The influence of isoenergy surface anisotropy and surface scattering kinetics on the conductivity of a thin metal layer

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Abstract. A kinetic theory of the conductivity of a thin metal layer in a longitudinal alternative electric field is constructed. We assume the layer thickness is much greater than the electron de Broglie wavelength and less than the skin layer depth. Therefore, the skin effect is neglected and electron energy spectrum quantization is not considered. The Soffer model is used as the boundary conditions for the Boltzmann equation. We suppose the roughness parameters of the upper and lower layer surface have different values. The Fermi surface is an ellipsoid of revolution, the main axis of which lies in the layer plane. The dependences of conductivity tensor components on the layer thickness, electric field frequency, Fermi surface anisotropy parameter, and surface roughness parameters are analyzed. The results are compared with the ones performed within the framework of diffuse-mirror boundary conditions and with experimental data.

1. Introduction
In this paper, the kinetic method is used to solve the problem of the electrical conductivity of a thin metal layer placed in a longitudinal ac electric field. We assumed that the layer thickness is much greater than the de Broglie wavelength of charge carriers and much less than the skin depth. In this case, the skin effect is not taken into account and quantum size effects associated with electron energy spectrum quantization are not considered. Such problems are decided by the standard kinetic method. Note that at room temperature in many typical metals, the mean free path of charge carriers lies in the range 10 – 100 nm, and the de Broglie wavelength is of the order of an interatomic distance. Modern technologies permit to grow layers with a characteristic size approximately several nanometers. Therefore, the situation, when it is necessary to allow surface scattering of charge carriers and ignore quantum size effects, is realistic in practice.

The kinetic method was used for solving such problems as the high-frequency conductivity of a thin metal [1] and semiconductor [2] layer in the view of diffuse and diffuse-mirror boundary conditions, ac conductivity of a thin conductive wire located in a longitudinal magnetic field [3].

A range of common materials (silicon, germanium, bismuth, etc.) have the isoenergy surface as a system including several ellipsoids of revolution. In this paper, we suppose the case of an ellipsoidal isoenergy surface, which is a natural generalization of frequently used spherically symmetric band structure. We also plan to use Soffer model [4], which takes into account the dependence of a specularity coefficient on a surface roughness parameter and an incidence angle of charge carriers on the layer surface.
2. Solving method and mathematical calculations

Figure 1. (a) Thin metal layer placed in a longitudinal electrical field; (b) Fermi surface form of material.

Let’s consider a thin layer of metal or degenerate $n$- or $p$-type semiconductor with the thickness $a$. An ac electric voltage with the frequency $\omega$ is applied to layer ends. The time-periodic electric field changes according to the law:

$$ E = E_0 \exp(-i\omega t), $$

(1)
affects conduction electrons and causes a deviation $f_1$ of their distribution function $f$ from the equilibrium Fermi-Dirac function $f_0$:

$$ f(v, z) = f_0(\varepsilon) + f_1(v, z), $$

(2)
where $\varepsilon$ and $v$ are an electron kinetic energy and velocity accordingly.

The equilibrium distribution function has the step approximation form:

$$ f_0(\varepsilon) = \begin{cases} 1, & 0 < \varepsilon < \varepsilon_F; \\ 0, & \varepsilon > \varepsilon_F. \end{cases} $$

(3)
There $\varepsilon_F$ is Fermi energy.

The Fermi surface represents an ellipsoid of revolution, the main axis of which is parallel to the $v_x$ axis (see figure 1). In this case, the electron kinetic energy takes the form:

$$ \varepsilon = \frac{m_1}{2} (v_y^2 + v_z^2) + \frac{m_\parallel}{2} v_x^2, $$

(4)
where $m_\parallel$ and $m_\perp$ are a longitudinal and transverse effective mass respectively.

The function $f_1$ obeys the kinetic Boltzmann equation in the relaxation time approximation $\tau$ and the approximation linear in an external field:

$$ \nu f_1 + v_z \frac{\partial f_1}{\partial z} - e(v \cdot E) \frac{\partial f_0}{\partial \varepsilon} = 0. $$

(5)
There $\nu = \tau^{-1} - i\omega$ is the complex scattering frequency, $e$ is an elementary charge. We note that the relaxation time is supposed to be a scalar and depends only on electron energy.

We note the Soffer model [4] permits as boundary conditions for the equation (5) and takes into account the dependence of the specularity coefficients of a lower and upper layer surface $q_1$ and $q_2$ on the roughness parameters $g_1$ and $g_2$ on the layer surface:

$$ \begin{align*}
  &f_1(v_z, 0) = q_1(g_1, \vartheta)f_1(-v_z, 0); \\
  &f_1(-v_z, \alpha) = q_2(g_2, \vartheta)f_1(v_z, \alpha); \\
  &q_1(g_1, \vartheta) = \exp(-(4\pi g_1 \cos \vartheta)^2); \\
  &q_2(g_2, \vartheta) = \exp(-(4\pi g_2 \cos \vartheta)^2); 
\end{align*} $$

(6-8)
\[ g_1 = \frac{g_{s1}}{\lambda_F}; \quad g_2 = \frac{g_{s2}}{\lambda_F}. \]  

(9)

There \( g_{s1} \) and \( g_{s2} \) are respectively, the root-mean-square height of the surface relief for the lower and upper layer boundaries; \( \lambda_F \) is the electron de Broglie wavelength at the Fermi surface. If an each of the parameters \( q_1 \) and \( q_2 \) is a constant \((0 \leq q_1 \leq 1, 0 \leq q_2 \leq 1)\), the expression (6) describes the Fuchs diffuse-specular boundary condition model.

For the found nonequilibrium distribution function of conduction electrons, we can calculate the current with the density defined by the following expression

\[ j = -2e \left( \frac{m_0}{\hbar} \right)^3 \int v f_1 d^3 v, \]  

(10)

where \( h \) is Plank constant, \( m_0 = (m_\perp^2 m_\parallel)^{1/3} \).

Since the isoenergy surface is an ellipsoid of revolution, the layer integral conductivity represents as the 2nd rank tensor. If the main axis of this ellipsoid is parallel to the abscissa (figure 1), the conductivity tensor is diagonal:

\[ \sigma = \begin{pmatrix} \sigma_\parallel & 0 \\ 0 & \sigma_\perp \end{pmatrix}; \quad \sigma_\parallel = \int_0^a \frac{j_x}{E_x} dz; \quad \sigma_\perp = \int_0^a \frac{j_y}{E_y} dz. \]  

(11)

At the case of an arbitrary axis direction of the ellipsoid of revolution, the expression for the conductivity tensor is as follows:

\[ \sigma = \begin{pmatrix} \sigma_\parallel \cos^2 \chi + \sigma_\perp \sin^2 \chi & (\sigma_\parallel - \sigma_\perp) \cos \chi \sin \chi \\ (\sigma_\parallel - \sigma_\perp) \cos \chi \sin \chi & \sigma_\parallel \sin^2 \chi + \sigma_\perp \cos^2 \chi \end{pmatrix} \]  

(12)

where \( \chi \) is the angle between the main axis of the ellipsoid and the abscissa.

We note it is convenient for calculating the integral (10) to take advantage the following coordinate system \( v = (V, \theta, \phi) \) in the velocity space. The components of the Cartesian system are related to the above one by the following correlations:

\[ \begin{align*}
    v_x &= V \sqrt{m_0/m_\parallel} \sin \theta \cos \phi \\
    v_y &= V \sqrt{m_0/m_\perp} \sin \theta \sin \phi \\
    v_z &= V \sqrt{m_0/m_\perp} \cos \theta
\end{align*} \]  

(13)

After performing a series of mathematical calculations in the view of (13), we obtain the following expressions for the conductivity tensor components:

\[ \sigma_{0\parallel\perp} = \sigma_0 \Sigma_{0\parallel\perp}(x_0, y_0, k, g_1, g_2); \quad \sigma_{0\parallel\perp} = ne^2\tau/m_{\parallel\perp}; \]  

(14)

\[ \Sigma_{0\parallel\perp} = \frac{x_0}{z_0} \left(1 - \frac{3}{\pi} \int_0^{\pi/2} \Phi_{\perp\perp}(\phi) \sin^3 \theta \chi \left(\frac{z_0^\phi k}{\cos \theta}\right) d\theta d\phi\right); \]  

(15)

\[ \chi(p) = \frac{1}{p} \frac{(1 - \exp(-p))}{2 - q_1 - q_2 + (q_1 + q_2 - 2q_1q_2) \exp(-p)} \frac{1 - q_1q_2 \exp(-2p)}{1 - q_1q_2 \exp(-2p)}. \]  

(16)

\[ z_0 = \frac{av}{v_F} = \frac{a}{v_F \tau} - i \frac{a\omega}{v_F} = x_0 - iy_0; \quad \xi = \frac{z}{a}; \quad k = \frac{m_\parallel}{m_0}; \quad \Phi_{\perp}(\phi) = \cos^2 \phi; \quad \Phi_{\perp}(\phi) = \sin^2 \phi. \]  

(17)

There \( \Sigma_{\parallel} \) and \( \Sigma_{\perp} \) are dimensionless conductivity tensor components depending on dimensionless parameters: the layer thickness \( x_0 \), electrical field frequency \( y_0 \), ellipticity parameter \( k \), which characterizes isoenergy surface anisotropy and the roughness parameters of a lower and upper layer.
surfaces $g_1$ and $g_2$. The parameters $q_1$ and $q_2$ are defined by the expressions (7), (8), where $\cos \theta$ is expressed in the view:

$$\cos^2 \theta = \frac{\cos^2 \theta}{1 - (1 - k^3) \sin^2 \theta \cos^2 \varphi}.$$  \hfill (18)

3. Result analysis

Figure 2 shows the dependences of the non-dimensional longitudinal component of the integral conductivity tensor on the specularity coefficient and the roughness parameter of the upper surface for the different ellipticity parameters $k$. In this figure the results (dashed curves) are compared with calculations carried out within the framework of diffuse-mirror boundary conditions (solid curves). We see dashed curves 4 and 5 behave non-monotonically, in contrast to solid curves 1 and 2. At $g_2 = 0 - 0.2$ ($q_2 = 0.8 - 1$), the conductivity rapidly decreases with growing $g_2$ (with reducing $q_2$). At $g_2 > 0.4$ ($q_2 < 0.6$), the conductivity practically does not change. The results based on the Fuchs and Soffer models coincide each other at a purely specular scattering, as well as in the case of one specular and one diffuse surface (at $k < 1$). At the values $q_1 = q_2 = 1$ ($g_1 = g_2 = 0$) all curves converge to one point corresponding to the classical conductivity of a macroscopic sample ($\Sigma_{||} = 1$).

In figure 3 the dependences of the dimensionless longitudinal (solid curves) and transverse (dashed curves) components of the conductivity tensor on the ellipticity parameter $k$ are built. Surface roughness parameters are assumed to be the same ($g_1 = g_2 = g$). We observe at the value $k < 1$, the solid curves lie below the dashed ones, and at $k > 1$, it is the reciprocal situation: the solid curves lie above the dashed ones. This is due to the follow reason. At $k < 1$, the longitudinal electron effective mass $m_{||}$ is greater than the transverse one $m_{\perp}$, hence the longitudinal conductivity should be less than the transverse one. A different situation occurs at $k > 1$: $m_{||}$ is less than $m_{\perp}$ and the longitudinal conductivity is greater than the transverse one as a consequence. We see in figure 3 with growing the ellipticity parameter, the layer conductivity increases and tends to unity at large $k$ value. This is due to the fact that charge carriers have large transverse and small longitudinal effective masses, move mainly along the layer and don’t scatter practically at layer boundaries. Therefore, at $k \to \infty$, we obtain a classical result for the conductivity of a massive sample ($\Sigma_{||,\perp} \to 1$).

In figure 4 we construct the dependences of the module of the dimensionless longitudinal component of the conductivity tensor on the ellipticity parameter $k$ at the dimensionless electric field frequency $\gamma_0 = 3$. Oscillations are observed that decay with a growth of the ellipticity parameter. As the surface roughness parameters increase, the oscillations become less pronounced. For the case of different roughness parameters (curves 4 and 5 in figure 4), the oscillation period is less than for the case of the same ones.

In figures 5 and 6 we plot the dependences of the modulus and argument of the dimensionless longitudinal component of the conductivity tensor on the dimensionless electric field frequency $\gamma_0$ at the ellipticity parameter value $k = 4$. Solid curves are calculations in the view of the Fuchs model, and dashed curves are calculations within the Soffer model. We suppose the specular coefficients (roughness parameters) of layer surfaces are the same ($q_1 = q_2 = q$, $g_1 = g_2 = g$). With increasing frequency, the modulus of conductivity decreases, and the argument grows and tends to $\pi/2$. We see the slope of the dashed curves is greater than the one of the solid curves. The greatest difference between the calculations obtained within the framework of two boundary condition models is observed for diffuse scattering ($q = 0$, $g = 1$) and reaches 50% at $\gamma_0 = 0$.

In figure 7 we built the dependences of the resistivity of thin bismuth films grown on mica substrates on the thickness at the temperature 77 K. The solid curve is a theoretical calculation, points are experimental data of the work [5]. The electron Fermi surface in bismuth consists of three symmetrically located ellipsoids of revolution, the main axes of which are parallel to the film plane. The angle between the main axes is the same and equals 120°. Based on (12), the bismuth film conductivity can be determined as follows:
\[ \sigma = \sum_{i=1}^{3} \sigma_{i}^{Lx} = \sum_{i=1}^{3} \left\{ \sigma_{i} \cos^{2} \left( \chi + i \frac{2\pi}{3} \right) + \sigma_{\perp} \sin^{2} \left( \chi + i \frac{2\pi}{3} \right) \right\} = \frac{3}{2} (\sigma_{\parallel} + \sigma_{\perp}). \]  

(19)

where \( \sigma_{i}^{Lx} \) is the conductivity tensor component of the \( i \)-th ellipsoid.

We observe in figure 7 with decreasing film thickness, the resistance grows. The theoretical calculations agree with experimental data at the film thickness \( a < 80 \text{ nm} \). In the case when the film thicknesses less than 80 nm, the size dependence of the resistance is oscillating. The authors of [5] explain this behavior by the transition from the classical size effect to the quantum one. Indeed, the de Broglie wavelength of electrons in bismuth in the direction perpendicular to the film plane is 67 nm [5]. Therefore, at thicknesses comparable to or less than the above, it is necessary to use a mathematical apparatus that takes into account the charge carrier energy spectrum quantization. It will allow describing further the oscillating size dependences of the film resistance.

**Figure 2.** The dependences of the non-dimensional longitudinal conductivity tensor component on the specularity coefficient \( q_2 \) (roughness parameter \( g_2 \)) of an upper layer surface at \( x_0 = 0.1, y_0 = 0 \) and \( q_1 = 1 \) \( (g_1 = 0) \): 1, 4 \(- k = 0.1; 2, 5 - k = 1; 3, 6 - k = 4. \)

**Figure 3.** The dependences of the non-dimensional longitudinal and transverse conductivity tensor component on the ellipticity parameter \( k \) at \( x_0 = 0.1, y_0 = 0 \): 1, 4 \( g = 0.05 \); 2, 5 \(- g = 0.15 \); 3, 6 \(- g = 1. \)

**Figure 4.** The dependences of the non-dimensional longitudinal conductivity tensor component on the ellipticity parameter \( k \) at the value \( x_0 = 0.1, y_0 = 3 \): 1 \(- g_1 = g_2 = 0.05; 2 - g_1 = g_2 = 0.13; 3 - g_1 = g_2 = 1; 4 - g_1 = 0, g_2 = 0.13; 5 - g_1 = 0, g_2 = 1. \)

**Figure 5.** The dependences of the non-dimensional longitudinal conductivity tensor component module on the non-dimensional electric field frequency \( y_0 \) at the value \( x_0 = 0.1, k = 4 \): 1 \(- q = 0, g = 1; 2, 5 - q = g = 0.6; 3, 6 - q = 0.95, g = 0.05. \)
4. Conclusions

In the present paper, the dependences of the conductivity tensor components of a thin metal layer on the layer thickness, the electric field frequency, the Fermi surface ellipticity parameter, and the surface roughness parameters are analyzed. The conductivity dependences oscillations on the ellipticity parameter $k$ are discovered. These oscillations decay with increasing $k$ and the roughness parameters. In the case of different roughness parameters, the oscillation period is shorter than in the case of the same ones.

The results are compared with the calculations carried out in terms of the Fuchs boundary conditions. The results obtained taking into account the Fuchs and Soffer models coincide each other at specular and diffuse (at $k < 1$) surface scattering.

A comparative analysis of theoretical calculations with experimental data for bismuth film resistivity is carried out. The constructed theoretical model agrees with experiment at the film thickness $a \geq 80$ nm (i.e., is greater than the de Broglie wavelength of electrons in bismuth).

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