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Magnetic field dependence of electrical transport properties in acceptor doped bismuth

Kajal Krishna Dey
Department of Physics, Banwarilal Bhalotia College, Asansol
P.O.Ushagram, Dist.Burdwan Pin Code-713303, West Bengal, India

Abstract: *Measurements were made on the Hall coefficient and transverse magnetoresistance of bismuth alloys containing small amount of gallium and indium as functions of magnetic filed at different constant temperatures. Change of sign of the Hall coefficient with magnetic field is observed at low temperature. Change of sign of the Hall coefficient with rise in temperature is a common phenomenon in case of acceptor doped semiconductor. But a reversal of sign in the Hall coefficient with magnetic field is not that commonly observed. Values of the magnetoresistance and Hall coefficient strongly vary with magnetic field strength. The magnetoresistance does not obey the quadratic dependence on magnetic field strength. The observed results may be a consequence of the particular band structure which allows the presence of different kinds charge carriers with high and strongly anisotropic mobilities.*

Keywords**:** *bismuth, electrical transport, Hall coefficient, magnetoresistance, semimetal*

I. Introduction

Bismuth has a small valence and conduction band overlap, three small L point electron Fermi pockets, and a T point hole Fermi pocket, which gives an equal (small) number of both charge species at the Fermi level.[1] L and T refer to symmetry points in the reduced Brillouin zone of bismuth. Bismuth is a semimetal which plays an important role in solid-state physics. The electrical transport properties of bismuth and its alloys have been a subject of interest due to the overlap. Bismuth has an extremely small Fermi surface. So this material provides the remarkable possibility to observe strong effects induced by the presence of external fields, i.e., magnetic field and temperature, even if these external forces are of moderate amplitude. Investigations on the properties of alloys of bismuth are important because various devices are being developed by using alloys of bismuth. [2,3] Several bismuth-containing oxides have been found to be high-T_C superconducting material.[4,5] Bismuth-antimony alloys have applications in peltier cooling modules and in infrared detectors. Extensive investigations of the transport properties of bismuth doped with impurities like lead, tin, tellurium, antimony etc have been made.[6-9] In the last few years, a series of experiments has once again drawn the attention of the community to elemental bismuth and challenged our understanding of this material. Few experiments clearly indicated that the question of transport in bismuth was still not understood. [10] In fact, similar questions still existed for the standard resistivity as well. [11] A material of much long term interest with many interesting properties bismuth has recently been found to host a variety of exotic electronic phenomena, including phase transitions at high field. There has been extensive interest in the transport properties of bismuth because of its unusual behavior that is exhibited due to the low density and very high mobilities of carriers. Bismuth behaves like a metal though not strictly metallic. Its behavior is in between a metal and a semiconductor. Both the holes and electrons are found to be responsible for the transport properties.

The band structure of pure bismuth may be considered to consist of a pair of light mass bands (L_C for electrons and L_V for holes) at six symmetrically related positions in **k**-space (six half ellipsoid) and a heavy mass hole band (T_V) at two positions in **k**-space (two half ellipsoid). These six half ellipsoids for each of the electrons and light holes in the Brillouin zone may be considered as three whole ellipsoids centered at L-point and two half ellipsoids for the heavy holes as one whole ellipsoid centered at T-point. The energy spectrum of bismuth has been investigated in a large number of experimental and theoretical papers. [12-14] However, right up to the present time models describing the spectrum of carriers at the points L and T in the reduced Brillouin zone, as well as certain important parameters of the spectrum have not been given unique values, owing to the complexity of the band structure of bismuth and the strong anisotropy of its properties. At acceptor impurity concentrations below 0.1 at.% the lattice parameters of bismuth do not vary markedly [13] and the effect of the acceptors is apparently only to make the electron and hole concentrations unequal and to change the electron and hole mobilities. Additional complications are caused by the anisotropic nature of the relaxation time, [15] the strongly non-parabolic nature of the dispersion law for carriers at the L-extrema. [16, 17]

The purpose of this work is to re-examine the transport properties of doped semimetal. We present here the results of the magnetic field variation of the Hall coefficient and magnetoresistance study of gallium and indium doped bismuth single crystal.

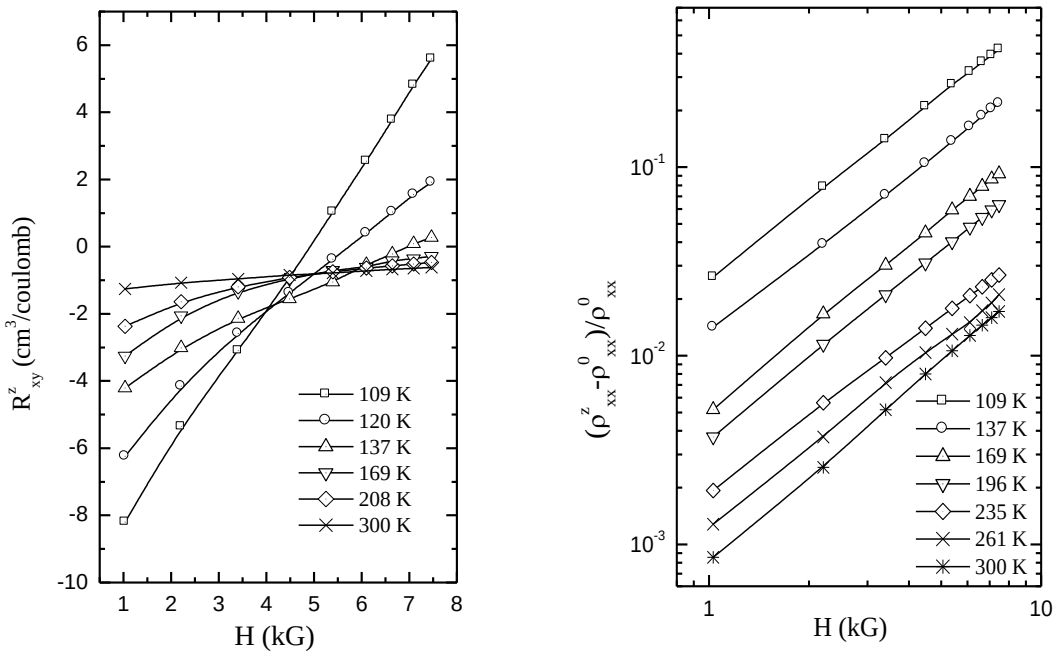
II. Experiments And Results

Single crystals of bismuth (Bi) doped with gallium (Ga) and indium (In) were prepared by the vertical Bridgeman technique using a modified Bridgeman furnace. The percentages of doping of the studied samples, as determined by EDX Analytical System (ISIS Link, Oxford Instruments, U.K.) are shown in Table I. The thin and small portions were cut and then ground into rectangular shapes of dimension 1cm × 0.3cm × 0.1cm for measurements.

Table I. Prepared samples and their percentages of impurity.

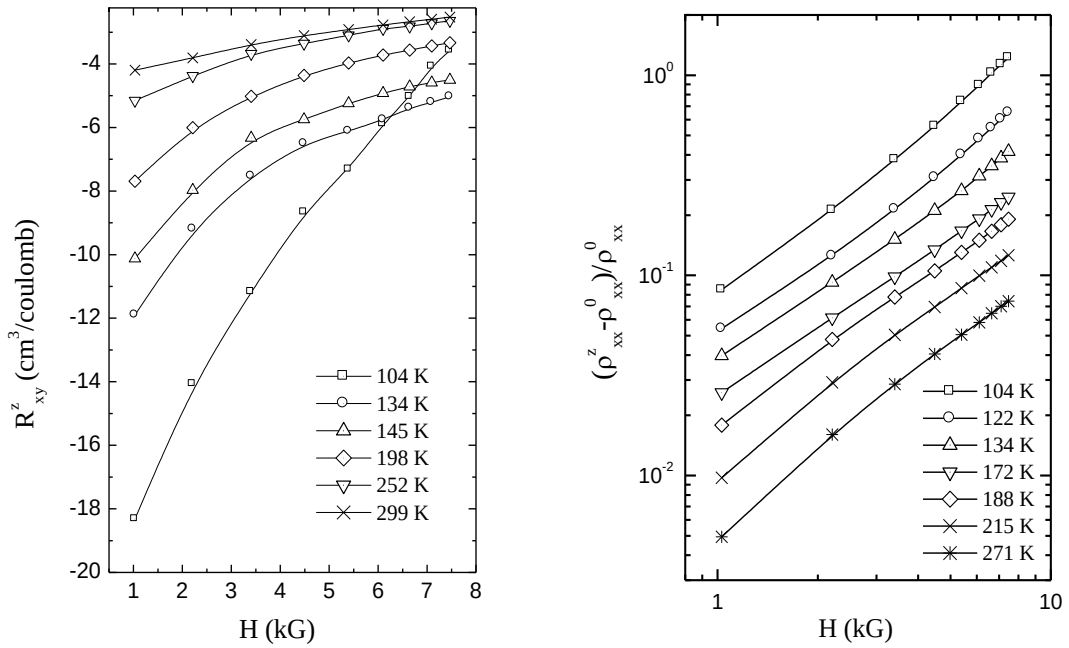
alloys	sample number	weighted atomic %
Bi-In	S1	0.15
Bi-Ga	S2	0.22

The crystallographic axes are usually referred to as the binary, the bisectrix, and the trigonal or c-axis, pertaining to the x-, y-, and z-axes respectively. The current was applied in the direction perpendicular to the trigonal axis and magnetic field was applied parallel to the trigonal axis. Figures 1 and 2 show the magnetic field variation of the Hall coefficient (R_{xy}^{z}) and transverse magnetoresistance $(\rho_{xx}^{z} - \rho_{xx}^{0})/\rho_{xx}^{0}$ of the samples. The values of the magnetoresistance and Hall coefficient strongly vary with the magnetic field strength. Hall coefficient is found to be negative and it approaches to the positive value with the increase of magnetic field. A change of sign of R_{xy}^{z} with magnetic field is observed at three low temperatures for the sample S2. The magnetoresistance does not show strictly quadratic dependence on magnetic field strength.



(a) **(b)**

Fig. 1 Magnetic field dependence of the (a) Hall coefficient and (b) transverse magnetoresistance of 0.22 at% gallium doped bismuth at different constant temperatures indicted in the figures.



(a) **(b)**

Fig. 2 Magnetic field dependence of the (a) Hall coefficient and (b) transverse magnetoresistance of 0.15 at% indium doped bismuth at different constant temperatures indicted in the figures.

III. Theoretical Consideration

Bismuth is pentavalent and from the two atoms in the unit cell ten valence electrons originate. They would fill a whole number of bands if a slight band overlap did not occur. Due to this overlap a few electrons are accumulated in the next-higher band, leaving an equal number of holes in a nearly filled band. Both these electrons and holes act as free carriers. Based on infrared transmission experiments [18], Lax [19] proposed an ellipsoidal-non-parabolic model for the Fermi surface of bismuth which has been found to work quite well in explaining physical properties.

One axis of each electron ellipsoid is parallel to a crystallographic axis (binary axis having 1 or x), the other two axes of each ellipsoid are tilted with respect to the other crystallographic axes (trigonal axis having 3 or z and bisectrix axis having 2 or y). According to the relation of energy versus wave-vector proposed by Lax, the electron ellipsoids can be described as

$$E_e\left(1+\frac{E_e}{E_g}\right)=\frac{\hbar^2}{2m_0}\left(\alpha_{11}^{(e)}k_x^2+\alpha_{22}^{(e)}k_y^2+\alpha_{33}^{(e)}k_z^2+2\alpha_{23}^{(e)}k_yk_z\right)$$

where E_e is the electron Fermi energy, E_g is the band gap between the two light mass bands(L_C and L_V), and $\alpha_{ij}^{(e)}$ is the component of reciprocal electron mass tensor $\boldsymbol{\alpha}^{(e)}$ in unit of $(1/m_o)$; m_o being the free electron mass. This is known as the Lax or ellipsoidal-non-parabolic model. The three light hole ellipsoids are also of the same form as the three electron ellipsoids. The Fermi surface of heavy holes is described by one set of ellipsoid with its axis of revolution parallel to the trigonal axis. The ellipsoid of revolution for heavy hole is of the form

$$E_{h1}=\frac{\hbar^2}{2m_0}\left(\alpha_{11}^{(h1)}\left(k_x^2+k_y^2\right)+\alpha_{33}^{(h1)}k_z^2\right)$$

where E_{h1} is the heavy hole Fermi energy and $\alpha_{ij}^{(h1)}$ is the component of reciprocal heavy hole effective mass tensor $\boldsymbol{\alpha}^{(h1)}$.

Figure 3 shows a schematic diagram of energy bands in bismuth showing a projection of energy bands L_C, T_V and L_V on a two-dimensional plane. E_C is the lowermost available energy level in the L_C band and $E_V^{(h1)}$ and $E_V^{(h2)}$ are the uppermost available energy levels in the T_V and L_V bands respectively. As bismuth has sufficient number of electrons to fill the band T_V, we get a Fermi level E_F^0 in the region of overlap due to the distribution of electrons among the energy states of T_V and L_C in that region. L_V and L_C bands will give rise to light mass holes and electrons respectively as free carriers and the T_V band to heavy mass holes. Gallium and indium are elements of group III and so they act as acceptor impurity to bismuth. Acceptor impurity takes

electrons from both the overlapping bands, thereby increasing the number of holes and decreasing the number of electrons. The Fermi level then moves to a lower energy to a position E_F^a .

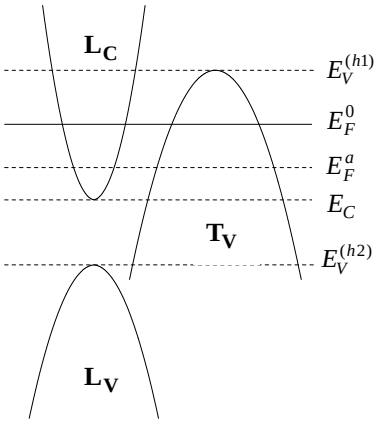


Fig. 3 Schematic diagram of the electron and hole bands**.**

For electrons and light holes we use Lax model or ellipsoidal-non-parabolic band. If $N_0^{(h1)}$ and $N_0^{(e)}$ represent the densities of holes and electrons in the two bands T_V and L_C at T=0K, we then have

$$N_0^{(h1)} = \int_{E_F^0}^{E_V^{(h1)}} C_{h1}\left(E_V^{(h1)} - E\right)^{1/2} dE \qquad \text{and} \qquad N_0^{(e)} = \int_{E_C}^{E_F^0} \frac{df_L^{(e)}}{dE} dE$$

where $C_{h1} = \frac{4\pi}{h^3}\left\{2m_0\mathbf{m}^{(h1)^{1/3}}\right\}^{3/2}$ and $f_L^{(e)} = \frac{8\pi}{h^3}\left\{2m_0\mathbf{m}^{(e)^{1/3}}\left(E - E_C\right)\left(1 + \frac{E - E_C}{E_g}\right)\right\}^{3/2}$

$\mathbf{m}^{(h1)}$ is the effective mass tensor of heavy holes in T_V band and and $\mathbf{m}^{(e)}$ is that for electrons at the bottom of the L_C band.

The densities of the carriers in bands T_V and L_C in the impure sample will become

$$N_i^{(h1)} = \int_{E_F^a}^{E_V^{(h1)}} C_{h1}\left(E_V^{(h1)} - E\right)^{1/2} dE \qquad \text{and} \qquad N_i^{(e)} = \int_{E_C}^{E_F^a} \frac{df_L^{(e)}}{dE} dE$$

If N_a be the density of acceptor impurity centers added then

$$N_i^{(h1)} + N_i^{(e)} = \left(N_0^{(h1)} + aN_a\right) + \left(N_0^{(e)} - bN_a\right)$$

where a and b are the fractions of acceptor centers taking away electrons from the bands T_V and L_C respectively and are therefore proportional to the density of states in T_V and L_C; (a>b and a+b=1). The total density of impurities added will be

$$N_{imp} = \left|\Delta N_i^{(h1)}\right| + \left|\Delta N_i^{(e)}\right|$$

$$\Delta N_i^{(h1)} = N_i^{(h1)} - N_0^{(h1)} \quad \text{and} \quad \Delta N_i^{(e)} = N_0^{(e)} - N_i^{(e)}$$

If the concentration of impurity is increased the impurity will take more electrons from the bands and for a sufficient percentage of impurity the Fermi level E_F^a moving to the lower energy, may enter into the region of L_V band. As a result, there will be created more holes in T_V and L_V bands and L_C band will be devoid of electron. The above expressions relate the concentration of impurities and the number of free carriers with the consequent shift of the Fermi level.

The theoretical three band model for pure as well as doped bismuth predicts the Hall coefficient and the transverse megnetoresistivity with the magnetic filed H along z-axis as

$$R_{xy}^z = \frac{\frac{1}{e} \times A_1}{A_1^2 H^2 + A_2^2} \text{ and } \rho_{xx}^z = \frac{\frac{1}{e} \times A_2}{A_1^2 H^2 + A_2^2}$$

where the following terms have been taken as A_1 and A_2 in the above expressions,

$$\frac{N^{(h1)}\mu_1^{(h1)^2}}{1 + \mu_1^{(h1)^2} H^2} + \frac{N^{(h2)}\mu_1^{\{h2\}}\mu_2^{\{h2\}}}{1 + \mu_1^{(h2)}\mu_2^{(h2)} H^2} - \frac{N^{(e)}\mu_1^{\{e\}}\mu_2^{\{e\}}}{1 + \mu_1^{(e)}\mu_2^{(e)} H^2} = A_1$$

$$\frac{N^{(h1)}\mu_1^{(h1)}}{1+\mu_1^{(h1)^2}H^2}+\frac{N^{(h2)}\bar{\mu}^{(h2)}}{1+\mu_1^{(h2)}\mu_2^{(h2)}H^2}+\frac{N^{(e)}\bar{\mu}^{(e)}}{1+\mu_1^{(e)}\mu_2^{(e)}H^2}=A_2$$

$\mu_1^{(h1)}$ is the (isotropic) mobility of heavy holes in the xy-plane, $\mu_1^{(e)}$ and $\mu_2^{(e)}$ are the electron mobilities taken for each electron ellipsoid in the xy-plane and $\mu_1^{(h2)}$ and $\mu_2^{(h2)}$ are those for light holes respectively. $\bar{\mu}^{(e)}\left(=\frac{\mu_1^{(e)}+\mu_2^{(e)}}{2}\right)$ and $\bar{\mu}^{(h2)}\left(=\frac{\mu_1^{(h2)}+\mu_2^{(h2)}}{2}\right)$ are the average mobilities of electrons and light holes in the xy-plane respectively. The resistivity in the absence of magnetic field is then given by

$$\rho_{xx}^0=\frac{1}{e\left(N^{(h1)}\mu_1^{(h1)}+N^{(h2)}\bar{\mu}^{(h2)}+N^{(e)}\bar{\mu}^{(e)}\right)}$$

The transverse magnetoresistance is then given by

$$\frac{\Delta\rho}{\rho_{xx}^0}=\frac{\rho_{xx}^z-\rho_{xx}^0}{\rho_{xx}^0}$$

3.1 Effect of Magnetic Field

Let us now see what happens to the electrons in metals when a magnetic field is applied. For simplicity, we consider the situation at T=0K. For the same reason, the electrons with spin parallel and antiparallel to the direction of magnetic field (H) are shown in Fig.4a in two groups so that all the states below the Fermi level E_F^0 are occupied and those above E_F^0 are empty. If a magnetic field is applied, there will be an unstable situation due to the shift in energy of electrons in the two halves (see Fig.4b) and a number of electrons with antiparallel spin will enter the group of parallel ones. In equilibrium both halves are again filled to the same level E_F' as shown in Fig.4c. In equilibrium at E_F', the density of states in the right half (parallel spin) is greater than that in the left half (antiparallel spin) and it is expected that, $\delta_2>\delta_1$. This means that the Fermi energy is lowered by the application of magnetic field by an amount $\delta_2-\delta_1$. Here δ_2 and δ_1 are such that $\delta_2+\delta_1=2\mu_B H$. If $\mu_B H<< E_F^0$, it is evident that the shift $\delta_2-\delta_1$ will have no significant effect. In the case of metals while finding the spin paramagnetism of free electrons this difference is never considered because there E_F^0 ~few eV and for ordinary fields ~10kG, $\mu_B H \sim 10^{-4}$eV. In the present case of bismuth, the Fermi surface is small $\sim 10^{-2}$eV. [20] So the small change in the Fermi energy due to the application of the magnetic field will cause a small change in the distribution of free carriers. Since there are two overlapping bands, this small change in the distribution of free carriers will cause an unequal change in the distribution of holes and electrons in doped bismuth because the density of states of the two bands above the Fermi surface are different. This change will of course not be able to produce any significant change in the properties where the contribution of carriers are additive. But it may produce a significant effect in those properties where the contribution from holes and electrons oppose each other. If the Fermi energy is lowered, there will be a gain in the number of holes over electrons. Since $\delta_2-\delta_1 \propto H$, the gain in holes will increase with H making R_{xy}^z positive with increasing field.

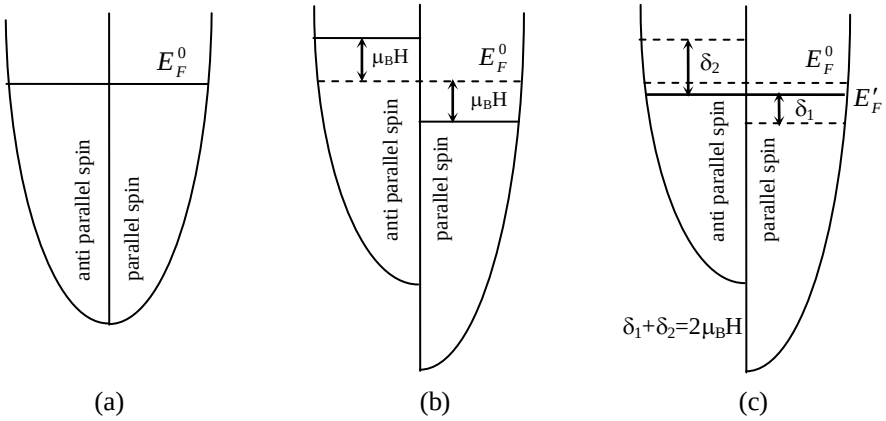


Fig. 4 (a) H=0, (b) unstable situation in presence of H, (c) equilibrium position in presence of H.

3.2 Effect of Temperature

When small amount of acceptor impurity is added, the Fermi level may lie within the overlap region. As the temperature rises, electrons from T_V will go to the vacant states in L_C, thereby increasing the number of free electrons in L_C and the same number of holes will be created in the band T_V. From L_V, excited electrons will go to both T_V and L_C. Electrons, those go to the vacant states in T_V, decrease the number of holes in T_V and those go to L_C, increase the number of free electrons. Also the total number of electrons excited from L_V will give rise the same number of holes in L_V. Number of electrons in the L_C band grows faster with temperature than the holes.

The density of electrons excited from one band to another can be calculated as a function of temperature using the Fermi-Dirac distribution function f(E), like this,

$$N_i = \int_E^{E+dE} g(E')f(E')dE' \; ; \quad g(E') = \text{density of states at energy } E'$$

The two important factors responsible for the temperature variation of mobility are phonons and ionized impurity atoms. Any arbitrary carrier mobility, when scattering mechanism occurs independently, is determined by

$$\frac{1}{\mu} = \frac{1}{\mu_{imp}} + \frac{1}{\mu_{lat}}$$

where μ_{imp} represents scattering due to impurity ions and μ_{lat} represents scattering due to phonons.

When the concentration of ionized donors or acceptors is high, the charge carriers suffer Rutherford scattering due to the presence of such ions. The scattering of electrons at low temperatures is dominated by ionized impurity atoms with approximate power law, $\mu \propto T^{3/2}$ and at high temperatures lattice scattering ($\mu \propto T^{-3/2}$) becomes more prominent. Experimental observations however are not always in precise accord with this formula.

IV. Conclusion

In the present samples electrons are present as minority carrier. Since R_{xy}^z is negative at low magnetic fields, it is concluded from the above expression of R_{xy}^z that the electron mobilties exceed the hole mobilities. It is clear that the carrier properties are represented by many a parameters, viz. the densities of free carriers and the strongly anisotropic mobilities. If the energy band structure shown in Fig.3 is correct for the dilute bismuth alloys, the electrons which are thermally excited into the conduction band can contribute to the conduction phenomena. The masses of the electron and light hole change with the position of the Fermi level according to the built-in-property of the Lax ellipsoidal-non-parabolic band model. The effective mass and the relaxation time determine the mobility of the carrier. The density of electrons in L_C is sufficient at low temperature and the mobilities of electrons are much greater than those of holes. Then it is possible that the effective contribution of electrons towards the Hall coefficient is greater than that of holes, which makes the Hall coefficient negative. The number of electrons in the L_C band grows faster with temperature than the holes. It is expected that the ratio of the density of lighter holes to that of a heavier holes changes as the carrier distribution deviates from complete degeneracy with the increase in temperature. The increases in the concentration of three types of carriers to a great extent decrease the magnitudes of the Hall coefficient and magnetoresistance. Zero field resistivity shows the temperature dependence of approximately T^2. [21] This result indicates the dominating contribution of phonon scattering over the ionized impurity scattering. So the effect of phonon scattering might also be there in the higher temperature limits.

For closed Fermi surface with equal number of holes and electrons, the magnetoresistance varies as H^2 and for unequal number of electrons and holes, it saturates at high field limit. [22] In the present case it varies as H^n where the values of n are in the range $1.3<n<1.5$ for gallium doped and $1.15<n<1.5$ for indium doped sample. With increasing temperature it approaches an approximately quadratic dependence on field strength. At very low temperature it may saturate in the high field limit. [1]

The results here point to the variation of the concentration of three different types of carriers. The observed behaviours are accounted for qualitatively in terms electronic band structure and the change of carrier concentration with differences in their masses (mobility) and the scattering mechanism with temperature.

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