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The effect of energy bands on the amplification of surface phonons in thin bismuth films

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Abstract. The effect of energy bands on the amplification coefficient of Rayleigh waves in thin bismuth films is investigated quantum mechanically in the gigahertz frequency region. It is shown that the amplification coefficient for the modified non-ellipsoidal non-parabolic model is much closer than that for the non-ellipsoidal non-parabolic (NENP) model to that for the ellipsoidal parabolic model or the ellipsoidal non-parabolic model in the low-temperature limit. Therefore the NENP model in the thin bismuth films does not explain very well the electronic transport properties in the gigahertz region at very low temperatures.

The constant-energy wavevector surface of bismuth differs considerably from the simple spherical surface of the degenerate electron gas. From theoretical calculations (Cohen 1961) and experimental results (Koch and Jensen 1969, Dinger and Lawson 1970, 1971, 1973), it was pointed out that the energy band of bismuth follows the Cohen non-ellipsoidal non-parabolic (NENP) energy band model. However, the magneto-optical results (Maltz and Dresselhaus 1970, Vecchi *et al* 1976) and the longitudinal magnetostriction (Michenaud *et al* 1981, 1982) supported the Lax ellipsoidal non-parabolic (ENP) energy band model (Lax 1958). McClure and Choi (1977) presented a new energy band model for bismuth electrons which is more general than those currently in use. They showed that it can fit the data for a large number of magneto-oscillatory and resonance experiments. This new energy band model is called the McClure–Choi modified non-ellipsoidal non-parabolic (MNENP) energy band model.

The interaction between acoustic waves and conduction electrons provides a useful tool for investigating the electronic band structure of matter. Acoustic waves can be propagated along the boundary of an elastic half-space (Ezawa 1971), the amplitude of which falls off rapidly as one goes away from the surface. Such elastic excitations are called Rayleigh waves (Grishin and Kaner 1972). The surface phonons are the quanta of elastic waves that satisfy the proper boundary condition on solid surfaces (Ezawa 1971). They are to be used in place of the bulk phonons when one is dealing with surface phenomena. In semimetals such as bismuth, the interaction of elastic surface waves with conduction electrons is dominated by the deformation potential coupling in solids. The deformation of the crystals due to the surface waves determines directly the deformation potential force acting on the conduction electrons. The amplification coefficient of

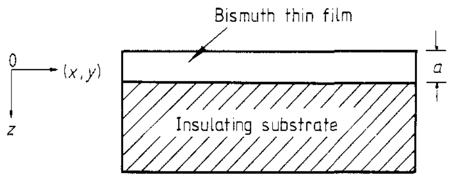

Figure 1. A thin layer with the thickness a of a thin bismuth film and an insulating material. Rayleigh waves propagate parallel to the surface of the film (x–y plane).

Rayleigh waves can be calculated using the Born approximation. In this paper, we report on our study of the effect of energy bands on the amplification of Rayleigh waves in thin bismuth films using the quantum mechanical treatment.

A thin layer with a thickness a of a semimetal such as bismuth is grown epitaxially on an insulating substrate with the same elastic properties as the semimetal layer. For simplicity, the analysis is made for an isotropic medium occupying the half-space $z \geqslant 0$ with a stress-free boundary parallel to the x–y plane as shown in figure 1. We fix Rayleigh waves of wavevector $\boldsymbol{q}$ along the [110] direction. It is assumed that the potential along the z axis is a square well which has infinitely high potential barriers at $z = 0$ and $z = a$, neglecting possible depletion layers at both sides near $z = 0$ and $z = a$. Under this approximation, the field operator $\psi(\boldsymbol{r})$ of conduction electrons in the second quantisation can take the form (Tamura and Sakuma 1977)

$$\Psi(\boldsymbol{r}) = \left(\frac{2}{V}\right)^{1/2} \sum_{n=1}^{\infty} \sum_{\boldsymbol{k}} b_{\boldsymbol{k}n} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}) \sin\left(\frac{n\pi z}{a}\right)$$
$$= \left(\frac{1}{S}\right)^{1/2} \sum_{n=1}^{\infty} \sum_{\boldsymbol{k}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}) \varphi_n(z) b_{\boldsymbol{k}n} \qquad (1)$$

where $\boldsymbol{r} = (\boldsymbol{x}, z) = (x, y, z)$, $\boldsymbol{k} = (k_x, k_y)$, $V = aS$ is the volume of the film with a surface area S, $b_{\boldsymbol{k}n}$ and its Hermitian conjugate $b^{\dagger}_{\boldsymbol{k}n}$ are annihilation and creation operators respectively, of conduction electrons, satisfying the commutation relation of Fermi type. The energies $E_{\boldsymbol{k}n}$ of conduction electrons in bismuth are given by the following different types of relation.

(i) For the MNENP model,

$$E_{\boldsymbol{k}n}(1 + E_{\boldsymbol{k}n}/E_g) = \hbar^2 k_x^2/2m_1 + (\hbar^2 k_y^2/2m_2)(1 - n^2\pi^2\hbar^2/2m_3 E_g a^2) + \hbar^4 k_y^4/4m_2^2 E_g - \hbar^4 k_x^2 k_y^2/4m_1 m_2 E_g + n^2\pi^2\hbar^2/2m_3 a^2 \qquad n = 1, 2, 3, \ldots . \qquad (2a)$$

(ii) For the NENP model,

$$E_{\boldsymbol{k}n}(1 + E_{\boldsymbol{k}n}/E_g) = \hbar^2 k_x^2/2m_1 + \hbar^2 k_y^2/2m_2 + \hbar^4 k_y^4/4m_2^2 E_g + n^2\pi^2\hbar^2/2m_3 a^2 \qquad n = 1, 2, 3, \ldots . \qquad (2b)$$

(iii) For the ENP model,

$$E_{\boldsymbol{k}n}(1 + E_{\boldsymbol{k}n}/E_g) = \hbar^2 k_x^2/2m_1 + \hbar^2 k_y^2/2m_2 + n^2\pi^2\hbar^2/2m_3 a^2 \qquad n = 1, 2, 3, \ldots . \qquad (2c)$$

(iv) For the ellipsoidal parabolic (EP) model,

$$E_{\boldsymbol{k}n} = \hbar^2 k_x^2/2m_1 + \hbar^2 k_y^2/2m_2 + n^2\pi^2\hbar^2/2m_3 a^2 \qquad n = 1, 2, 3, \ldots . \qquad (2d)$$

E_g is the energy gap between the conduction and valence bands, and m_1, m_2 and m_3 are the effective masses of electrons along the x, y and z axes, respectively.

The surface-phonon field operator is written, using well known eigenfunctions for the Rayleigh wave (Ezawa 1971), as

$$u(r) = \sum_q \left(\frac{\hbar}{2\rho\omega_q S}\right)^{1/2} [a_q u_q(z) \exp(\mathrm{i}q \cdot x) + a_q^\dagger u_q^*(z) \exp(-\mathrm{i}q \cdot x)] \tag{3}$$

where ρ is the mass density of the medium, $q = (q_x, q_y)$ is the wavevetor of Rayleigh waves, $\omega_q = c_R|q|$ is the surface-phonon angular frequency and c_R is the velocity of Rayleigh waves. a_q and its Hermitian conjugate $a_q^\dagger$ are the annihilation and creation operators, respectively, for the surface-phonon field, obeying commutation relations of the Bose type. The explicit forms of the wavefunction $u_q(z)$ are

$$u_q^j(z) = \mathrm{i}(q_j/q)(q/J)^{1/2}[\exp(-\gamma qz) - [2\gamma\sigma/(1+\sigma^2)] \exp(-\sigma qz)] \qquad j = (x, y) \tag{4}$$

$$u_q^z(z) = -\gamma(q/J)^{1/2}[\exp(-\gamma qz) - [2/(1+\sigma^2)] \exp(-\sigma qz)] \tag{5}$$

where γ, σ and J are constants defined by the velocity c_l of the longitudinal sound wave and the velocity c_t of the transverse sound wave as

$$\gamma^2 = 1 - (c_R/c_l)^2 \tag{6}$$

$$\sigma^2 = 1 - (c_R/c_t)^2 \tag{7}$$

and

$$J = (\gamma - \sigma)(\gamma - \sigma + 2\gamma\sigma^2)/2\gamma\sigma^2. \tag{8}$$

In the semimetal-like bismuth, the conduction electrons interact with the surface phonon through the deformation potential which is proportional to the dilation caused by the acoustic field. Using the Green function method with the Born approximation, the amplification coefficient of the surface phonon can be obtained as

$$\alpha = \frac{\omega_q x}{4\pi c_R k_B T} \sum_{i,j} [C(q)]^2 |\Phi_{ij}^D(q)|^2 \int \mathrm{d}k \int \mathrm{d}\varepsilon \,\mathrm{sech}^2[(\varepsilon - E_F)/2k_B T]$$
$$\times \delta(\varepsilon - E_{ki})\delta(\varepsilon + \hbar\omega_q x - E_{k-q,j}) \tag{9}$$

where $C(q) = C/\varepsilon_l(q)$, $\varepsilon_l(q) = 1 + (6\pi e^2 N c_l^2/\varepsilon_0 q^2 c_R^2 E_F)$, C is the deformation potential, ε_0 is the static dielectric constant, N is the electron concentration, E_F is the Fermi energy, $\delta(x)$ is the Dirac δ-function, $x = v/c_R - 1$ is the drift parameter for the drift velocity v of electrons and

$$\Phi_{nn'}^D(q) = -\left(\frac{\hbar q^2}{2\rho c_R J}\right)^{1/2} \left(\frac{c_R}{c_l}\right)^2 \int_0^a \varphi_{n'}^*(z) \exp(-\gamma qz)\varphi_n(z)\,\mathrm{d}z. \tag{10}$$

The relevant values of physical parameters for bismuth (Harrison 1960, Fal'kovskiĭ 1968) are $m_1 = m_0/172$, $m_2 = m_0/0.8$, $m_3 = m_0/88.5$ (m_0 is the free-electron mass), $\rho = 9.8\ \mathrm{g\ cm^{-3}}$, $N = 2.75 \times 10^{17}\ \mathrm{cm^{-3}}$, $\varepsilon_0 = 10$, $c_R = 2.9 \times 10^5\ \mathrm{cm\ s^{-1}}$, $c_l = 4.9 \times 10^5\ \mathrm{cm\ s^{-1}}$, $c_t = 3.8 \times 10^5\ \mathrm{cm\ s^{-1}}$, $E_g = 0.0153\ \mathrm{eV}$, $E_F = 0.0276\ \mathrm{eV}$, $C = 10\ \mathrm{eV}$, $a = 1\ \mu\mathrm{m}$ and $x = 50$ (corresponding to an applied electric field E of 480 mV cm^{-1}). The frequency

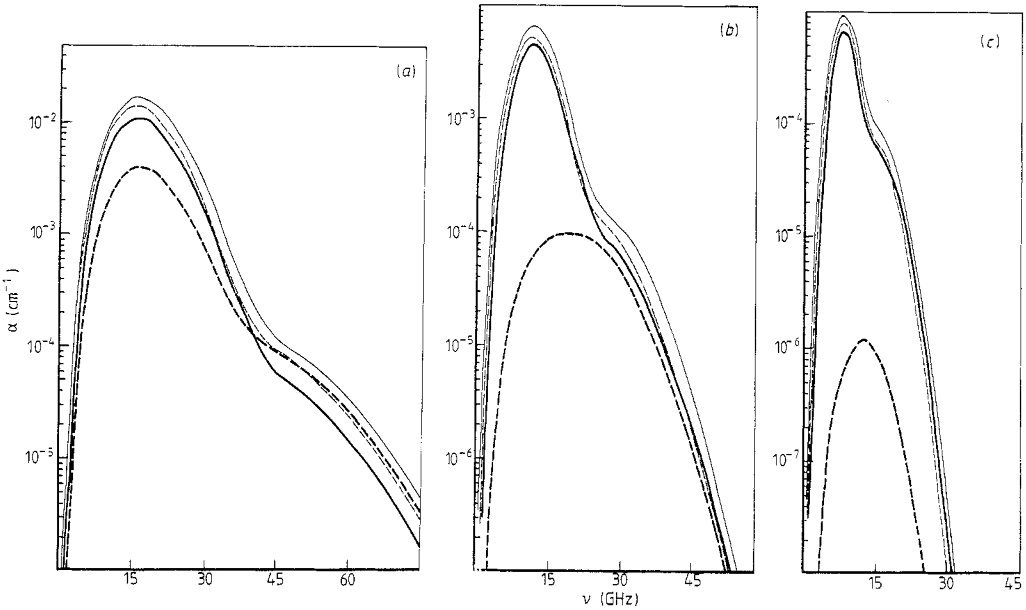

Figure 2. Amplification coefficient of Rayleigh waves against frequency in bismuth films with $x = 50$ ($E = 480\,\text{mV cm}^{-1}$) and $a = 1\,\mu\text{m}$ at (a) $T = 77$ K, (b) $T = 19.7$ K and (c) $T = 4.2$ K: ———, MNENP model; ----, NENP model; ———, ENP model; ----, EP model.

($\nu = \omega_q/2\pi$) dependence of the amplification coefficient for temperatures T of 77, 19.7 and 4.2 K is shown in figure 2.

It can be seen that the amplification coefficient increases rapidly with increasing frequency and, after reaching a maximum point, the amplification coefficient decreases on further increase in frequency. From figure 2(a) for a temperature of 77 K, it can be seen that in the lower-frequency region the amplification coefficient for the MNENP model is close to those for the ENP and EP models, while in the higher-frequency region the amplification coefficient for the NENP model is close to those for the ENP, EP and MNENP models. For a temperature of 19.7 K as shown in figure 2(b), the amplification coefficient decreases more rapidly with increasing frequency than for a temperature of 77 K as shown in figure 2(a) after passing the maximum point. It can also be seen that the amplification coefficients for the EP, ENP and MNENP models become much closer, while the inflection point in the amplification coefficient for the NENP model disappears with decreasing temperature. Moreover, when the temperature is 4.2 K, the difference between the amplification coefficient of the NENP model and those of the EP, ENP and MNENP models becomes larger. However, the amplification coefficients for these four types of model become closer in the high-frequency region. This is because the energy band of conduction electrons plays an important role in the low-frequency region, while in the high-frequency region the Rayleigh waves become important in the electronic transport in thin bismuth films. By comparing equations (2a), (2c) and (2d) with equation (2b), it can be seen that the correction term $\hbar^4 k_y^4/4m_2^2 E_g$ in the NENP model causes quite an over-correction of the energy band in bismuth. Thus some other correction terms, $-\hbar^4 k_y^2 \pi^2 n^2/4m_2 m_3 E_g a^2$ and $-\hbar^4 k_x^2 k_y^2/4m_1 m_2 E_g$, in the MNENP model could reduce the over-correction of the NENP model. This energy band effect will become more important at low temperatures and in the low-frequency region. Consequently, for thin bismuth films the amplification coefficient for the NENP model deviates from those for the EP, ENP and MNENP models in the low-temperature region and the gigahertz frequency region. From our present study concerning Rayleigh waves in thin bismuth films, it is shown that the NENP model did not explain very well the electronic transport property in the low-temperature region and the gigahertz frequency region.

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