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The Temperature Dependence of Electrical Transport Properties in Indium Doped Bismuth

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Abstract:
Measurements were made on the electrical resistivity at zero magnetic field, magnetoresistivity and Hall coefficient of bismuth alloys containing small amounts of indium as function of temperature in the range 100 - 300K for different magnetic field strengths. The Hall coefficient is observed to be negative in all the cases. Resistivity increases with temperature as it does in metals. The values of the magnetoresistivity and Hall coefficient strongly vary with the magnetic field strength. This is a consequence of the particular band structure which allows the presence of different kinds charge carrier with high and strongly anisotropic mobilities.

Keywords: *Hall coefficient, electrical resistivity, magnetoresistivity, bismuth*

1. Introduction

Bismuth is a semimetal which plays an important role in solid-state physics. It 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 of the Brillouin zone of bismuth. 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). The six half ellipsoids for each of the electrons and holes in the Brillouin zone may be considered as three whole ellipsoid centered at *L*-point and two half ellipsoids for the heavy holes as one whole ellipsoid centered at *T*-point. 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 impurity. Extensive investigations of the transport properties of bismuth doped with impurities like lead, tin, tellurium, antimony etc have been made. [2-5] 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. The recent experiments clearly indicated that the question of transport in bismuth was still not understood. [6] In fact, similar questions still existed for the standard resistivity as well. 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 holes and electrons are found to be responsible for the transport properties.

The purpose of this work is to reexamine the transport properties of doped semimetal. We present here the results of the resistivity, Hall coefficient and magnetoresistivity study of indium doped bismuth single crystal.

2. Experiments and Results

Single crystals of bismuth doped with indium 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 the ground into rectangular shapes of dimension 1cm x 0.3cm x 0.1cm for measurements.

Alloys	Sample Number	Weighted Atomic %
Bi-In	S1	0.02
Bi-In	S2	0.15

Table 1: Prepared Samples and Their Percentages of Impurity.

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, 2 and 3 show the temperature variation of the zero field resistivity (ρ_{xx}^{0}), magnetoresistivity (ρ_{xx}^{z}) and Hall coefficient (R_{xy}^{z}) of the samples. Resistivity increases with temperature nonlinearly.

Magnetoresistivity at low field decreases first in the low temperature range and then increases. It decreases exponentially with temperature at higher field strength. The Hall coefficient is negative throughout the range of temperature investigated (100-300K). The negative value decreases with temperature.

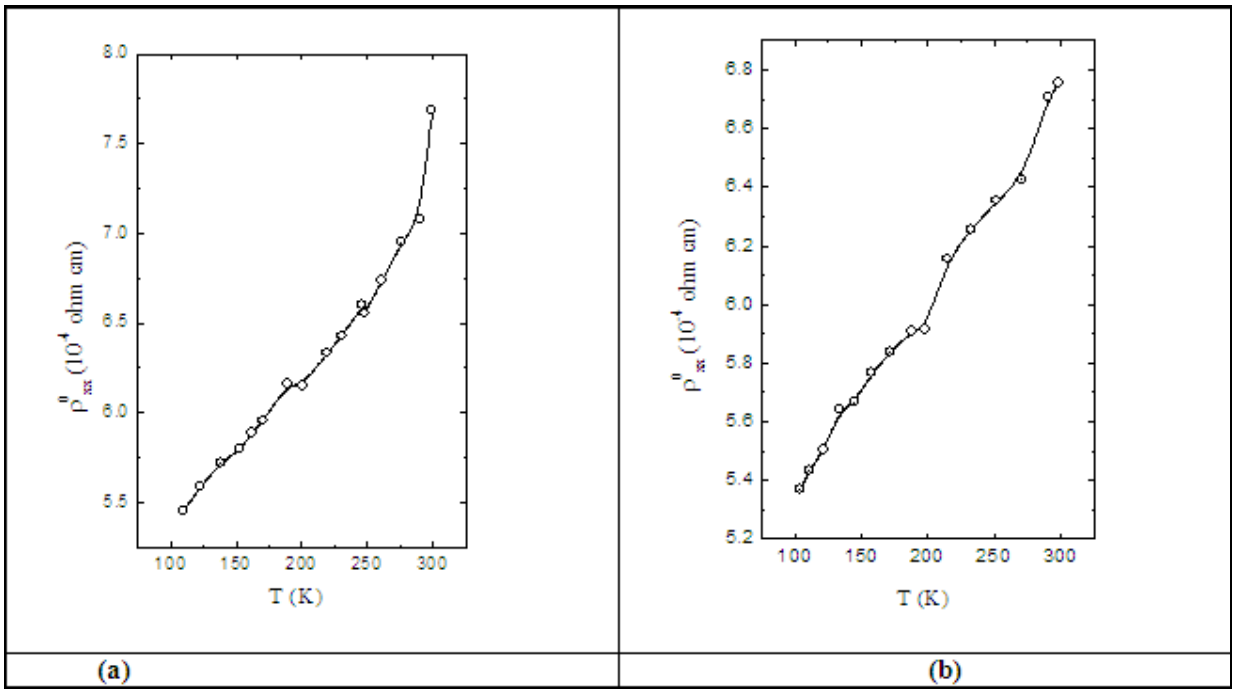

Figure 1: Temperature dependence of the resistivity in the absence of magnetic field: (a) 0.02 at% indium and (b) 0.15 at% indium doped bismuth

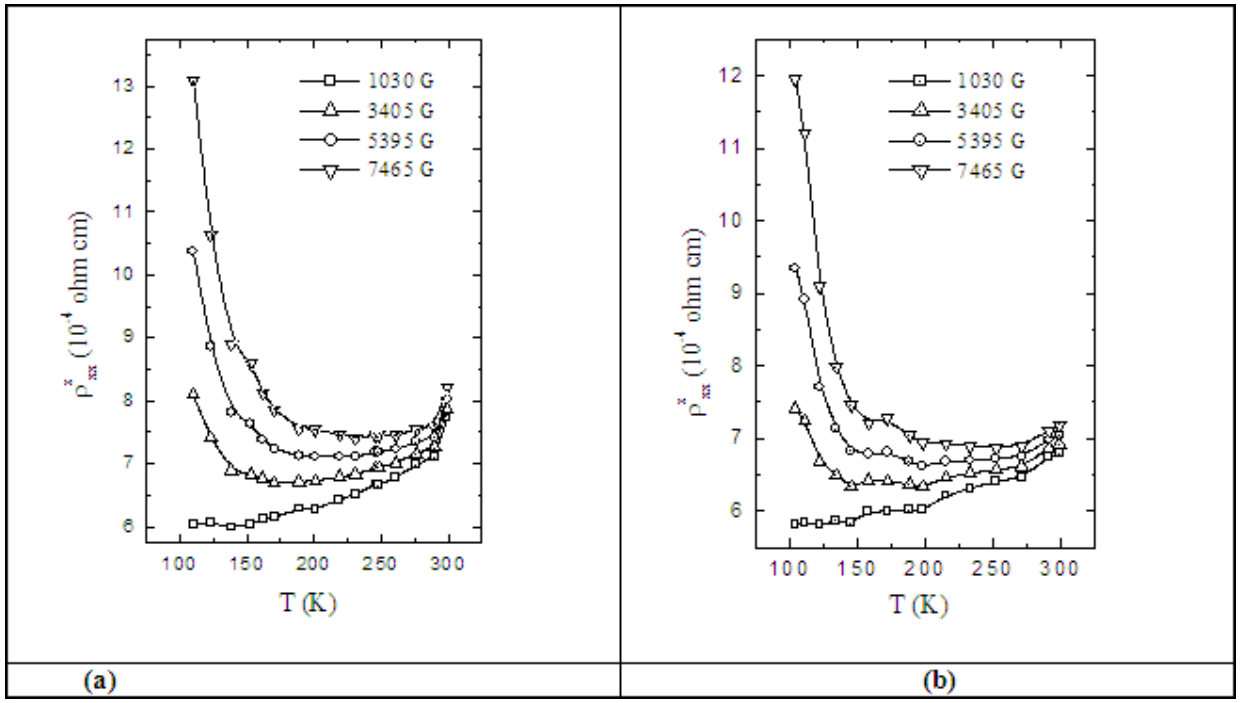

Figure 2: Temperature dependence of the magnetoresistivity: (a) 0.02 at% indium (b) 0.15 at% indium doped bismuth. Applied magnetic field strengths are indicated in the figure.

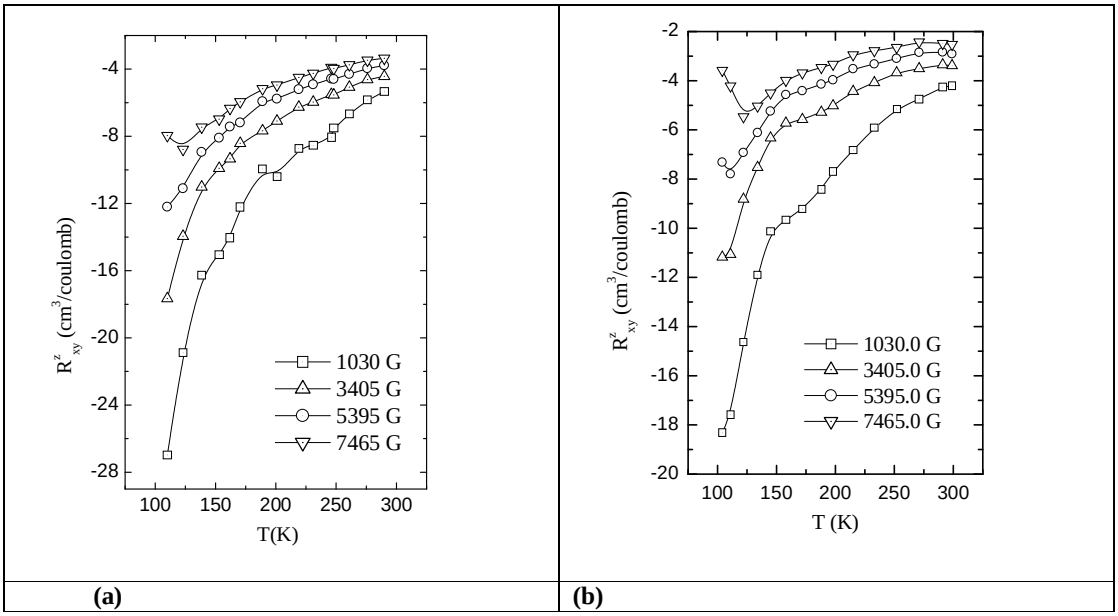

Figure 3: Temperature dependence of the Hall coefficient: (a) 0.02 at% indium (b) 0.15 at% indium doped bismuth. Applied magnetic field strengths are indicated in the figure.

3. Discussion

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 [7], Lax [8] 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 $\alpha_{ij}^{(e)}$ the components 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 hole 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 components of reciprocal heavy hole effective mass tensor $\boldsymbol{\alpha}^{(h1)}$.

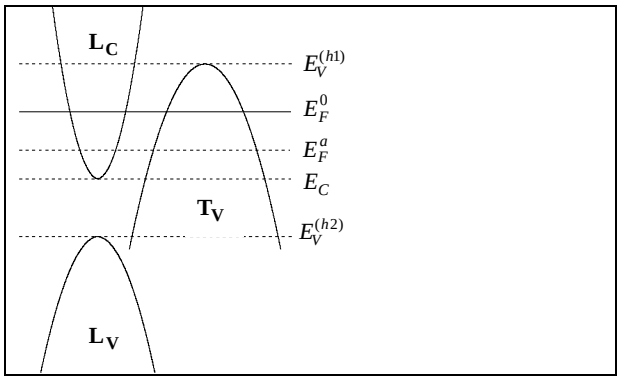

Figure 4: Schematic diagram of the electron and hole bands.

Figure 4 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 the that region. L_C and L_V bands will give rise to light mass electrons and light mass holes respectively as free carriers and the T_V band to heavy mass holes. Indium is an element of group III and so it should act as an 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.

The theoretical three band model for pure as well as doped bismuth predicts the Hall coefficient in the *xy*-plane with the magnetic filed *H* along *z*-axis as

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

and the transverse megnetoresistivity in the presence of magnetic field H along *z*-axis as

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

where A_1 and A_2 are given by,

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

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

Here $\mu_1^{(h1)}$ 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. $\overline{\mu}^{(e)}\left(=\frac{\mu_1^{(e)}+\mu_2^{(e)}}{2}\right)$ and $\overline{\mu}^{(h2)}\left(=\frac{\mu_1^{(h2)}+\mu_2^{(h2)}}{2}\right)$ 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

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

The mobility associated with scattering due to lattice vibrations for non-polar crystals varies as $T^{-3/2}$. Experimental observations however are not always in precise accord with this formula. When the concentration of ionized donors or acceptors is high, the charge carriers suffer Rutherford scattering due to the presence of such ions. The characteristic of the ionized impurity scattering is the approximate power law, $\mu \propto T^{3/2}$. The two important factors responsible for the temperature variation of mobility are phonons and ionized impurity atoms. We consider that the three groups of carriers stand in the same ratio when scattered by phonons and the impurity ions. 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. The scattering of electrons at low temperatures are dominated by impurity atoms, at high temperatures lattice scattering becomes more prominent.

If the energy band structure shown in Fig.4 is correct for the dilute bismuth alloys, the electrons which are thermally excited into the conduction band can contribute to the conduction phenomena. Resistivity shows the temperature dependence of approximately T^2. This indicates the dominating contribution of phonon scattering over the ionized impurity scattering.

From the above expressions of R_{xy}^z and ρ_{xx}^z it is clear that the magnitude as well as the sign of the Hall coefficient and magnetoresistivity depend on the number of free carriers, their nature and their mobility at the temperature under consideration. . The carrier density depends on the position of the Fermi level. So the value of R_{xy}^z and ρ_{xx}^z at any particular temperature will also depend on the position of the Fermi level. In the present case, a very low amount of acceptor impurity is added to pure bismuth so that the Fermi level lies within the overlap region. The number of electrons in the L_C band grows faster with temperature than the holes. The density of electrons in L_C is sufficient and the mobility of electrons is much greater than that 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. Magnetoresistivity curves show an initial decrease in the low temperature region and then grow slowly in the

higher temperature. This initial decrease is rapid at higher field strengths. At higher temperatures 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 that go to the vacant states in T_V decrease the number of holes in T_V and those going 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. The increase in the concentration of three types of carriers to a great extent in this way decreases the magnitudes of the Hall coefficient and magnetoresistivity. The effect of phonon scattering might be the most important one in the slow increase of the magnetoresistivity at higher temperature.

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. As the impurity concentration increases, the density of holes in T_V band becomes larger and with a shift of the Fermi level to a lower energy thermal excitation of electrons from L_V starts at lower temperature. So it is possible that both the Hall coefficient and magnetoresistivity starting with lower magnitudes show similar types of variations for higher doping concentration. The Hall coefficient magnitude at higher magnetic field strength increases initially with temperature to attain a maximum negative value and decreases. This increase in the Hall coefficient versus temperature curves can be explained in terms of the change of the ratio of the density of a hole to that of the density of a hole with a smaller value of mobility. This situation is similar to the case of the impurity conduction of a semiconductor. It is expected that the ratio of the density of lighter hole to that of a heavier hole changes as the carrier distribution deviates from complete degeneracy with the increase in temperature.

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

4. References

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