Journal of Magnetics 4(4), 111-114 (1999)

Temperature Dependence of Galvanomagnetic Properties in Thin Bi Film

S. W. Nam

Department of Physics, Korea University, ChoChiWon 339-700, Korea

(Redeived 30 October 1999)

Numerical calculation for temperature dependence of galvanomagnetic properties of thin bismuth film is pursued. The quasi-two dimensional system is treated in the perturbation formalism of previous study, where realistic screened potential due to impurity is assumed to be the only scattering channel. The potential is separated into pure two dimensional part and the remaining presumed perturbation part. Relaxation time and mobilities for both electron and hole are evaluated, then temperature dependence of the Hall coefficient and magnetoresistance is obtained. The broad minimum of magnetoresistance is manifested, and the interpretation under the kinetic theory is made. Thickness dependence of the quantities are also shown, which are in good agreement with the expected quantum size effect.

1. Introduction

Bi is very typical material in studying the kinetic properties of thin film structure: Small density of state effective mass for electron in trigonal direction gives rise to a large separation of the energy subbands, so that we can observe the quantum size effect from 250 Å up to a few thousand Å thicknesses of the film. It's oscillatory behavior of transport quantities with respect to the thickness is well known experimentally [1-6] and theoretically [7, 8]. On the other hand, the details of the kinetic mechanism are not clear for this low charge carrier density material. The role of versatile scattering channels of impurity, phonon, or surface needs to be separated out from each other [9]. Surface charge concentration and boundary condition for the wavefunction can change the physical quantities substantially [6]. These effects are expected to answer the abnormal behavior of resistivity, Hall coefficient, and the magnetoresistance at low temperature range [1, 2].

Among the various origins of scattering channels, the effect of impurity is the most fundamental, in that we can learn from it how to treat a potential in thin film structure generally. Especially, the impurity is more important for the scattering at lower temperature than the phonon.

Thus, dynamic consideration for the scattering mechanism of the charge carriers due to a potential center in the quasi-two dimensional (Q2D) system is requested in the first principle theoretical study. In the previous study [10-12], the scattering mechanism in the Q2D geometry is formulated in the peculiar perturbation scheme. For the case of very thin film the Hamiltonian is separated into pure 2D part and the remaining part, but the perturbation potential is expected to be smaller when the thickness is reduced. The valid thickness for the perturbation theory is quite large, ~500 Å, for Bi film.

We introduce the perturbation theory in section 2, and apply this to thin Bi film at lower temperature range. We need numerical calculation to determine basic quantities, like chemical potential and charge concentration. The relaxation times and mobilities for electron and hole are also evaluated in section 3, and the galvanomagnetic quantities are calculated. In section 4, we discuss the validity and limits of this formulation.

2. Formulation

Theoretical study of very thin film structure is naturally implied to treat it as 2D system. A typical way of projecting the motion of charge carriers onto a plane is to take an integral over perpendicular direction [13], which is a sort of averaging with respect to the quantum states of perpendicular coordinates. In a MOSFET structure [14] boundary condition for the potential well determines the wavefunction in a self-consistent way.

In the present study we adopt the perturbation theory [12], calculating the dynamic scattering amplitude in a film structure, including screening by the itinerant charges. We notice that the potential in the thin film expressed by 2D projection of real coordinates is almost the same as the 3D potential, then take the difference as the perturbation Hamiltonian. Quantum mechanical calculation gives rise to the scattering amplitude, which depends on thickness and especially on the screening parameter. The total scattering amplitude is obtained by $F(\theta)=f(\theta)+f'(\theta)$, where $f(\theta)$ is the scattering amplitude for pure 2D Hamiltonian with the 'projected' potential, and $f'(\theta)$ is the perturbing term which

is proportional to the scattering matrix of the perturbation between incident and scattered waves $\langle k|H'|k'\rangle$. We assume that only the intra-subband scattering is important, since the inter-subband transition between the nearest subbands vanishes in our formulation. Total scattering rate is the sum of each subband scattering rate. For n-th subband the momentum relaxation time is evaluated as

$$\frac{1}{\tau_n(k)}=\frac{2\pi n_i e^4}{\hbar^2 k_F^2}\left[\left(\frac{\pi}{k^2}-\frac{\pi q}{k^2}\frac{1}{\sqrt{4k^2+q^2}}\right)+8I_n(q,d)T(k,q)+2\pi I_n^2(q,d)\right] \quad (1)$$

where n_i is the impurity concentration in the sample, k_F is the Fermi wave vector, d is the thickness, and q is the screening parameter. The first term is the pure two dimensional contribution, which is calculated from the scattering amplitude due to screened impurity potential in 2D system. The second and the third terms represent the effect of finiteness of thickness;

$$I_n(q,d)=2\pi e^2\int_{-d/2}^{d/2}dz|\phi_n(z)|^2\int_0^\infty d\rho\rho H'(\rho, z; q) \quad (2)$$

is obtained from the matrix element of the perturbation, and

$$T(k, q)=\int_0^\pi d\theta\ \frac{\sin^2(\theta/2)}{\sqrt{q^2+4k^2\sin^2(\theta/2)}} \quad (3)$$

is nothing but the confluent hypergeometric function ${}_2F_1$ (1/2, 3/2; 2; $-4k^2/q^2$). Thermal average of the momentum relaxation time for each subband yields the relaxation time;

$$\left\langle\frac{1}{\tau_n}\right\rangle=\frac{\int_0^\infty dEE(\partial f_o/\partial E)[1/\tau_n(E)]}{\int_0^\infty dEE(\partial f_o/\partial E)} \quad (4)$$

where f_o is the Fermi distribution function for each charge carrier.

3. Numerical Results

Assuming the usual compensation condition for the electron and hole charges in semimetallic Bi, we write

$$3\gamma_e\sum_{s=1}^{\infty}\ln(1+e^{(\mu_e-\varepsilon_e s^2)/k_BT}) =\gamma_h\sum_{s=1}^{\infty}\ln(1+e^{(\mu_h-\varepsilon_h s^2)/k_BT}), \quad (5)$$

where $\gamma_e=m_e k_B T/\pi\hbar^2 d$, $\gamma_h=m_h k_B T/\pi\hbar^2 d$ and the factor of 3 on the electron side is due to three-fold degeneracy along the trigonal direction. μ_e and μ_h are the chemical potentials of two charge carriers, and ε_e and ε_h are the quantized energies along the perpendicular direction of the film respectively. Although the energy quantization for the hole is very small compared with the electron case, we keep the subband summation, instead of treating it continuum as other authors did [1, 2]. This equation is solved for the chemical potentials and the concentration of electron and hole, along with the condition for the energy band overlap of semimetallic Bi, $\mu_e+\mu_h=\Delta$. Δ=30 meV is used for the present study. Temperature and thickness dependences of these quantities are important in determining the temperature dependence of galvanomagnetic properties. Energy overlap transforms itself into insulator by reducing the thickness down to 250 Å. The observation of semimetal - insulator transition still arouse some skepticism [15], but we take $d>300$ Å for investigation of electric transport phenomena.

Another important parameter in the present study is the screening, since the kinetic scattering by a more realistic impurity is considered here in the perturbation scheme. Screening parameter in Bi is not known precisely yet. However, in order to take into account real feature of scattering potential other than the simple delta shape potential [7], we consider the Thomas-Fermi screening parameter in the intermediate range, ~k_F. The Fermi wave vector for d=400 Å at T=5 K is $k_F=1.2\times10^6$ cm^{-1}. In this case the screening potential extends out to an order of 100 Å, still smaller than the thickness that we are considering, therefore the perturbation theory is still valid.

According to the numerical evaluation, temperature dependence of chemical potential and concentration is prominently sensitive, but thickness dependence is negligible; μ_e decreases by 2% for 300 Å to 700 Å change, but it varies substantially with temperature, 20% increase for 5 K to 50 K. Inclusion of the perturbation terms decreases the relaxation time more for the thinner films compare with the pure two dimensional term. On the other hand the Fermi energy on denominator is larger for the thinner films, so that these opposite tendencies make the relaxation time less sensitive to the quantum size effect.

3.1. Relaxation time and mobilities

Fig. 1 shows the temperature dependence of mobilities for electron and hole in the temperature range of T=5-150 K. Mobility, $\mu_i=e\langle\tau_i\rangle/m_i$, is proportional to the inverse of thermal average of scattering rate, Eq. (4), which is generally expected to have increasing behavior with temperature for any charge carrier [2], since more charge carriers are supposed to be involved in the scattering process at higher temperature. However, scattering rate for electron in the present study reveals a decreasing behavior with increasing temperature. We understand this behavior as a consequence of competition between temperature dependence of quantum mechanical momentum scattering rate $1/\tau(k)$ and that of thermal average: (i) Momentum scattering rate is roughly proportional to the inverse of chemical potential, so that the larger the speed of charge carriers at high temperature the smaller the scattering cross section. (ii) When taking thermal average through df_o/dE, more charge carriers are involved at higher temperature, so that the number of scattering events increases. In the case of electron the first fac-

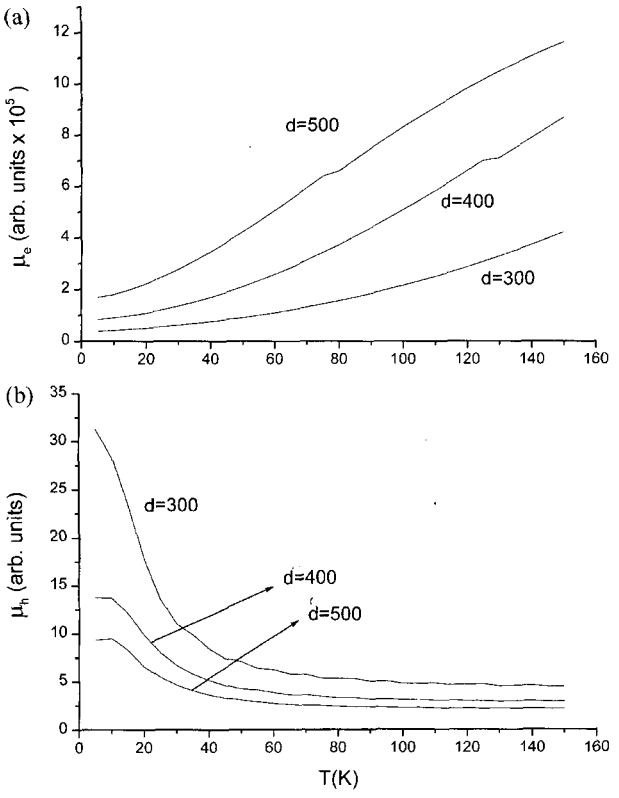

Fig. 1. (a) Temperature dependence of electron mobility for various thickness (in Å). (b) Temperature dependence of hole mobility for various thickness (in Å).

tor is more important; since the chemical potential increases substantially fast with temperature. On the other hand, for the hole channel the chemical potential decreases as $\mu_p = \Delta - \mu_n$ with increasing temperature, so that momentum scattering rate increases with temperature. The second factor for hole still helps it increase. However; the magnitude for the hole mobility is negligibly small (4 orders smaller than for electron) due to its huge effective mass compared with electron case. Though the hole mobility is small enough to be neglected in calculation of resistivity and Hall coefficient, it will be considered importantly when evaluating the magnetoresistance together with the oscillatory behavior.

We observe a small oscillating behavior in mobility results, superposed onto the above mentioned temperature dependence. It manifests the quantum size effect: As a new subband is started to supply more charge carriers according to df_0/dE, a new contribution of scattering amplitude is added to that of old subband(s). The subband level spacing in the perpendicular direction to the film plane is 11.7 meV for electron and 0.234 meV for hole when thickness $d = 400$ Å. Thus, the period of oscillation would be 135 K and 2.7 K respectively. This effect resembles the Landau level character in the de Haas-van Alphen effect.

Electron mobilities for thinner films exhibit lower values, but it is in opposite way for hole mobilities. We interpret it in the scheme of present perturbation theory; a potential cross section will block the incident beam of electrons in the film, but thicker film would leave more free space for itinerant electrons to reduce the effective value in the parenthesis of Eq. (1). However, the momentum scattering rate which is divided by the chemical potential, is again determined by the competition between the kinetic and thermal considerations.

Thickness dependence of relaxation time is also checked, It suggests the oscillatory behavior with a period of ~300 Å for electron. As the thickness is increased, a new subband is started to be filled, so that more scattering events contribute to the scattering amplitude. The period is verified through the self-consistent solution of compensation equation and the overlap relation.

3.2. Hall constant and Magnetoresistance

The expression of Hall coefficient and magnetoresistance for two charge carrier model [16] can be rewritten in terms of mobilities:

$$R_H = \frac{1}{nec}\frac{\mu_e - \mu_h}{\mu_e + \mu_h} \tag{6}$$

$$\frac{\Delta\rho}{\rho H^2} = \frac{1}{c^2}\mu_e\mu_h \tag{7}$$

Since the ratio of hole to electron effective masses, m_{hole}/m_{el} ~50, for (111) direction in Bi, R_H is not much different from the electron dominant result R_H~1/nec. Fig. 2 does not show any anomalous peak at lower temperature, which is shown in several experimental works [1, 2, 6]. As is mentioned in those papers this anomaly might come from the surface charge concentration and(or) other scattering channels like phonon and surface roughness, among which we anticipate that the phonon is the most important channel since the experimental results show a strong temperature dependence.

Magnetoresistance (MR) reveals the most interesting result in Fig. 3: It shows broad minimum at about T=20-80 K, which is also obtained in the experimental study [2, 6]. Since MR depends on the product of the mobilities of both charge carriers only, this is the place where we can not neglect hole mobility. The present qualitative study shows

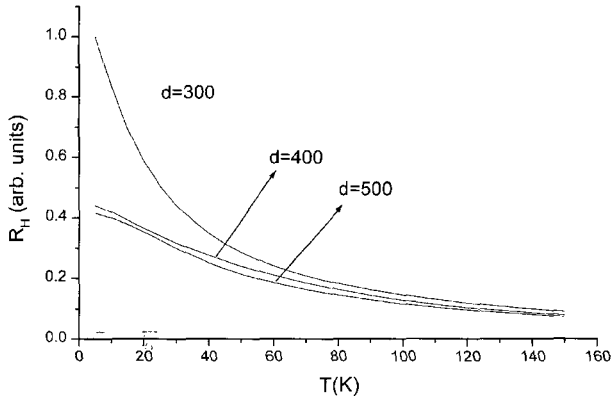

Fig. 2. Hall coefficient as a function of temperature. d in Å.

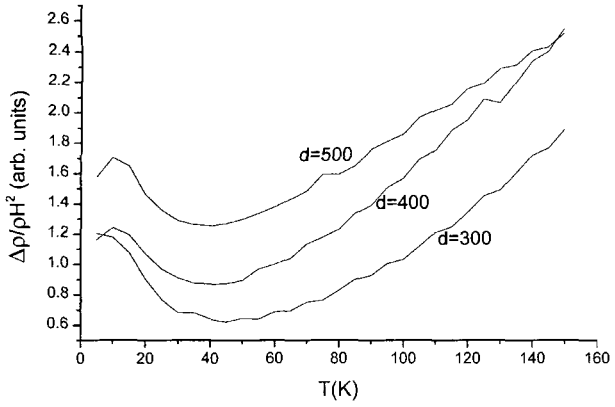

Fig. 3. Magnetoresistence as a function of temperature. d in Å.

that the perturbation theory of calculating scattering amplitudes can elucidate the role of several charge carriers, especially that of hole. The thickness dependence of MR is also understood by the enhancement of scattering process for thinner film. The existence of minimum in the present formulation manifests itself that the scattering mechanisms for electron and hole show opposite character. This behavior also stems on the fact that the momentum scattering rate is determined by pure mechanical consideration of finding scattering cross section. A few of the small bumps in the figure is believed that the quantum size effect is exhibited at the specific thickness. We also note that only the impurity channel scattering gives rise to a deep minimum, which is understandable since the phonon channel is depressed in the lower temperature range.

4. Discussion

We persue a quantitative calculation of temperature dependence of galvanomagnetic properties of Bi by first principle calculation. Temperature dependence comes in through density, chemical potential, and Fermi distribution function in a complicated way. Since the contribution of surface charge concentration [6] is excluded, the peak in the Hall coefficient is not observed in the present calculation. However, the temperature dependence of magnetoresistance shows the broad minimum, which is a consequence of kinetic effect in quantum scattering. Thus, the perturbation theory could be a way of understanding of microscopic transport in thin film system.

The validity of this formalism should always be questioned, since the smallness of the perturbation potential is not guaranteed in the first place. General rule for validity of the theory is known as $k_F d \ll 1$. [10, 11] In the present study, we numerically test the validity by checking the magnitude of $I_n(q, d)$ comparing with the pure 2D Hamiltonian; we confirm that the perturbation terms are about 10%, or smaller than the pure 2D term when d ~400 Å and $k_F < q < 5k_F$.

Finally, we point out the limits of the study: Scattering channels other than impurity scattering, like phonons, or surface scattering are not included in the present study. The importance of phonons is growing when the temperature approaches the Debye value, and the effect of surface roughness scattering [17] should be taken into account for the realistic consideration. On the other hand, the condition for the compensation of electron and hole concentrations is not applied, especially for thinner films [15].

References

[1] Yu. F. Ogrin, et al., Soviet Physics JETP **26**, 714 (1968).
[2] N. Garcia, Y. H. Kao and M. Strongin, Phys. Rev., **B5**, 2029 (1972).
[3] K. Liu, C. L. Chien and P. C. Searson, Phys. Rev., **B58**, R14681(1998).
[4] V. Yu. Kashirin and Yu. F. Komnik, Phys. Rev., **B50**, 16845 (1994).
[5] Yu. F. Komnik, et al., Phys. Rev., **B50**, 15298 (1994).
[6] Yu. F. Komnik, et al., Soviet Physics JETP **33**, 364 (1971).
[7] V. B. Sandomirskii, Soviet Physics JETP **25**, 101 (1967).
[8] V. A. Tavgar and V. Ya. Demikhovskii, Soviet Physics Uspekhi **11**, 644 (1969).
[9] K. Hirakawa and H. Sakaki, Phys. Rev., **B33**, 8291 (1986).
[10] J. Heo and S. W. Nam, Sae Mulli **36**, 619 (1996).
[11] S. W. Nam, Phys. Stat. Sol. (b) **209**, 329 (1998).
[12] S. W. Nam and Y. C. Lee, Proc. Stat. Phys., Sigapore, 122 (1998).
[13] P. J. Price, Ann. Phys., **133**, 217 (1981).
[14] F. Stern, Phys. Rev. Lett., **44**, 1469 (1980).
[15] C. A. Hoffman, et al., Phys. Rev., **B48**, 11431 (1993).
[16] Ziman, 'Electrons And Phonons', Oxford, 494 (1960).
[17] D. Calecki, Phys. Rev., **B42**, 6909 (1990).