistivity parallel and perpendicular to c-axis of all the materials is found to decrease with increase in temperature at higher temperatures.

- The slopes of ln$\rho$ vs. 1000/T for low temperature limit give the activation energy for creation of the hole in the valance band while the slope for high temperature range gives the activation energy for electrons and holes in conduction and valance bands.

- The decrease in resistivity with decrease in the selenium content in the compounds can be attributed to decrease in activation energy. This decrease in activation energy with selenium atoms can be due to higher atomic states in selenium rich compound than the tellurium rich compound.

- Obtained values of the carrier concentrations ($10^{16}$ to $10^{17}$ cm$^{-3}$) and Hall co-efficient for all the materials confirmed the semiconducting and n-type nature of them.

- Seebeck coefficients of all the materials are found to be of the order of 0.8 mV/K. The high Seebeck coefficient of MoSe$_{2-x}$Tex is due to the selenium incorporated into the compound. The thermoelectric power for transition metal selenides compounds is high compared to the transition metal tellurides because selenium is more semiconducting than tellurium.

- From the obtained values of scattering constant for MoSe$_{1.75}$Te$_{0.25}$ and MoSe$_{1.5}$Te$_{0.5}$ single crystals it is confirmed that the piezoelectric scattering is dominant in these single crystals. While in cases of MoSeTe, MoSe$_{0.5}$Te$_{1.5}$ and MoSe$_{0.25}$Te$_{1.75}$ optical mode lattice scattering is dominant.
REFERENCES