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Study of the Transverse Magnetoresistance of Bismuth Nanowires by Solution of the Boltzman Equation

Janipour Bidsardareh, Vahid
Department of Mathematics
Islamic azad university , Gachsaran branch,Iran
Gachsaran,Iran
Email: Vahidjanipor@yahoo.com

Zare Bidsardareh, Moslem
Department of Physics
Islamic azad university , Gachsaran branch,Iran
Gachsaran,Iran
Email: Mzare@mail.yu.ac.ir

Abstract –**The effects of sample size on the galvanomagnetice properties of semimetal nanowire are investigated. Transverse magnetoresistance is calculated within a Boltzman Transport Equation approach.The obtained values for transverse magnetoresistance are in good agreement with the experimental results reported by Heremans for Bismuth nanowire. Temperature dependence of the transverse magnetoresistance of cylindrical Bi nanowires is studied too.**

Key Words-Boltzman Equation , Magnetoresistance , Size effect , Ellipsoidal Fermi Surface , Specular reflection,Bismuth.

I. INTRODUCTION

The galvanomagnetic transport properties of the semimetal nanowires have been a great interest in recent years, experimentally [1, 2, 3]. Among the semimetals, Bismuth semimetal with a rhombohedral structure have increasing attention and distinct it with the other like samples for a number of reasons: Firstly, the carrier concentration is much smaller by a factor of 10 000 compared to most metals, at low temperatures, resulting in a relatively large resistivity, in spite of the long mean free path and wavelength. Secondly, the electron mean free path at liquid Helium temperatures in bulk Bi can be on the order of a millimeter [4], resulting in strong ballistic effects [5]. Thirdly, the carrier effective masses are small and highly anisotropic so that they lead to increased quantum confinement effects, with a large spatial extension of the electron wave function. At low carrier density, semimetal-semiconductor phase transitions can occur for critical wire diameter d_c [6,7,8]. Furthermore, at this phase transitions a significant enhancement is expected in the thermoelectric figure of merit over bulk Bi [7].

There are two types of size effects observable in thin metal samples. The ordinary size effect (OSE) which is seen when the charge carrier mean free path (MFP) is comparable with or greater than the sample diameter , results in a resistivity which is higher than the bulk values , due to the additional scattering of the charge carriers at the sample surface. When the de Broglie wavelength of an electron is comparable to the dimensions of the sample, quantum size effect (QSE) became important and deviations from the bulk behavior in transport properties are expected. The QSE manifests itself in the oscillatory behavior of the electron density of states. Although a number of studies have been carried out on the size effect on the conductivity of thin films [9], quantum holes [10] and superlattices [11], only a small amount of progress has been achieved for the size effect on the magnetoresistance of nanowires, theoretically [3, 12]. Size effect in the thin metallic films (with a spherical Fermi surface) was given by Fuch-Sondheimer, firstly [13] and scattering of the carriers from the surface is characterized by a parameter *P*, the fraction of the carriers which reflected on the boundary surface, speculary. Price studied the size effect in thin metallic films with ellipsoidal Fermi surfaces and deducted that for specular reflection the conductivity approaches a finite limit for every thin films [14]. However, in general the longitude and transverse magnetoresistance have been calculated numerically [15, 16, 17]. In this paper, galvanomagnetic properties of Bi nanowires were explained by Parrott theorem by solution of the Boltzmann Transport Equation. In previous work [18] the special resistivity of Bi thin wire is calculated per an ellipsoidal electron pocket and the results is verified by Gurvitch experimental results [16]. In this paper transverse magnetoresistance of bismuth–like cylindrical nanowires (with three ellipsoid electron pockets) has been calculated using parrott theorem [19] extension. Transverse magnetoresistance dependence of radius, temperature and magnetic field, was studied too. The values of transverse magnetoresistance deduced our calculation are in good agreement with the experimental results, reported by Heremans *et al* [17] for Bismuth nanowires.

II. THEORY

In order to study the size effect on the galvanomagnetic transport properties of nanowires, suppose that the sample is in the form of a long cylindrical with circular cross section of radius *R*. To this end the equation of the surface of wire can be written as

$$\hat{\mathbf{m}}\cdot\mathbf{x} = R \qquad (1)$$

Where $\hat{\mathbf{m}}$ is the unit vector, normal to the surface and $\mathbf{x}$ is a position vector. By using the distribution function of carriers f_k , then current density can be expressed as

$$\mathbf{J} = \frac{e}{4\pi^3}\int \mathbf{V}(k) f_k \mathrm{d}^3 k \quad (2)$$

Where k is the wave vector and $\mathbf{V}$ is the velocity vector of carriers. To carry out this calculation we need to determine distribution function of carriers f_k that should be realized by Boltzmann differential equation and using of suitable boundary conditions. In presence of electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$ the BTE can be written as

$$-(\mathbf{V}.\nabla T)\,\partial f_k/\partial T - \frac{e}{\hbar}(\mathbf{E}+\mathbf{V}\times\mathbf{B}).\,\partial f_k/\partial k = -\,\partial f_k/\partial t\,\Big|_{scatt} \quad (3)$$

Where ∇T is the temperature gradient. Let us suppose that differ of equilibrium distribution f_k° function with conservative distribution function f_k is trivial, thus we can write [20]

$$f_1 = f_k - f_k^{\circ} \quad (4)$$

Where

$$f_k^{\circ} = \frac{1}{\exp(\frac{\varepsilon_k - \mu}{K_\beta T}) + 1}$$

Substituting equation (4) into equation (3) and use of relaxation time approximation (RTA)

$$\frac{\partial f}{\partial t}\Big|_{scatt} = -\frac{f_1}{\tau} \quad (5)$$

Where τ is the effective relaxation time, and regarding

$$\frac{e}{c}(\mathbf{V}\times\mathbf{B}).\,\partial f_\circ/\partial k = \frac{e}{c}(\mathbf{V}\times\mathbf{B}).\,\partial\varepsilon_k\partial f_k^{\circ}/\partial k\partial\varepsilon_k = \frac{e}{c}(\mathbf{V}\times\mathbf{B}).\hbar\mathbf{V}\,\partial f_\circ/\partial\varepsilon_k = 0 \quad (6)$$

Then the BTE is given by

$$\mathbf{V}.\nabla_x f_1 + \frac{f_1}{\tau} - \frac{e}{\hbar}\mathbf{E}.\nabla_k f_\circ - \frac{e}{\hbar}\mathbf{V}\times\mathbf{B}.\nabla_k f_1 = 0 \quad (7)$$

The Fermi energy surfaces for the conduction electrons of Bismuth are ellipsoidal and that therefore for solving equation (7) first with a suitable transformation coordinate, change the ellipsoidal Fermi surface into a spherical surface. To this end, a dyadic $\mathbf{A}$, considered so that $\mathbf{A}.\mathbf{A} = \boldsymbol{\alpha}$, then the energy equation of Fermi surface can be expressed as

$$\mathrm{E} = \frac{\hbar^2}{2m_\circ}\boldsymbol{\kappa}.\boldsymbol{\alpha}.\boldsymbol{\kappa} = \frac{\hbar^2}{2m_\circ}\omega^2 \quad (8)$$

Where $\boldsymbol{\alpha}$ is the reciprocal effective mass ratio dyadic, and ω is the wave vector in new coordinate system. Other parameters also have been changed into forms in new coordinate $(\mathbf{u}=\mathbf{A}^{-1}\cdot\mathbf{V}, \boldsymbol{\varepsilon}=\mathbf{A}\cdot\mathbf{E}, \mathbf{y}=\mathbf{A}^{-1}\cdot\mathbf{x})$, the BTE transforms into

$$\mathbf{u}\cdot\nabla_y f_1 + \frac{f_1}{\tau} - \frac{e}{m_\circ}\boldsymbol{\varepsilon}.\nabla_u f_\circ + \frac{e}{m_\circ}\mathbf{u}.\boldsymbol{\alpha}.\nabla_u f_1\times\mathbf{B} = 0 \quad (9)$$

Where y is the position vector, $\mathbf{u}$ is the velocity and $\boldsymbol{\varepsilon}$ is the electric field in new space. In this space, f_1 can be written in the form [21]

$$f_1 = -\mathbf{u}.\chi\frac{\partial f_\circ}{\partial\eta} \qquad (\eta = \frac{\mathrm{E}}{K_\circ T}) \quad (10)$$

Selecting unit vector $\mathbf{n}$ ($\mathbf{n} = \frac{\mathbf{A}\cdot\hat{\mathbf{m}}}{(\hat{\mathbf{m}}\cdot\boldsymbol{\alpha}\cdot\hat{\mathbf{m}})^{1/2}}$) in direction of radius of wire, χ just becomes function of r [16]. Substituting for f_1 from equation (10) into equation (9) we obtain BTE in terms of its components finally

$$u_r\frac{\partial\chi_i}{\partial r} + \frac{\chi_i}{\tau} + \frac{e\varepsilon_i}{K_\circ T} + \frac{e}{m_\circ}\alpha_{ij}\xi_{ijk}\chi_k B_l = 0 \quad (11)$$

ξ_{ijk} is the Levi-Civita symbol. Solving the above differential equations with the suitable boundary conditions, functions χ will be determined.

III. Determination Of χ In Presence Of Magnetic Field

In practice, we usually employ a simple phenomenological description according to which a fraction p of the incident carriers are specularelly reflected, as if by a highly polished mirror, whilst the remainder are scattered diffusely in all directions uniformly, without reference to the direction of the incident radiation. That is too say, there is probability (1-p) that the expectation value of the carrier velocity will be zero after reflection. (reflected diffusely). Perhaps we may define p as the polish of the surface. In this case, Expanding Fuchs boundary conditions to cylindrical wire, we have

$$\begin{cases}\chi_r(-u_r, R') = -p\chi_r(u_r, R') \\ \chi_z(-u_r, R') = p\chi_z(u_r, R')\end{cases} \quad (12)$$

Where $R' = \frac{R}{(\hat{\mathbf{m}}.\boldsymbol{\alpha}.\hat{\mathbf{m}})^{1/2}}$ is the wire radius in y space.

Applying the boundary conditions (12) and supposing that the magnetic field is in the1-direction, with replacing different values of the reverse effective mass tensor, then equation (11), can be expressed as

$$u_r\frac{\partial\chi_1}{\partial r} + \frac{\chi_1}{\tau} + \frac{e\varepsilon_1}{K_\circ T} = 0 \quad (13)$$

$$u_r\frac{\partial\chi_2}{\partial r} + \frac{\chi_2}{\tau} + \frac{e\varepsilon_2}{K_\circ T} + \frac{e}{m}\alpha_{22}B_1\cos\phi\chi_3 - \frac{e}{m}\alpha_{23}B_1\cos\phi\chi_2 = 0 \quad (14)$$

$$u_r\frac{\partial\chi_3}{\partial r} + \frac{\chi_3}{\tau} + \frac{e\chi_3}{K_\circ T} + \frac{e}{m}\alpha_{32}B_1\cos\phi\chi_3 - \frac{e}{m}\alpha_{32}B_1\cos\phi\chi_2 = 0 \quad (15)$$

Here ϕ is the angle between normal vector and the 3-axsis. At first approximation, because of α_{22} being much smaller in comparison with other components of the effective mass tensor, we neglect the third term in equation (14). These equations (13) and (14) have the solutions for the components

$$\chi_r = \chi_1 = -\frac{e\tau\varepsilon_1}{K_\circ T}[1 - F_1(u)e^{-(\frac{r}{\tau u_r})} \quad (16)$$

$$F_r = F_1 = \frac{(1+p)\exp(-\frac{R'}{u_r\tau})}{1+p\exp(-\frac{2R'}{u_r\tau})}$$

$$\chi_z = \chi_2 = -\frac{e\varepsilon_2}{K_\circ TD}[1-F_2(u)e^{(-\frac{rD}{u_r})}] \quad (17)$$

$$F_z = F_2 = \frac{(1-p)\exp(-\frac{R'D}{u_r})}{1-p\exp(-\frac{2R'D}{u_r})}$$

$$D = \frac{1}{\tau} - \frac{e}{m}\alpha_{32}B_1$$

In y space current density is changed and may be written as fallow

$$\mathbf{J} = \frac{e}{4\pi^3}\int \mathbf{u}(k)f_1(k)d^3\omega \quad (18)$$

Where $\boldsymbol{\omega} = \frac{m_\circ}{\hbar}\mathbf{u}$. The local conductivity, which a function of r can be written down by averaging σ_r, σ_z over r

$$\sigma_r = \sigma_0[1-\frac{3}{2K}\int_\circ^1 \frac{(1+p)\exp(-\frac{K}{\mu})}{1+p\exp(-\frac{2K}{\mu})}[1-e^{\frac{-K}{\mu}}]\frac{\mu^4}{\sqrt{1-\mu^2}}d\mu] \quad (19)$$

$$\sigma_z = \frac{\sigma_0}{\tau D}[1-\frac{3}{2\tau DK}\int_\circ^1 \frac{(1-p)\exp(-\frac{DK\tau}{\mu})}{1-p\exp(-\frac{2DK\tau}{\mu})}[1-e^{\frac{-DK\tau}{\mu}}]\mu^2 d\mu] \quad (20)$$

$$\sigma_0 = \frac{2e^2\sqrt{2m_\circ}}{3K_\circ T\hbar^3\pi^2}\int \tau\varepsilon^{3/2}\frac{\partial f_\circ}{\partial\eta}$$

Let us assume that $K = \frac{R'}{l}$ and $\mu = \sin\theta$. Where $l(T)$ is the carrier mean free path, θ is the angle between direction of carrier motion with wire surface and σ_0 is the bulk conductivity of a single band of electrons. Symmetry consideration show that the conduction tensor for each ellipsoid pocket, in space can be written as

$$\boldsymbol{\sigma} = \frac{1}{(\det\alpha)^{1/2}}\{\sigma_z\boldsymbol{\alpha} + (\sigma_r - \sigma_z)\frac{\boldsymbol{\alpha}.\mathbf{mm}.\boldsymbol{\alpha}}{\mathbf{m}.\boldsymbol{\alpha}.\boldsymbol{\alpha}}\} \quad (21)$$

In primitive space, let us suppose that the normal vector in the 1-direction (it means that the magnetoresistance is transverse, by noting that magnetic field was in the 1-direction), then the effective conductivity in direction of current flow (axis of cylindrical wire) can be expressed as [19]

$$\sigma_{zz} = \frac{1}{(\det\alpha)^{1/2}}\sum_{i=1}^{3}\{\sigma_z\alpha_{22}^i + (\sigma_r - \sigma_z)\frac{\alpha_{21}^i\alpha_{12}^i}{\alpha_{11}^i}\} \quad (22)$$

Where normal vector is in the 1-direction, and α_{kl}^i is the components of the reciprocal effective mass ratio tensor for ith electron pocket. To distinguish between the different ellipsoids, we use a superscript running from 1 to 3.

IV. RESULTS AND DISCUSSIONS BY NUMERICAL CALCULATIONS

Bulk bismuth is a semimetal with a $(R\bar{3}m)$ crystal structure and a small band overlap $(\Delta_0 = -38\,\text{mev})$. The Fermi surface consist of a single ellipsoidal hole pocket and three ellipsoidal, anisotropic electron pockets [22]. Note that for Bi the mobility of holes is much smaller than the mobility of electrons so, then the electrical conductivity is determined by electrons [22, 23]. Electrical resistivity of nanowire is determined by equation 24, to this end we require the components of the effective mass tensor (for three ellipsoidal Fermi surfaces), bulk conductivity and variation type of scattering parameter. Assuming that 1, 2, 3 directions are in direction of binary, bisectrix and trigonal axes sequentially, then effective mass tensor for an ellipsoidal pocket is of the form

$$\alpha_{ij}^1 = \begin{pmatrix} \alpha_1 & 0 & 0 \\ 0 & \alpha_2 & \alpha_4 \\ 0 & \alpha_4 & \alpha_3 \end{pmatrix} \quad (23)$$

Since $\alpha_1 = 119, \alpha_2 = 1.31, \alpha_3 = 102, \alpha_4 = 8.6$. While two other tensors, are determined by rotation by 120° and 240° around the trigonal axis [19].

Whereas we decided to compare the result of this analysis method with experimental values reported by Heremans *et al*, then we consider that the wires are single crystal, with their long axes oriented in the bisectrix-trigonal plane, about 19° from the bisectrix axis [17]. Therefore we can obtain the components of $\boldsymbol{\alpha}$ in the experimental coordinates system, by use of the parrot theory [19].

Resistivity of bulk bismuth is presented in various papers, theoretically [24] and experimentally [25], which may be written as

$$\rho_b = 3.88\times10^{-7}T \ \ (\Omega\, cm) \quad (24)$$

Now we wish to know the form of the p function. No theory of the scattering of electrons at the surface has existed, capable of enabling a calculation of *p* to be made, so that assuming it to be a constant was a reasonable first approximation. Let us assume that $p = 1$ when $\mu \langle \mu_0$ and $p = 0$, when $\mu \rangle \mu_0$. Where corresponds to an angle, so that for angles smaller than a μ_0 value, reflection is speculary. By noting this assumption and Substituting mentioned parameters into equation (19), equation (20) and use of equation (24), the transverse magnetoresistance for Bi nanowires can be calculated and plotted versus temperature, magnetic field and wire diameter. We have numerically evaluated the theoretical transverse magnetoresistance ratios, and the results are plotted in figures 1 to 4. The values of $\bar{\mu}_0$ $(\bar{\mu}_0 = \frac{\mu_0^1+\mu_0^2+\mu_0^3}{3})$ are presented in table1, for the five radii in various magnetic fields. As can be seen as the radius decreases, the value of $\overline{\mu}_0$ increases and the specular reflection of the carriers from the boundary decreases and so less magnetic size effect in the magnetoresistance of the wires is expected. On the other hand, as small value of B (corresponds to a large value of $\overline{\mu}_0$), is an indication of a large amount of diffusion of the carriers on the boundary and therefore a more pronounced magnetic size effect is expected.

TABLE I. $\overline{\mu}_0$ VALUES FOR VARIOUS DIAMETERS AND MAGNETIC FIELDS

	B=1T	B=2T	B=3T	B=4T	B=5T
R=7nm	0.600	0.598	0.580	0.520	0.513
R=28nm	0.548	0.536	0.524	0.512	0.498
R=36nm	0.432	0.422	0.417	0.403	0.399
R=70nm	0.291	0.280	0.254	0.241	0.236
R=200nm	0.203	0.183	0.161	0.143	0.101

V. CONCLUSIONS AND INTERPRETATION OF THE GRAPHS

By generalizing the surface scattering theory of fuchs, over nanowires, with multiple ellipsoidal fermi surfaces, transverse magnetoresistance versus temperature, magnetic field and wire diameter is calculated. Experimental data reported by Heremens *et al* [15] (the dashed lines) and theoretical calculations obtained in this research (the solid curves) are plotted in figures 1 and 2. As seen from the figures, although many other factors like, lattice defects, impurity and noncrystal state are effective on the carrier scattering , it is clear that our results can give adequate agreement with the experimental data for (B<3T). As shown in the figures, for (B>3T) the sharp disparity between them is observed, because of the variation of l and τ in presence of high magnetic field.

Figure 1(a) and figure 1(b) show the temperature dependence of the MR in the transverse direction. From these figures it is clear that the magnetic size effects can be observed at low temperatures when MFP of carriers is with the same order at the sample size. It should be pointed out that the magnetic behaviors of semimetals have been studied extensively in these two temperature ranges. For example the low temperature (T<10k) data are dominated by the localization effects [24], which increases as the temperature is decreased. In the temperature rang $(1o^{\circ}K \leq T \leq 300^{\circ}K)$, the temperature dependence of the longitude MR coefficient has been used to identify the semimetal-semiconductor phase transitions[26] which is calculated to occur as the wire diameter decreases below about 65nm.

Referring to figures, it can be seen that firstly, by increasing the magnetic field, TMR will be increased for all radii. Secondly, for temperature greater than a critical value, TMR will be unchangeable, approximately. These critical temperature for R=7nm and R=28nm diameter, are about $1o^{\circ}\mathrm{K}$. In a certain temperature, TMR versus Bi nanowire diameter, for various magnetic fields are plotted in figure 2(a) and figure 2(b). As shown in these figures, in curve of each magnetic fields, in a critical diameter, TMR varied dramatically from a single value. In $T = 1o^{\circ}\mathrm{K}$, critical radius is $d_c = 33.4\mathrm{nm}$ and in $T = 2o^{\circ}\mathrm{K}$ is $44.5nm$, averagely.

In fact these radii were those where semimetal-semiconductor phase transitions can occur. Because in these diameters the effect of confinement (QSE) is to raise the electron energies and lower the hole energy, thus removing the overlap $(\Delta_0 = -38\,mev)$. When the wire diameter is reduced below a critical value, an energy gap opens up and wires become semiconducting. The critical diameter for nanowire oriented along the trigonal axis is calculated as $d_c = 53\mathrm{nm}$ by Bejenari *et al* [7] and is 32.5nm for nanowire oriented along the bisectrix axis [7]. Also reported by Zhang Z *et al* for the binary, trigonal and bisectrix directions, $d_c \approx 30\mathrm{nm}$, $45nm$ and $81\mathrm{nm}$, respectively [26]. Here it is worth mentioning that there is a close relationship between critical radius, calculated in this article and electrons Cyclotron radius ($r_c = 40\mathrm{nm}$) of the wire [17] and critical diameters (that phase transitions occur), which will be studied in consequent works.

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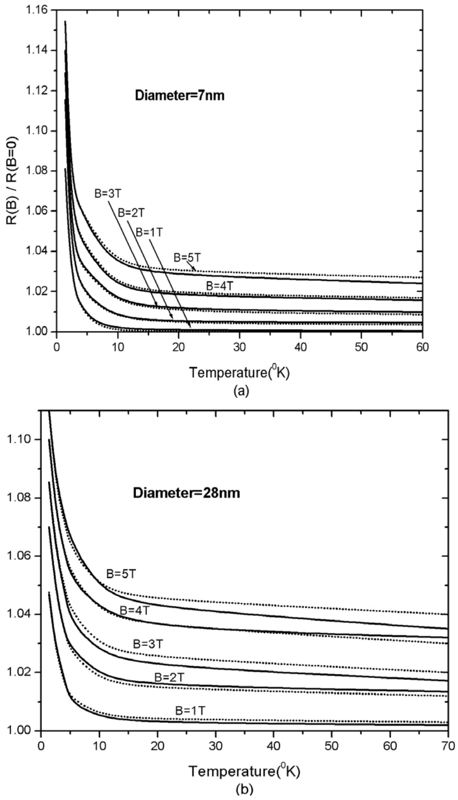

Figure 1. Temperature dependence of the TMR Bi nanowire, normalized to the resistance of zero field at the same temperature in the filed rang $1T \leq B \leq 5T$. (a) R=7nm diameter and (b) R=28nm diameter.

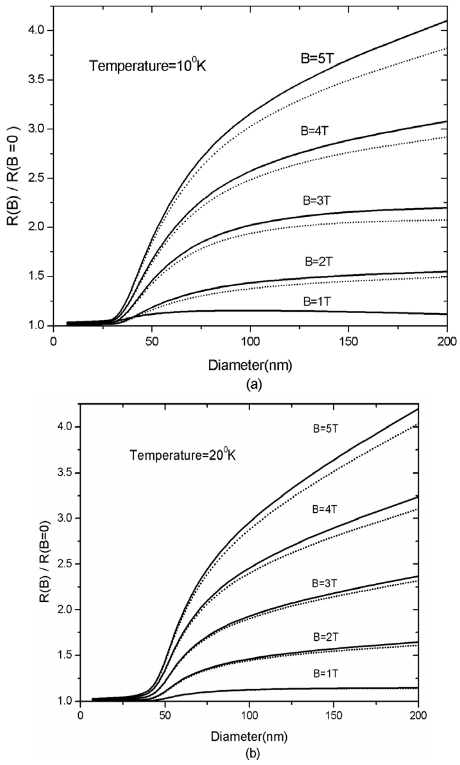

Figure 2. Diameter dependence of the Bi TMR, normalized to the resistance of zero field at the same temperature in the filed rang $1T \leq B \leq 5T$,(a) $T = lo^{\circ} K$ and (b) $T = 2o^{\circ} K$.