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Abstract

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ANISOTROPIC SCATTERING OF ELECTRONS BY IONIZED IMPURITIES

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The anisotropy of electron scattering by ionized impurities may be caused by anisotropy of the electron energy spectrum and by anisotropy of the scattering potential itself. The latter occurs in noncubic crystals, in which the dielectric constant is anisotropic. We shall consider the dielectric constant to be scalar. Generalization to the case of a tensor dielectric constant presents no fundamental difficulties.

The further assumptions are as follows:

1. The electron energy spectrum has the form

$$\varepsilon = \sum_{i=1}^{3} \frac{\hbar^2 k_i^2}{2m_i}, \qquad m_1 = m_2, \quad m_3 > m_1. \tag{1}$$

2. The electrons are in a weak electric field. There is no magnetic field.

The potential of an ionized impurity center has the form

$$V = \frac{e_0^2}{\chi r} e^{-r/a}, \tag{2}$$

where e_0 is the electron charge, χ is the dielectric constant of the crystal, and a is the screening radius.

In the Born approximation, for the matrix element of the transition we obtain

$$V_{\mathbf{k}\mathbf{k}'} = \frac{4\pi e_0^2}{\chi} \frac{1}{(\mathbf{k} - \mathbf{k}')^2 + 1/a^2}. \tag{3}$$

In what follows it will be convenient to use "deformed" coordinates,

$$\xi_i = \frac{\hbar}{\sqrt{2m_i \varepsilon}} k_i. \tag{4}$$

The direction of the vector $\vec{\xi}$ in a spherical coordinate system with the polar axis directed along the axis of rotation of the ellipsoid of constant energy will be characterized by the angles ϑ_0 and φ_0, and the direction of the vector $\mathbf{q} = \vec{\xi} - \vec{\xi}\,'$ by the angles ϑ and φ. Then for the probability $W_{\mathbf{k}\mathbf{k}'}$ of scattering of an electron by N ionized impurities, from (3) we obtain

$$W_{\mathbf{k}\mathbf{k}'} = \frac{N\pi^3 e_0^4 \hbar^3}{2\varepsilon^2 m_3^2 \chi^2 \left[\left(\cos^2\vartheta + \frac{m_1}{m_3}\sin^2\vartheta\right)\cos^2\theta + \gamma^2\right]^2}\,\delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}); \tag{5}$$

here $\pi - 2\theta$ is the scattering angle (the angle between $\vec{\xi}$ and $\vec{\xi}'$),

$$\gamma^2 = \hbar^2/8a^2 m_3 \varepsilon. \tag{6}$$

For $m_1 = m_3$, (5) becomes the well-known expression for the probability of isotropic scattering.

We calculated the quantity γ^2 for Ge and Si as a function of temperature and of the number of ionized impurities. The screening radius a was calculated from formula (1)

$$a^{-2} = \frac{16\pi^2 e_0^2 m^{*3/2}(2\pi kT)^{1/2}}{\chi h^3}\,F_{-1/2}(\mu^*). \tag{7}$$

In this formula, in the case of the multi-ellipsoid model, m^* should be understood as the density-of-states mass. The reduced chemical potential was calculated analytically from the formulas given in (^{2}), with the energy ε replaced by kT. It turned out that in the temperature range $5°\mathrm{K} \le T \le 100°\mathrm{K}$ and when N varies within $10^{14} \le N \le 10^{17}$, the quantity $\gamma^2 \le 10^{-2}$ and is mainly $> 10^{-6}$. Only for Si at $T < 10°\mathrm{K}$ does γ^2 become much smaller ($\lesssim 10^{-10}$). It is clear from (5) that for small γ^2 the role of the anisotropic term $\left(\cos^2\vartheta + \frac{m_1}{m_3}\sin^2\vartheta\right)\cos^2\theta$ is large, and, consequently, the anisotropy of the scattering may be large.

Let us write the kinetic equation in the form:

$$\hat{D}n_k^{(0)} + \sum_{k'} W_{kk'}(n'_{k'} - n'_k) = 0. \tag{8}$$

Here n'_k is the nonequilibrium addition to the distribution function; $n_k^{(0)}$ is the equilibrium distribution function; $\hat{D}n_k^{(0)}$ is the free term of the kinetic equation, having the form

$$\hat{D}n_k^{(0)} = -\frac{e_0}{\hbar}\frac{\partial n_k^{(0)}}{\partial\varepsilon}\sum_i \frac{\partial\varepsilon}{\partial k_i}E_i, \tag{9}$$

where **E** is the external electric field.

We expand n'_k in a series in spherical functions $Y_{lm}(\vartheta_0\varphi_0)$:

$$n'_k = \sum_{lm} X_{lm}(\varepsilon)\, Y_{lm}(\vartheta_0\varphi_0). \tag{10}$$

The solution of equation (8) can be reduced to the solution of two infinite systems of algebraic equations for X_{lm}:

$$\sum_{l} B_{kl}(m)\, X_{lm} = D_m \delta_{k1}; \tag{11}$$

$m = 0,\ 1,\ -1;$ k and l are odd; here

$$D_1 = -e_0\sqrt{\frac{4\pi\varepsilon}{3m_1}\frac{\partial n_k^{(0)}}{\partial\varepsilon}}\,(E_1 + iE_2), \tag{12}$$

$$D_{-1} = -D_1^*, \qquad D_0 = -e_0\sqrt{\frac{8\pi\varepsilon}{3m_3}\frac{\partial n_k^{(0)}}{\partial\varepsilon}}\,E_3.$$

The coefficients $B_{kl}(m)$ are determined by the scattering probability $W_{kk'}$ and depend, consequently, on the parameters γ^2 and m_1/m_3. They possess the following symmetry properties:

$$B_{kl}(m) = B_{lk}(m), \qquad B_{kl}(m) = B_{kl}(-m). \tag{13}$$

Since the nonequilibrium addition to the distribution function is needed in order to calculate fluxes whose components are proportional to first-order spherical functions, it is sufficient for us to determine X_{1m} from system (11). The calculation we carried out showed that the coefficients $B_{kl}(m)$ for not very large k and l increase as $|k-l|$ increases. Nevertheless, X_{1m} can be determined with good accuracy from only the first two equations of system (11), putting $X_{lm} = 0$ for $l > 2$. Introducing the notation

$$g_m = \frac{B_{13}^2(m)}{B_{11}(m)B_{33}(m) - B_{13}^2(m)}, \tag{14}$$

we now obtain for X_{1m}

$$X_{1m} = \frac{D_m}{B_{11}(m)}(1 + g_m). \tag{15}$$

Fig. 1

Figure 1: Fig. 1

Comparing the distribution function

$$\bar{n}'_k = \sum_m X_{1m} Y_{1m}(\vartheta_0 \varphi_0), \tag{16}$$

which in fact determines the fluxes calculated by us, with the known expression

$$n'_k = -\frac{\partial n_k^{(0)}}{\partial \varepsilon} e_0 \sum_{i=1}^{3} \tau_i v_i E_i, \tag{17}$$

we obtain for the components of the relaxation-time tensor τ_i

Fig. 1

$$\tau_3 \equiv \tau_{\parallel} = \frac{1}{B_{11}(0)}(1+g_0), \qquad \tau_1 = \tau_2 \equiv \tau_{\perp} = \frac{1}{B_{11}(1)}(1+g_1). \tag{18}$$

All coefficients $B_{kl}(m)$ entering into (18) can be computed exactly.

Figure 1 shows graphs of the quantities g_0 and g_1 as functions of γ^2 for Ge and Si at $\gamma^2 < 10^{-2}$. It is seen from the graphs that g_0 and g_1 depend very weakly on γ^2. They decrease slowly as γ^2 increases, i.e., as the anisotropy decreases. For $\gamma^2 < 10^{-3}$ for Ge and for any γ^2 for Si, g_m makes only a small correction to the expressions for τ_i.

Restricting ourselves, in calculating $B_{11}(m)$, to terms $\sim \gamma^2$ (then the formulas for $B_{11}(m)$ will be valid for $\gamma^2 < 10^{-2}$) and introducing the notation:

$$\beta^2 = \frac{m_3 - m_1}{m_1}, \tag{19}$$

we obtain

$$B_{11}(0) = \frac{3\pi N e_0^4 \sqrt{2m_3}}{8\chi^2 m_1 \varepsilon^{3/2} \beta^3} \Bigg\{ 2 \bigg(\operatorname{arc\,tg} \beta - \frac{\beta}{1+\beta^2} \bigg) \ln \frac{1}{\gamma^2} - 2 \operatorname{arc\,tg} \beta \ln(1+\beta^2) + 4L(\operatorname{arctg} \beta) + (1+\beta^2) \Bigg[\operatorname{arctg} \beta + \tag{20}$$

$$B_{11}(1) = \frac{4\pi N e_0^4 \sqrt{2m_3}}{8\chi^2 m_1 \varepsilon^{3/2} \beta^2} \Bigg[[(\beta^2 - 1) \operatorname{arc\,tg} \beta + \beta] \ln \frac{1}{\gamma^2} - 2\beta^2 \operatorname{arc\,tg} \beta - (\beta^2 - 1) \operatorname{arc\,tg} \beta \ln(1+\beta^2) + 2(\beta^2 - 1)L(\tag{21}$$

Here $L(t)$ is the Lobachevsky function, tabulated in (3).

The dependence of $\tau_\parallel$ and $\tau_\perp$ on energy is determined mainly by the factor $\varepsilon^{3/2}$ entering into $B_{11}(m)$. In addition, the dependence of the relaxation time on energy is also affected by the multiplier in the curly brackets in $B_{11}(m)$ and g_m. The latter factors somewhat weaken the dependence of τ_i on energy. Figure 2 shows the dependence of the ratio $\tau_\parallel/\tau_\perp$ on $\lg\gamma^{-2}$ for Ge and Si, and Fig. 3 shows the dependence of this ratio on $m_\parallel/m_\perp$ at various γ^2. For γ^2 so small that in expressions (20) and (21) for $B_{11}(m)$, and in analogous expressions for g_m, only the term with $\ln\gamma^{-2}$ may be retained, $\tau_\parallel/\tau_\perp = 11.4$ for Ge and 3.8 for Si. These values are very close to the values of $\tau_\parallel/\tau_\perp$ calculated by Herring[4]. If, however, in calculating $\tau_\parallel/\tau_\perp$ for the indicated γ^2 one discards g_m, then one obtains $\tau_\parallel/\tau_\perp = 12$ for Ge and 3.9 for Si, which agrees with Herring' s result. Herring carried out the calculation under the assumption that scattering occurs predominantly through small angles. This corresponds precisely to such small γ^2 that the term with $\lg\gamma^{-2}$ is the principal one in the expression for τ_i (the term corresponding to g_m, apparently, was not taken into account by Herring). From the data presented it is clear that Herring' s result is valid only for very small γ^2 ($\sim 10^{-14}$—10^{-16}), which are practically not realized in semiconductors.

Fig. 2
Fig. 2

Fig. 3
Fig. 3

In conclusion, let us note the following essential circumstance. From the fact that $B_{kl}(m)$ at small k and l increases with increasing $|k-l|$, it follows that even in the case when g in (15) may be neglected, the collision term in (8) cannot be expressed in the usual way through the components of the relaxation-time tensor (18). Therefore, when calculating various effects in a magnetic field, the kinetic equation should, generally speaking, again be reduced to a system of the type (13), and X_{1m} should be found from it.

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Note: Figure translations are in progress. See original paper for figures.