Calculation of the conductivity of a thin conductive layer taking into account Soffer boundary conditions and isoenergy surface anisotropy of conductor

O V Savenko, P A Kuznetsov and I A Kuznetsova

Microelectronics and General Physics Department, P G Demidov Yaroslavl State University, 14 Sovetskaya street, Yaroslavl 150003, Russia.

E-mail o.savenko@uniyar.ac.ru

Abstract. The task about the conductivity of a thin conductive layer in a longitudinal alternative electric field is solved. The relationship between layer thickness and charge carrier mean free path is arbitrary. The Soffer model is used as boundary conditions for Boltzmann equation. The isoenergy surface of a semiconductor is an ellipsoid of revolution. Analytical expressions are obtained for conductivity tensor components as functions of layer thickness, isoenergy surface anisotropy parameter, electric field frequency, surface roughness parameters, and chemical potential. The limiting cases of a degenerate and non-degenerate electron gas are considered. The dependences of conductivity tensor components on the above parameters are analyzed. The results obtained for cases of a degenerate and non-degenerate electron gas are compared. A comparative analysis of results is made with calculations in the view of diffuse-mirror boundary conditions and with known experimental data.

1. Introduction

The growing interest in the study of electrical and optical properties of thin conductive layers is due to the widespread use of thin-film structures in various fields of micro- and nanoelectronics, optoelectronics, microwave electronics, etc. Modern technologies make it possible to create nanomaterials with a characteristic size of the order of several nanometers. In this case, it is necessary for a theoretical description of the electrical characteristics of conductive layers, to take into account the surface charge carrier scattering. In fact, at room temperature the carrier mean free path lies in the range of 10 – 100 nm in many typical metals, and 10 – 1000 nm in typical semiconductors. If the layer thickness is much larger than the de Broglie wavelength of charge carriers, quantum effects associated with the discrete structure of charge carrier energy levels can be ignored. We note that the de Broglie wavelength takes a value proportional to 0.3 nm in metals (an interatomic distance) and 10 nm in semiconductors. In this case, it is sufficient to use the standard kinetic method as a mathematical apparatus, which consists in solving the Boltzmann kinetic equation with corresponding boundary conditions.

Most materials, such as silicon and germanium, have anisotropic properties. The isoenergy surface is a complex structure consisting of several rotation ellipsoids. Therefore, the electrical characteristics of thin conductive layers, taking into account the ellipsoidal energy zone, is an actual task. A systematic study of transport processes in thin layers is just beginning. In [1, 2], the problems of the conductivity of a thin inhomogeneous metal wire in the view of diffuse boundary conditions and the interaction of an electromagnetic radiation with a thin metal film in terms of diffuse-mirror boundary conditions were solved.
In present work, we decide the kinetic task about the conductivity of a thin conductive layer taking into account the Soffer model [3]. We assume the layer thickness is less than the skin layer depth. Therefore, the skin effect is not considered. The electric field is supposed to be uniform.

2. Solution method and mathematical calculations

We consider a thin conductive layer with a thickness \(a\) placed in a longitudinal alternative electric field with an intensity \(E\). The time-periodic electric field obeys to the law:

\[
E = E_0 \exp(-\imath \omega t),
\]

where \(\omega\) is an electric field frequency.

The isoenergy surface of a semiconductor is an ellipsoid of revolution, the main axis of which is parallel to \(v_x\) axis (figure 1(b)). Therefore the electron (hole) kinetic energy is as follow:

\[
\epsilon = \frac{1}{2} m \perp (v_y^2 + v_z^2) + \frac{1}{2} m \parallel v_x^2,
\]

where \(m\parallel\) and \(m\perp\) are respectively an electron (hole) longitudinal and transverse effective mass.

The electric field (1) acts to charge carriers and induces the distribution function deviation \(f_1\) from an equilibrium distribution function \(f_0\):

\[
f(v, z) = f_0(\epsilon) + f_1(v, z).
\]

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

\[
v f_1 + v_z \frac{\partial f_1}{\partial z} + e (v \cdot E) \frac{\partial f_0}{\partial \epsilon} = 0.
\]

There \(v = \tau^{-1} - i \omega\) is a complex scattering frequency, \(e\) is an electron (hole) charge. We note that, it is necessary for the strict kinetic description to take into account the anisotropy of charge carrier scattering. In this case, the relaxation time is a second-rank tensor. However, in many cases, the relaxation time can be considered a scalar that depends only on energy [4]. In this paper, we will be restricted to this approximation.

We use the Soffer model as a boundary condition to the equation (4). This model takes into account the dependence of mirror coefficients of lower \((q_1)\) and upper \((q_2)\) layer surfaces on roughness parameters \(g_1\) and \(g_2\) and the angle \(\vartheta\) between an electron (hole) velocity vector and layer surface normal:

\[
\begin{align*}
q_1(g_1, \vartheta) &= \exp(-(4\pi g_1 \cos \vartheta)^2); \\
q_2(g_2, \vartheta) &= \exp(-(4\pi g_2 \cos \vartheta)^2);
\end{align*}
\]

\[
g_1 = \frac{g_{s1}}{\lambda_F}; \quad g_2 = \frac{g_{s2}}{\lambda_F}.
\]

Figure 1. (a) Thin conductive layer in a longitudinal electric field; (b) Isoenergy surface form for a semiconductor.
There $g_{s1}$ and $g_{s2}$ are accordingly, the root-mean-square surface relief height for lower and upper layer boundary; $\lambda_F$ is the charge carrier de Broglie wavelength with Fermi level energy. In the case when each of coefficients $q_1$ and $q_2$ is a constant ($0 \leq q_1 \leq 1$, $0 \leq q_2 \leq 1$), the expression (5) describes the model of diffuse-mirror boundary conditions (Fuchs model).

The nonequilibrium distribution function of charge carriers allows us to calculate the current density:

$$j = 2e \left( \frac{m_0}{h} \right)^3 \int \nu f_\nu d^3 \nu,$$

(9)

where $h$ is the Plank constant, $m_0 = (m_1^2 m_2)$.

Since the constant energy surface is an ellipsoid of revolution, the layer integral conductivity represents a second-rank tensor:

$$\sigma = \begin{pmatrix} \sigma \parallel & 0 \\ 0 & \sigma \perp \end{pmatrix}; \quad \sigma \parallel = \int \frac{j_x}{E_x} dz; \quad \sigma \perp = \int \frac{j_y}{E_y} dz.$$

(10)

As the major and minor ellipsoid semi-axes are parallel to the coordinate axes $X$ and $Y$, the off-diagonal components of the conductivity tensor are equal to zero.

We note to calculate the integral, it is convenient to use the following coordinate system in the velocity space $v = (V, \theta, \phi)$. The components of the Cartesian system are related to the ones of the above system by the following relations:

$$\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} V \sqrt{m_0/m_\parallel} \sin \theta \cos \phi \\ V \sqrt{m_0/m_\perp} \sin \theta \sin \phi \\ V \sqrt{m_0/m_\perp} \cos \theta \end{pmatrix}.$$

(11)

After mathematical calculations series taking into account (11), we obtain the following expressions for conductivity tensor components:

$$\sigma \parallel \parallel = \sigma \parallel \perp \Sigma \parallel \perp \left( x_0, y_0, k, g_1, g_2, u_\mu \right);$$

$$\sigma \parallel \perp = ne^2 \tau / m \parallel \perp ;$$

$$\Sigma \parallel \perp = \frac{x_0}{z_0} \left( 1 - \frac{2}{\pi k} \int_0^{\pi/2} \int_0^{\pi/2} \frac{u^2 \Phi \parallel \perp (\phi) \exp((u - u_\mu))}{(\exp(u - u_\mu) + 1)^2} \sin^2 \theta \chi \left( \frac{z_0 \sqrt{k}}{\cos \theta} \frac{u_1}{u} \right) d \theta du d\phi \right) ;$$

$$\chi(p) = \frac{1}{p} \left( 1 - \exp(-p) \right) \frac{2 - q_1 - q_2 + (q_1 + q_2 - 2q_1q_2) \exp(-p)}{1 - q_1q_2 \exp(-2p)} ;$$

$$l_0 = \int_0^\infty \frac{\sqrt{u} du}{1 + \exp(u - u_\mu)} ; \quad u = \frac{m_0 V^2}{2k_0 T} ; \quad u_\mu = \frac{\mu}{k_0 T} ; \quad u_1 = \frac{m_0 v_1^2}{2k_0 T} ; \quad \xi = \frac{z}{a} ;$$

$$z_0 = \frac{a \nu_v}{v_1} = \frac{a - i \omega}{v_1} = x_0 - i y_0 ; \quad k = \frac{m_1}{m_0} ; \quad \Phi \parallel (\phi) = \cos^2 \phi ; \quad \Phi \perp (\phi) = \sin^2 \phi .$$

There $\Sigma \parallel$ and $\Sigma \perp$ are dimensionless conductivity tensor components depending on dimensionless parameters: layer thickness $x_0$, electric field frequency $y_0$, parameter $k$, which characterizes the isoenergy surface anisotropy (we call it the ellipticity parameter), roughness parameters $g_1$ and $g_2$, and chemical potential $u_\mu$. The parameters $q_1$ and $q_2$ are defined by the expressions (6), (7), where $\cos \theta$ is expressed as:

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

(16)

The parameters $x_0$, $y_0$, and $z_0$ normalized to the characteristic charge carrier velocity, which is determined similarly to the work [5].
3. Limited cases

Let’s consider the case of a degenerate electron gas corresponding to the condition $\mu/k_0T \gg 1$. The equilibrium distribution function takes the form of a step approximation:

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

(17)

There $\varepsilon_F$ is Fermi energy.

The expressions for dimensionless conductivity tensor components take the following form:

$$\Sigma_{\parallel,\perp} = \frac{x_0}{z_0} \left\{ 1 - \frac{3}{\pi} \int_0^{\pi/2} \int_0^{\pi/2} \Phi_{\parallel,\perp}(\varphi) \sin^3 \theta \chi \left( \frac{z_0 \sqrt{k}}{\cos \theta} \right) d\theta d\varphi \right\}.$$  

(18)

The case of a nondegenerate electron gas corresponds to the condition $\mu/k_0T \rightarrow -\infty$. The equilibrium distribution function takes the form of the classical Maxwell-Boltzmann distribution:

$$f_0(\varepsilon) = \exp \left( (\mu - \varepsilon)/k_0T \right) = A \exp \left( -\varepsilon/k_0T \right).$$

(19)

The expressions for dimensionless conductivity tensor components take the view:

$$\Sigma_{\parallel,\perp} = \frac{x_0}{z_0} \left\{ \frac{4}{\pi \sqrt{\pi}} \int_0^{\infty} \int_0^{\infty} u^{3/2} \exp(-u) \Phi_{\parallel,\perp}(\varphi) \sin^3 \theta \chi \left( \frac{z_0 \sqrt{k}}{\cos \theta} \right) \sin \gamma \left( \frac{u_1}{u} \right) du d\theta d\varphi \right\}.$$  

(20)

4. Result analysis

In figure 2 we show the dependences of the longitudinal component of the integral conductivity tensor on the specularity coefficient and the roughness parameter of an upper layer surface for various values of the ellipticity parameter $k$. In this figure we compare the results with the calculations in terms of diffuse-mirror boundary conditions. The calculations are made for the case of a nondegenerate electron gas. We see in contrast to the solid curves 1 and 2, corresponding to the ellipticity parameter value $k < 1$, the dashed curves 4 and 5 behave nonmonotonously. So, in the range $g_2 = 0 - 0.2$, the conductivity rapidly decreases with growing the roughness parameter. At the value $g_2 > 0.4$ the conductivity practically does not change. In the case of a purely specular reflection of charge carriers ($q_1, q_2 \rightarrow 1$ and $g_1, g_2 \rightarrow 0$), all the curves converge at one point. Therefore, the mirror surface does not affect the charge carrier distribution function and we observe a transition to the classical conductivity of a macroscopic sample ($\Sigma_{\parallel} \rightarrow 1$). In the case of one diffuse and another mirror surface and the ellipticity parameter value $k \leq 1$, the calculations obtained in the view of the Fuchs and Soffer models coincide.

Figure 3 shows the dependences of the dimensionless longitudinal component of the integral conductivity tensor on the surface roughness parameter $g$. Here and in the following figures, we assume the roughness parameters of upper and lower surfaces are the same ($g_1 = g_2 = g$). The solid curves are plotted for the case of a degenerate, and the dashed curves are plotted for the case of a non-degenerate electron gas. Figure 3 shows that the relative difference between solid and dashed curves increases with growing roughness parameter and reducing ellipticity parameter. The maximum relative difference between the solid and dashed curves is observed when the roughness parameter is equal to one and reaches 10%.

In figure 4 we built the dependences of the dimensionless longitudinal and transverse components of the conductivity tensor on the ellipticity parameter $k$. We see in this figure with growth of the parameter $k$ the dimensionless layer conductivity increases and tends to 1 at $k \rightarrow \infty$. This behavior can be explained as follow: for large values of the ellipticity parameter, the charge carriers have a small longitudinal effective mass and a large velocity component along the $X$ axis. The charge carriers practically do not scatter on the layer surface, we observe a transition to macroscopic conductivity ($\Sigma_{\parallel,\perp} \rightarrow 1$). Figure 4 shows that for $k < 1$ the solid curves lie below the dotted ones, and for $k > 1$ it is the opposite situation: the solid curves lie above the dotted ones.

In figures 5 and 6, the dependences of the dimensionless longitudinal component modulus and argument of the integral conductivity tensor on the dimensionless electric field frequency $\gamma_0$ are...
plotted. A reduction of the conductivity modulus with increasing \( y_0 \) is observed. This is due to the fact that the charge carrier system does not have time to respond to high-frequency oscillations of the electric field strength and behaves like a set of bound charges which does not contribute to the conductivity. The conductivity argument increases with growth of \( y_0 \). At the high-frequency limit, the conductivity becomes a purely imaginary quantity.

In figure 7 we built the dependence of the surface resistance logarithm of a thin \( p \)-silicon layer doped with phosphorus and located between the \( \text{SiO}_2 \) layers on the thickness. Points are experimental data from [6]. The solid curve is a theoretical calculation. Figure 7 shows that the theory agrees with experiment in the layer thickness range 100 – 150 nm. With a layer thickness of less than 50 nm, the experimental points lie above the theoretical curve. A possible reason for such discrepancy, as indicated in [6], is the influence of surface bound charges formed at \( \text{Si/SiO}_2 \) boundaries.

Figure 2. Dependences of the dimensionless longitudinal component of the integral conductivity tensor on the specularity coefficient \( q_2 \) (solid curves 1 – 3) and roughness parameter \( g_2 \) (dashed curves 4 – 6) of upper layer surface at \( x_0 = 0.1, y_0 = 0 \) and \( g_1 = 0 \) (\( q_1 = 1 \)): 1, \( 4 - k = 0.2 \); 2, \( 5 - k = 1 \); 3, \( 6 - k = 3 \). Dependencies are built for the case of a nondegenerate electron gas.

Figure 3. Dependences of the dimensionless longitudinal component of the integral conductivity tensor on the roughness parameter \( g \) at \( x_0 = 0.1, y_0 = 0 \); 1, \( 4 - k = 0.2 \); 2, \( 5 - k = 1 \); 3, \( 6 - k = 3 \). Dependencies are built for the case of a degenerate (solid curves 1 – 3) and nondegenerate (dashed curves 4 – 6) electron gas.

Figure 4. Dependences of the dimensionless longitudinal (solid curves 1 – 3) and transverse (dashed curves 4 – 6) component of the integral conductivity tensor on the isoenergy surface ellipticity parameter \( k \) at \( x_0 = 0.1, y_0 = 0 \): 1, \( 4 - g = 0.05 \); 2, \( 5 - g = 0.15 \); 3, \( 6 - g = 1 \). Dependencies are built for the case of a nondegenerate electron gas.

Figure 5. Dependences of the dimensionless longitudinal component modulus of the integral conductivity tensor on the dimensionless electric field frequency \( y_0 \) at \( x_0 = 0.1, k = 0.1 \): 1, \( 4 - g = 0.05 \); 2, \( 5 - g = 0.1 \); 3, \( 6 - g = 1 \). Dependencies are built for the case of a degenerate (solid curves 1 – 3) and nondegenerate (dashed curves 4 – 6) electron gas.
Figure 6. Dependences of the dimensionless longitudinal component argument of the integral conductivity tensor on the dimensionless electric field frequency $y_0$ at $x_0 = 0.1, k = 0.1$: 1, 4 – $g = 0.05$; 2, 5 – $g = 0.1$; 3, 6 – $g = 1$. Dependencies are built for the case of a degenerate (solid curves 1 – 3) and nondegenerate (dashed curves 4 – 6) electron gas.

Figure 7. Dependences of the surface resistance logarithm of a thin p-silicon layer on $a$. Points are the experimental data of the work [6]. Solid curves are the theoretical calculation at the values $y_0 = 0$, $k = g = 1$.

5. Conclusions
Analytical expressions are obtained for the integral conductivity of a thin conductive layer as a function of layer thickness, electric field frequency, surface roughness parameters, isoenergy surface ellipticity parameter and chemical potential. We observe a significant difference between the calculations obtained within the framework of Fuchs and Soffer boundary condition models. A comparative analysis of the results obtained for the limiting cases of a degenerate and non-degenerate electron gas is made. We show that the maximum relative difference between the dimensionless conductivity of metal and semiconductor layers is observed at diffuse scattering of charge carriers and reaches 10%. The results are compared with experimental data for the p-silicon layer. The agreement of theoretical calculations is observed at layer thicknesses greater than 100 nm. At thicknesses less than 50 nm, the experimental values of resistance are more than theoretical ones, which is associated with the influence of surface bound charges on layer conductivity.

References
[1] Kuznetsova I A, Romanov D N and Yushkanov A A 2019 Phys. Scr. 94 115805
[2] Kuznetsova I A, Romanov D N and Yushkanov A A 2019 Opt. Spectrosc. 127 328
[3] Soffer S B 1967 J. Appl. Phys. 38 1710
[4] Anselm A I 2006 Introduction to Semiconductor Theory (NJ: Prentice-Hall).
[5] Yushkanov A A, Savenko O V, Kuznetsova I A 2020 Phys. Scr. 95 045805
[6] Zhang P, Nordberg E P, Park B N, Celler G K, Knezevic I, Evans P G, Eriksson M A and Lagally M G 2006 New Journal of Physics 8 200