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Electron–phonon scattering and anisotropy of conductivity in quasi-two-dimensional systems

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Abstract. The inverse relaxation time tensor in quasi-two-dimensional systems is calculated for elastic electron scattering by both acoustic and optical phonons. It is shown that in the general case the relaxation time is anisotropic. Also, on the basis of the Boltzmann equation in the anisotropic relaxation time approximation the electrical conductivity in these systems is calculated. It is found that anisotropy of the conductivity is defined not only by the anisotropy of effective mass and the relaxation time but also by the ratio of the Fermi level to the one-dimensional conduction band half-width. A comparison with available experimental data has been carried out. Qualitative agreement of theory with experiment was obtained.

1. Introduction

The extensive use of layered materials of the transition-metal dichalcogenide type in modern applications as well as the observation of new physical properties due to the specific crystalline structure have led to active investigation of these materials in recent years [1–3]. The transport phenomena in such compounds with a quasi-two-dimensional (Q2D) electron gas have not been sufficiently well studied. This is because of the severe problem of charge carrier scattering. Thus, in [4], galvanomagnetic phenomena in layered conductors were investigated, but anisotropy of scattering was not taken into account and the relaxation time was assumed to be independent of energy.

In this paper the inverse relaxation time tensor is obtained for elastic electron scattering by acoustic and optical phonons. It is shown that, when electrons are scattered by polar optical and piezoacoustic phonons, the relaxation time in Q2D systems is anisotropic whereas, when electrons are scattered by acoustic and non-polar optical phonons, it is isotropic. Also the electrical conductivity in Q2D systems is calculated in the absence of a magnetic field. The conductivity is anisotropic too; the ratio of the conductivity in the plane of the layers to the conductivity in the direction normal to the plane of the layers depends on the ratio of the corresponding inverse effective-mass tensor components. Anisotropy of the conductivity also depends on the scattering mechanism and on the degree of conduction band filling.

2. Density of states and concentration

We consider the conductor with the Q2D dispersion relation having the following form [1, 5]:

$$\varepsilon(k) = \varepsilon_{\perp}(k_{\perp}) + \varepsilon_z(k_z). \tag{1}$$

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Here $\varepsilon_\perp(k_\perp) = \hbar^2 k_\perp^2/2m_\perp$, $k_\perp^2 = k_x^2 + k_y^2$, $\varepsilon_z(k_z) = \varepsilon_0[1 - \cos(ak_z)]$, ε_0 is the one-dimensional conduction band half-width in the direction of k_z, $k(k_x, k_y, k_z)$ is the wavevector of conduction electrons and a is the lattice constant in the direction perpendicular to the plane of the layers. In Q2D systems the effective mass is anisotropic and may be represented in the diagonal tensor form with the components $m_x^{-1} = m_y^{-1} = m_\perp^{-1}$, corresponding to the motion in the plane of the layers and $m_z^{-1} = m_\parallel^{-1} = \hbar^{-2}\varepsilon_0 a^2 \cos(ak_z)$ corresponding to motion in the direction normal to the plane of the layers.

The density of energy states in this case is given by [5]

$$g(\varepsilon) = \frac{m_\perp}{\pi^2\hbar^2 a} z(\varepsilon). \tag{2}$$

$$z(\varepsilon) = \begin{cases} \pi & \\ \cos^{-1}\left(1 - \dfrac{\varepsilon}{\varepsilon_0}\right) & \text{for} \quad \begin{cases} \varepsilon > 2\varepsilon_0 \\ \varepsilon < 2\varepsilon_0. \end{cases} \end{cases} \tag{3}$$

The equation giving the relationship of the chemical potential μ to the concentration n is obtained in the form

$$n = \frac{m_\perp k_0 T}{\pi^2\hbar^2} \int_0^{\pi/a} \ln\left[1 + \exp\left(\frac{\mu - \varepsilon_0}{k_0 T}\right)\right] \mathrm{d}k_z. \tag{4}$$

The integration in (4) can be performed analytically for a strong degenerate electron gas and a non-degenerate electron gas. In the case of the strong degenerate electron gas, equation (4) gives

$$n = \frac{m_\perp \varepsilon_0}{\pi^2\hbar^2 a}(\sin z_0 - z_0 \cos z_0). \tag{5}$$

Here $z_0 = z(\mu)$ is given by (3) at $\varepsilon = \mu$.

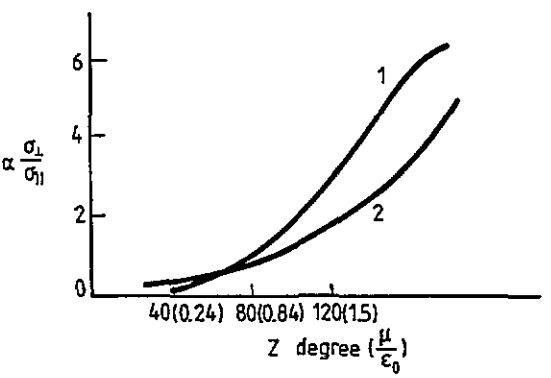

Figure 1. Dependence of the anisotropy of conductivity on z_0 and on the ratio μ/ε_0 for Q2D systems: curve 1, scattering by acoustic and non-polar optical phonons; curve 2, scattering by polar and piezoacoustic phonons; $\alpha = na^3\pi^2$.

In the case of the non-degenerate electron gas, equation (4) gives

$$n = \frac{m_\perp k_0 T}{\pi\hbar^2 a} \exp\left(\frac{\mu - \varepsilon_0}{k_0 T}\right) I\left(\frac{\varepsilon_0}{k_0 T}\right) \tag{6}$$

where

$$I\left(\frac{\varepsilon_0}{k_0 T}\right) = \int_0^{z_0} \exp\left(\frac{\varepsilon_0}{k_0 T} \cos z_0\right) \mathrm{d}z$$

is the Bessel integral at $z_0 = \pi$.

3. Relaxation time

In accordance with [6] the inverse relaxation time diagonal tensor components are

$$\frac{1}{\tau_i} = \sum_{k'} \left| 1 - \frac{k_i'}{k_i} \right| W_{kk'} \tag{7}$$

where $W_{kk'}$ is the probability of a transition from the k' state to the k state, $i = x, y, z$.

In the case when electrons are scattered by acoustic and non-polar optical phonons the probability of a transition is given by [7, 8]

$$W_{kk'} = C_0 \delta(\varepsilon_{k'} - \varepsilon_k). \tag{8}$$

Here $C_0 = (2\pi/\mathcal{M}\mathcal{N})(E_1^2/\hbar v_0^2)k_0 T$ for acoustic phonons, where E_1 is the deformation potential constant, $\mathcal{M}$ is the mass of an elementary cell, $\mathcal{N}$ is the number of elementary cells, and v_0 is the velocity of sound; $C_0 = (\pi E_0^2/\mathcal{N}_0 \mathcal{M}\omega_0)(\pi/a)^2$ for non-polar optical phonons, where E_0 is the optical deformation potential constant and $\mathcal{N}_0$ is the number of optical phonons with the maximum frequency ω_0 at the temperature T.

In the case when electrons are scattered by polar optical and piezoacoustic phonons the probability of a transition is [7, 9]

$$W_{kk'} = C_1 \frac{\delta(\varepsilon_{k'} - \varepsilon_k)}{|k - k'|^2}. \tag{9}$$

Here $C_1 = (8\pi^2 e^2/V\kappa^*)(k_0 T/\hbar)$ for polar optical phonons, where $\kappa^{*-1} = \kappa_\infty^{-1} - \kappa_0^{-1}$, κ_∞ and κ_0 are the high-frequency and static permittivity and V is the volume of the sample; $C_1 = 2\pi e^2 E_{pz}^2 k_0 T/\kappa^2 \mathcal{N}\mathcal{M} v_0^2 \hbar$ for piezoacoustic phonons, where E_{pz} is the piezoacoustic constant.

Equations (7)–(9) are satisfied in the approximation of an elastic process for electron–phonon interaction. The applicability of this approximation has been discussed in [7].

Inserting equations (8) and (9) into equation (7) and performing the integration over cylindrical coordinates $k_\perp'$, φ', k_z' convenient for this dispersion relation we obtain diagonal components of the relaxation time on the scattering by acoustic and non-polar optical phonons, given by

$$\frac{1}{\tau_x} = \frac{1}{\tau_y} = \frac{1}{\tau_z} = \frac{m_\perp C_0 V}{2\pi^2 \hbar^2 a} z \tag{10}$$

and on the scattering by polar optical and piezoacoustic phonons, given by

$$\begin{aligned} \frac{1}{\tau_x} = \frac{1}{\tau_y} = \frac{1}{\tau_\perp} &= \frac{m_\perp C_1 V}{8\pi^2 \hbar^2 k_\perp^2} \int_{-\pi/a}^{\pi/a} \left(1 - \frac{\mathcal{A}}{(\mathcal{A}^2 + \mathcal{B}^2)^{1/2}} \right) \theta(\varepsilon - \varepsilon_z') \, \mathrm{d}k_z' \\ \frac{1}{\tau_z} = \frac{1}{\tau_\parallel} &= \frac{m_\perp C_1 V a^2}{4\pi^2 \hbar^2 |k_z|} \int_{-\pi/a}^{\pi/a} \frac{|k_z' - k_z| \theta(\varepsilon - \varepsilon_z') \, \mathrm{d}k_z'}{(\mathcal{A}^2 + \mathcal{B}^2)^{1/2}} \end{aligned} \tag{11}$$

where $\mathcal{A} = 2\gamma[\cos(ak_z') - \cos(ak_z)] + a^2(k_z' - k_z)^2$, $\gamma = m_\perp/m_{z0}$, $m_{z0} = \hbar^2/\varepsilon_0 a^2$, $\mathcal{B} = 2ak_\perp(k_z' - k_z)$, $\theta(\varepsilon - \varepsilon_z') = 1$ for $\varepsilon - \varepsilon_z' > 0$, $\theta(\varepsilon - \varepsilon_z') = 0$ for $\varepsilon - \varepsilon_z' < 0$.

Analytical expressions for the relaxation time in the second case can be obtained with the approximation $|aq_z| = |a(k'_z - k_z)| \ll 1$:

$$\frac{1}{\tau_x} = \frac{1}{\tau_y} = \frac{1}{\tau_\perp} = \frac{m_\perp C_1 V}{4\pi^2\hbar^2 a k_\perp^2}\left(1 - \frac{1}{\{1 + a^2k_\perp^2/[\gamma^2\sin^2(ak_z)]\}^{1/2}}\right)z$$
$$\frac{1}{\tau_z} = \frac{1}{\tau_\parallel} = \frac{m_\perp C_1 V}{4\pi^2\hbar^2|k_z|[\gamma^2\sin^2(ak_z) + a^2k_\perp^2]^{1/2}}z. \tag{12}$$

The parameter $\gamma = m_z/m_{z0}$ may be assumed to be small in the sense that the motion normal to the layers plane is limited. Using this, equations (12) can be written as

$$\frac{1}{\tau_x} = \frac{1}{\tau_y} = \frac{1}{\tau_\perp} = \frac{m_\perp C_1 V}{4\pi^2\hbar^2 a k_\perp}z$$
$$\frac{1}{\tau_z} = \frac{1}{\tau_\parallel} = \frac{m_\perp C_1 V}{4\pi^2\hbar^2 a|k_z k_\perp|}z. \tag{13}$$

It should be noted that equations (11) and (13) for the relaxation time are obtained on account of the anisotropy of spectrum (1) only in the density of states.

Equations (11) and (13) can be represented in the general form

$$\frac{1}{\tau_\alpha} = \mathcal{A}_r\frac{g(\varepsilon)}{|k_\alpha k_\perp|^r} \tag{14}$$

where $r = 0$ corresponds to the acoustic and non-polar optical phonon scattering, $r = 1$ corresponds to the polar optical and piezoacoustic phonon scattering, $\alpha = \perp, z$ and $k_\alpha(k_\perp, k_z)$ denotes the longitudinal and the transverse components of wavevector. The values of $\mathcal{A}_r$ have been given in [7].

As seen from (14) the inverse relaxation time tensor components are proportional to the density of states. In the case when electrons are scattered by acoustic and non-polar optical phonons the energy dependence of the relaxation time is defined by the density of states $g(\varepsilon)$ and the relaxation time is isotropic, which corresponds to the result obtained in [10, 11]. In the other case when electrons are scattered by polar optical and piezoacoustic phonons, an additional dependence on wavevector components appears and the relaxation time becomes anisotropic.

4. Conductivity

Now, using the solution of the Boltzmann equation in the anisotropic relaxation time approximation for the components of the current density, one can obtain the following expression:

$$j_i = -en_0\left\langle \rho_i\frac{v_i^2}{\varepsilon_\perp}\right\rangle \tag{15}$$

where ρ_i are the components of the vector $\boldsymbol{\rho}(\varepsilon)$, which has the meaning of a generalized impulse force $\boldsymbol{\rho}(\varepsilon) = \hat{\tau}(\boldsymbol{k})\boldsymbol{\Phi}(\varepsilon)$ ($\boldsymbol{\Phi}(\varepsilon)$ is the generalized disturbing force causing a deviation from the equilibrium distribution and $\hat{\tau}(\boldsymbol{k})$ is the relaxation time tensor with the components defined by (7)), $-e$ is the charge on an electron, v_i is the electron velocity component,

$i = x, y, z$, and n_0 is given by $n_0 = m_\perp(\mu - \varepsilon_0)/\pi^2\hbar^2 a$. The angular brackets ($\langle\rangle$) have the following meaning:

$$\langle A\rangle = \frac{m_\perp}{2\pi^2\hbar^2 a n_0}\int_0^{z_0} dz \int_0^{2\pi} d\varphi \int_0^{\infty} \varepsilon_\perp \left(-\frac{\partial f_0}{\partial \varepsilon}\right) A\, d\varepsilon_\perp \tag{16}$$

where f_0 is the distribution function.

Using (15) for the diagonal tensor components of the electrical conductivity in the absence of magnetic field we have

$$\sigma_i = e^2 n_0 \left\langle \tau_i \frac{v_i^2}{\varepsilon_\perp}\right\rangle. \tag{17}$$

Inserting (14) into (16) for the conductivity components in the case of a degenerate electron gas after integration over $\varepsilon_\perp$ and φ, we obtain

$$\begin{aligned}\sigma_x &= \sigma_y = \sigma_\perp = \sigma_{0rx}\frac{k_0 T}{\mu - \varepsilon_0}\frac{\mathcal{T}_{0,0,r+1}}{z_0}\\ \sigma_z &= \sigma_\parallel = \sigma_{0rz}\delta\frac{\mathcal{T}_{r,2,r/2}}{z_0}.\end{aligned} \tag{18}$$

Here

$$\sigma_{0ri} = \frac{e^2 n_0 \tau_{0ri}}{m_i} \qquad \delta = \frac{\varepsilon_0}{\mu - \varepsilon_0}$$

$$\tau_{0rx} = \tau_{0ry} = \frac{\pi^2\hbar^2 a}{\mathcal{A}_r m_\perp}\left(\frac{2m_\perp k_0 T}{\hbar^2}\right)^r \qquad \tau_{0rz} = \frac{\pi^2\hbar^2}{\mathcal{A}_r m_\perp a^{r-1}}\left(\frac{2m_\perp k_0 T}{\hbar^2}\right)^{r/2}$$

$$\mathcal{T}_{k,l,m} = \int_0^{z_0} z^k \sin^l z \left[\mu^* - 2\varepsilon_0^* \sin^2\left(\frac{z_0}{2}\right)\right]^m dz \qquad \mu^* = \frac{\mu}{k_0 T} \qquad \varepsilon_0^* = \frac{\varepsilon_0}{k_0 T}.$$

One can obtain analytical expressions for the diagonal tensor components of the conductivity in the form

$$\begin{aligned}\sigma_x = \sigma_y = \sigma_\perp &= \sigma_{0rx}(\mu^* - \varepsilon_0^*)\left[1 + (r+1)\delta\frac{\sin z_0}{z_0} + r\frac{\delta^2}{2}\left(1 + \frac{\sin(2z_0)}{2z_0}\right)\right]\\ \sigma_z = \sigma_\parallel &= \sigma_{0rz}\frac{\delta}{2}\left(\frac{z_0}{2}\right)^r\left[\mu^* - 2\varepsilon_0^*\sin^2\left(\frac{z_0}{4}\right)\right]^{r/2}\left(1 - \frac{(r+1)\sin(2z_0)}{2z_0} + r\frac{\sin^2 z_0}{z_0^2}\right).\end{aligned} \tag{19}$$

On calculation of σ_z the integration in (18) can be performed approximately.

As seen from these expressions the ratio of the conductivity $\sigma_\perp$ along the layers to the conductivity $\sigma_\parallel$ across the layers depends on the ratio of the corresponding inverse effective masses $m_\perp^{-1}$ to m_{z0}^{-1}:

$$\frac{\sigma_\perp}{\sigma_\parallel} = C_r\left(\frac{m_{z0}}{m_\perp}\right)^{1-r/2} \tag{20}$$

where C_r is a coefficient depending on the scattering mechanism and on the degree of conduction band filling, i.e. the anisotropy of conductivity is defined not only by the

anisotropy of effective mass and the relaxation time but also by the ratio of the Fermi level to the one-dimensional conduction band half-width. When the Fermi level lies above the one-dimensional conduction band top for the ratio $\sigma_\perp/\sigma_\parallel (\mu > 2\varepsilon_0)$ we have

$$\frac{\sigma_\perp}{\sigma_\parallel} = \left(\frac{\mu}{\varepsilon_0}\right)^{1+r/2} \left(2\frac{m_{z0}}{m_\perp}\right)^{1-r/2}. \tag{21}$$

When the Fermi level lies within the one-dimensional conduction band ($\mu < 2\varepsilon_0$), the ratio $\sigma_\perp/\sigma_\parallel$ can be written

$$\frac{\sigma_\perp}{\sigma_\parallel} = 2\frac{m_{z0}}{m_\perp}\frac{\sin z_0 - z_0 \cos z_0}{z_0 - \cos z_0 \sin z_0} \tag{22}$$

$$\frac{\sigma_\perp}{\sigma_\parallel} = 2\left(\frac{m_{z0}}{m_\perp}\right)^{1/2} \frac{z_0 + 2z_0\cos^2 z_0 - 3\cos z_0 \sin z_0}{\sin(z_0/4)[1+2\cos(z_0/2)]^{1/2}[z_0^2 - z_0\sin(2z_0) + \sin^2 z_0]}. \tag{23}$$

Equations (20)–(23) allow us to define such important physical magnitudes as the parameter ε_0 of the energy spectrum, the effective-mass components $m_\perp$ and $m_\parallel$ and the parameter r of scattering in layered compounds from the measurements of conductivity anisotropy.

Using equations (5), (22) and (23) the ratio $\sigma_\perp/\sigma_\parallel$ can be represented as a function of z_0 only. Graphical representation of the dependence $(\sigma_\perp/\sigma_\parallel)(z_0)$ and the formula

$$\frac{m_{z0}}{m_\perp} = \frac{\tan z_0 - z_0}{\pi^2 n a^3}$$

will be informative for explicit determination of the effective-mass ratio.

The anisotropy of the effective mass in transition-metal dichalcogenides is large, e.g. $m_{z0}/m_\perp = 46$ for NbSe and $m_{z0}/m_\perp = 11$ for TaS_2 [12], which corresponds to our approximation. The anistropy of conductivity is also large: $\sigma_\perp/\sigma_\parallel = 20$ and $\sigma_\perp/\sigma_\parallel = 50$ for NbSe and TaS_2, respectively; $\sigma_\perp/\sigma_\parallel = 200$ for MoS_2 [13]. Using equation (21) for $m_{z0}/m_\perp = 10$ we obtain $\sigma_\perp/\sigma_\parallel \simeq 10^2$, which is in qualitative agreement with the above experimental data.

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