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Interaction of an electromagnetic H-wave with an „insulator-semiconductor-insulator“ nanostructure in the view of semiconductor band structure anisotropy

© I.A. Kuznetsova, O.V. Savenko

Demidov State University,
150003 Yaroslavl, Russia

e-mail: savenko.oleg92@mail.ru

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The problem of electromagnetic H-wave interaction with a layered „insulator–semiconductor–insulator“nanostructure is solved. We assume that the semiconductor layer thickness can be comparable to or less than the charge carrier de Broglie wavelength. Charge carrier surface scattering is taken into account by the Soffer boundary conditions. The electromagnetic wave frequency is less than the plasma resonance frequency. The constant energy surface is an ellipsoid of revolution. Analytical expressions are obtained for the reflection, transmission and absorption coefficients. Calculations are performed for the limiting cases of a degenerate and nondegenerate electron gas. We analyze the dependences of the optical coefficients on dimensionless parameters: the semiconductor layer thickness, the electromagnetic wave frequency and incidence angle, the chemical potential, the ellipticity parameter, the insulating layer permittivities, and the „semiconductor-insulator“interface roughness parameters.

Keywords: layer nanostructure, Liouville equation, de Broglie wavelength, Soffer model, optical coefficients.

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Introduction

For the time being, the basis of all semiconductor nanoelectronics is layered nanostructures consisting of semiconductor, metal and dielectric layers. The use of nanocoatings in solar energy is of particular interest to researchers. Developments are being implemented to increase the ability of solar cells to effectively convert electromagnetic radiation into electrical energy [1–4]. As studies have shown, flexible solar cells based on GaAs [2] have the highest efficiency (approximately 35%). Studies are being carried out to increase the energy efficiency of solar cells by growing filamentary nanostructures with antireflective properties on the surface of a nanolayer [3]. An urgent task is to improve the physical parameters of optical devices by applying semiconductor nanocoatings [5].

For the time being, technological methods are being actively improved that allow to grow nanostructures, the thickness of the layers of which can be several atomic layers. In this case, for a theoretical description of transport phenomena in nanolayers, it is required to take into account the quantization of the energy spectrum of charge carriers. There is a number of theoretical papers in the literature in which, to calculate the electrical and optical parameters of nanolayers, a model of an electron gas enclosed in a quantum well with smooth walls was reviewed [6–8]. At small thicknesses, surface roughness at the atomic level significantly affects the phenomena of charge carrier transport in a nanolayer, so there is a need to generalize the models used in the papers [6–8] to the case of an uneven surface.

The issue of taking into account surface scattering to solve quantum problems on the static conductivity of a thin metal film was considered in the papers [9–13]. In the papers [9–11] the Green's function method was used, according to which the surface carrier scattering was reviewed as a perturbation potential. The task of finding wave functions in a quantum well was reduced to determining the Green's function by solving the Dyson equation. In the papers [12,13] the direct calculation of the surface collision integral was carried out. In the papers [14–16] the Soffer boundary conditions method [17] was used to calculate the electrical and galvanomagnetic parameters of a conducting nanolayer. The same method was used to construct theoretical models of the interaction of electromagnetic radiation with a semiconductor nanolayer [18] and with a layered nanostructure „dielectric-semiconductor-dielectric“ [19]. Let us note that in the papers [18,19] the case of a semiconductor with a spherical band structure was reviewed.

Nanolayers of silicon and germanium are widely used in nanoelectronics and solar energy. The constant energy surface in such semiconductors has a non-spherical shape and consists of several spheroids. In this paper, we summarize the theoretical model constructed in the paper [19] to the case of an ellipsoidal shape of the semiconductor constant energy surface.

Problem formulation

Let us review a nanostructure, which is a semiconductor nanolayer of thickness a, placed between two insulating layers with different dielectric constants. A plane monochromatic electromagnetic wave is incident on a layered nanostructure. Let us introduce the coordinate system so that the coordinate axes X and Y are directed in parallel to the plane of the nanolayer, so is the axis Z — nanolayer inward. The case of the H-configuration of an electromagnetic wave is considered, i.e. the electric field strength vector is parallel to the X axis. The dielectric layers are non-magnetic, and the top insulating layer is non-absorbing.

The semiconductor nanolayer thickness can be comparable or less than the de Broglie wavelength of the charge carrier. In this case, the energy spectrum of charge carriers in the direction perpendicular to the plane of the nanostructure is quantized. It is assumed that the constant energy surface is an spheroid with the main axis parallel to the plane of the nanolayer. There is a review of the cases when the axis of rotation is parallel and perpendicular to the electric field strength vector (let's call them the longitudinal and transverse directions of the axis, respectively, to the electric field). The expression for the total energy of an electron (hole) has the form

$$\varepsilon_l = \frac{m_{\parallel,\perp}}{2} v_x^2 + \frac{m_{\perp,\parallel}}{2} v_y^2 + \varepsilon_{zl}, \tag{1}$$

where $\varepsilon_{zl} = (\pi\hbar l)^2/(2m_\perp a^2)$ — the eigenvalue of the charge carrier energy in the lth sub-band, $m_\parallel$ and $m_\perp$ — the longitudinal and transverse effective masses of the electron (hole), respectively, the first index at m in expression (1) corresponds to the longitudinal direction of the main axis of the ellipsoid, and the second index — transverse direction, $\hbar$ — Planck's constant.

The present paper suggests a small deviation of the system of the charge carriers from the equilibrium state. In this case, the Liouville equation can be reduced to the following form [15]:

$$-i\omega f_l + v_{zl}\frac{\partial f_l}{\partial z} + \frac{e\mathbf{E}}{\hbar}\frac{\partial f_l}{\partial \mathbf{k}_\parallel} = -\frac{f_l - f_l^{(0)}}{\tau}, \tag{2}$$

where τ — relaxation time, ω — electromagnetic wave frequency, f_l — charge carrier distribution function on the ith sub-band, playing the role of a diagonal element of the density matrix ρ_{ll}, $f_l^{(0)}$ — equilibrium distribution function, $\hbar$ — Planck's constant, $\mathbf{E}$ — electric field strength, v_{zl} — z - component of the charge carrier velocity in the l- th sub-band, e — electron (hole) charge.

The function f_l has the following expansion [15]

$$f_l(z, \mathbf{k}_\parallel, t) = f_l^{(0)} + f_l^{(1)}(z, \mathbf{k}_\parallel)\exp(-i\omega t), \tag{3}$$

$$f_l^{(0)} = \frac{1}{1 + \exp((\varepsilon_l - \mu)/k_0 T)}, \tag{4}$$

where $f_l^{(1)}$ — non-equilibrium correction, μ — chemical potential, k_0 — Boltzmann constant, T — temperature.

Let us note that in the case of an ellipsoidal band structure of a semiconductor, the relaxation time is a second-rank tensor [14,15,20]:

$$\tau = \begin{pmatrix} \tau_{\parallel,\perp} & 0 & 0 \\ 0 & \tau_{\perp,\parallel} & 0 \\ 0 & 0 & \tau_\perp \end{pmatrix}. \tag{5}$$

Here the first index corresponds to the longitudinal orientation of the main rotation axis of the ellipsoid of constant energy, and the second index corresponds to the transverse orientation. Parameter $\tau_\parallel$ represents the characteristic time for establishing an equilibrium state of a system of charge carriers under the action of an external force directed parallel to the main axis of the spheroid, respectively, and $\tau_\perp$ — perpendicular to the main axis. To find the correction to the distribution function in the case of a longitudinal orientation of the rotation axis of a constant energy ellipsoid, it is required to substitute the parameter $\tau_\parallel$ into equation (2), and in the case of a transverse orientation — $\tau_\perp$.

The boundary conditions are described by the Soffer model [17], which takes into account the dependence of the reflection coefficients of the surfaces of the $q_{1,2}$ nanolayer on the $g_{1,2}$ roughness parameters and the charge carrier incidence to the internal surface of the ϑ nanolayer:

$$\begin{cases} f_l^{(1)+} = q_1(g_1, \vartheta) f_l^{(1)-} & \text{if } z = 0, \\ f_l^{(1)-} = q_2(g_2, \vartheta) f_l^{(1)+} & \text{if } z = a, \end{cases} \tag{6}$$

$$q_{1,2}(g_{1,2}, \vartheta) = \exp\left(-(4\pi g_{1,2}\cos\vartheta)^2\right), \tag{7}$$

$$g_{1,2} = \frac{g_{s1,2}}{\lambda_B}, \tag{8}$$

where $f_l^{(1)\pm}$ — the functions of the distribution of the electrons (holes) with a positive and negative projection of the wave vector on the axis Z, $g_{s1,2}$ — the mean square height of the surface relief of the lower and upper surface, respectively, λ_B — the de Broglie wavelength of the charge carrier.

The current density and integral conductivity in the case of longitudinal and transverse orientations of the rotation axis of a constant energy ellipsoid are determined by the expressions [14,15]

$$j_{\parallel,\perp} = \frac{2ek_{z1}}{(2\pi)^3}\sum_l \iint v_x\left(f_{l\parallel,\perp}^{(1)+} + f_{l\parallel,\perp}^{(1)-}\right)dk_x dk_y, \tag{9}$$

$$\sigma_{a_{\parallel,\perp}} = \int_0^a \frac{j_{\parallel,\perp}}{E_x}\,dz, \tag{10}$$

where k_{z1} — z- component of the wave vector of the charge carrier located in the first sub-band, $f_{l\parallel}^{(1)\pm}$ and $f_{l\perp}^{(1)\pm}$ — respectively, non-equilibrium corrections to the distribution functions of charge carriers in the case of longitudinal and

transverse directions of the main axis of a constant energy ellipsoid.

The present study suggests that the range of the electromagnetic-radiation frequencies is limited from above the frequency of the plasma resonance. The electromagnetic wave is weak, so the effects related with the quantum nature of the electromagnetic radiation are not taken into account. The behavior of an electromagnetic wave can be described by Maxwell's equations, which can be used to determine optical coefficients:

$$\begin{cases} \frac{\partial E_x}{\partial z} = ikH_y, \\ \frac{\partial H_y}{\partial z} - ik(1-\sin^2\theta)E_x = -\frac{4\pi}{c}\, j. \end{cases} \tag{11}$$

Here k — the module of the wave vector, θ — the incidence of the electromagnetic wave, c — the speed of light in vacuum.

Mathematical calculations

The task is solved by the method similar to the given studies in the paper [15]. Solving equation (2) taking into account the boundary conditions (6), substituting the expression for the distribution function in (9) and (10), we obtain the following expression for the integral conductivity:

$$\sigma_{a\parallel,\perp} = \frac{8\pi e^2 a k_0 T v_{z1}}{\nu_{\parallel,\perp} m_{\parallel,\perp}\sqrt{m_\parallel m_\perp}}\left(\frac{m_0}{h}\right)^3 \times \sum_{l=1}^{\infty} \ln\left(\exp\left(\frac{\mu-\varepsilon_{zl}}{k_0T}\right)+1\right)\left(1-\chi(\Omega_{\parallel,\perp})\right), \tag{12}$$

$$\chi(p) = \frac{1}{2p}(1-e^{-p})\frac{2-q_1-q_2+(q_1+q_2-2q_1q_2)e^{-p}}{1-q_1q_2e^{-2p}}, \tag{13}$$

$$m_0 = \sqrt[3]{m_\parallel m_\perp^2},\ \ \Omega_{\parallel\perp} = \frac{a\nu_{\parallel,\perp}}{v_{zl}}. \tag{14}$$

Here the designation $\nu_{\parallel,\perp} = \tau_{\parallel,\perp}^{-1} - i\omega$ — complex scattering frequencies of the charge carrier moving in directions parallel and perpendicular to the main axis of the constant energy ellipsoid, respectively, v_{z1} — z - component of the charge carrier velocity in the first sub-band is introduced.

The relationship between the reflectance R, transmittance T, absorption A and integral conductivity σ_a (12) will be obtained using the results of the paper [21]:

$$R = \left|\frac{\sqrt{\varepsilon-\sin^2\theta}(\bar{p}+p_1p_2)+\cos\theta(\bar{p}-p_1p_2)}{\sqrt{\varepsilon-\sin^2\theta}(1+\bar{p})+\cos\theta(1-\bar{p})}\right|^2, \tag{15}$$

$$T = \cos\theta \mathrm{Re}\left(\sqrt{\varepsilon-\sin^2\theta}\right) \times \left|\frac{p_2-p_1}{\sqrt{\varepsilon-\sin^2\theta}(1+\bar{p})+\cos\theta(1-\bar{p})}\right|^2, \tag{16}$$

$$A = 1-R-T, \tag{17}$$

$$\bar{p} = \frac{p_1+p_2}{2},\ \ \varepsilon = \frac{\varepsilon_2}{\varepsilon_1},\ \ p_1 = -1,\ \ p_2 = \frac{\sqrt{\varepsilon_1}\cos\theta - B}{\sqrt{\varepsilon_1}\cos\theta + B}, \tag{18}$$

$$B = \frac{2\pi\sigma_a}{c\cos\theta}, \tag{19}$$

where ε_1 and ε_2 — dielectric constants of the upper and lower insulating layers.

Let us note that in the paper [21] the case of mirror boundary conditions and a spherical constant energy surface was reviewed.

Expressions (15)–(19) can be used when reviewing the ellipsoidal band structure if the electric field strength vector is oriented parallel or perpendicular to the rotation axis of the ellipsoid. In this situation, the current density vector will be parallel to the electric field strength. In case of a longitudinal direction of the main axis of a constant energy ellipsoid, it is necessary to substitute $\sigma_{a\parallel}$ into formula (19), and in case of a transverse orientation — $\sigma_{a\perp}$.

Putting the expression for $\sigma_{a\parallel,\perp}$ into the function B (20), we get

$$B_{\parallel,\perp} = \frac{16\pi^2 e^2 a k_0 T v_1}{c\cos\theta v_{\parallel,\perp} m_{\parallel,\perp}\sqrt{m_\parallel m_\perp}}\left(\frac{m_0}{h}\right)^3 \times \sum_{l=1}^{\infty} \ln\left(\exp\left(\frac{\mu-\varepsilon_{zl}}{k_0T}\right)+1\right)\left(1-\chi(\Omega_{\parallel,\perp})\right), \tag{20}$$

where $B_\parallel$ corresponds to the longitudinal direction of the main axis of the ellipsoid, and $B_\perp$ — transverse one.

To analyze the obtained expressions, it is required to introduce dimensionless parameters

$$u_{zl} = \frac{\varepsilon_{zl}}{k_0T},\ \ u_\mu = \frac{\mu}{k_0T}, \tag{21}$$

$$x_0 = \frac{a}{\lambda_{B\perp}},\ \ x_\lambda = \frac{\Lambda}{\lambda_{B\perp}},\ \ y_0 = \omega\tau_{0\nu}, \tag{22}$$

$$z_{0\parallel,\perp} = \nu_{\parallel,\perp}\tau_{0\nu} = \frac{\tau_{0\nu}}{\tau_{\parallel,\perp}} - i\omega\tau_{0\nu} = \kappa_{\parallel,\perp} - iy_0, \tag{23}$$

$$\rho = \frac{v_{0\nu}}{c},\ \ y_p = \omega_p\tau_{0\nu},\ \ \gamma = \frac{m_\perp}{m_0}, \tag{24}$$

where Λ — free path of charge carriers taking into account volume scattering, $\tau_{0\nu}$ — scalar relaxation time in a macroscopic sample, determined through the longitudinal and transverse components of the relaxation tensor τ_ν as follows:

$$\tau_{0\nu} = \sqrt[3]{\tau_{\nu\parallel}\tau_{\nu\perp}^2}. \tag{25}$$

Parameters u_{zl} and u_μ —characterize, respectively, the discrete component of the total energy of the charge carrier and the chemical potential, normalized to k_0T; y_0 and y_p — respectively, the product of the frequency of the electromagnetic wave and the plasma frequency ω by the parameter $\tau_{0\nu}$. Parameters x_0 and x_λ represent the thickness of the nanolayer and the free path of charge carriers, normalized to the de Broglie wavelength of the charge carrier $\lambda_{B\perp}$ in the direction perpendicular to the plane of

the nanostructure;ρ — the ratio of the characteristic speed of the charge carrier $v_{0\nu}$ to the speed of light (characteristic speeds will be discussed below).

The parameter $z_{0\|,\perp}$includes the ratio of the scalar relaxation time in a macroscopic sample to the longitudinal (transverse) component of the relaxation time tensor. Let us find the connection between the longitudinal (transverse) components of the relaxation tensor τ and the scalar relaxation time τ_0, defined similarly to (25). From the expression for the total energy of the charge carrier (1) it follows that the ratio between the major and minor semi-axis of the spheroid in velocity space is equal to $\sqrt{m_\perp/m_\|}$ In this paper, it is assumed that the parameter Λ is determined by scattering on impurities and crystal lattice defects and does not depend on the thickness of the semiconductor nanolayer. The average charge carrier velocity is inversely proportional to the relaxation time. The ratio between the longitudinal and transverse components of the relaxation tensor will be equal to $\sqrt{m_\|/m_\perp}$. From what has been said

$$\tau_0\sqrt[3]{\tau_\|\tau_\perp^2} = \sqrt[6]{\frac{m_\|}{m_\perp}}\,\tau_\perp = \sqrt{\frac{m_0}{m_\perp}}\,\tau_\perp, \tag{26}$$

$$\tau_0 = \sqrt[3]{\frac{m_\perp}{m_\|}}\,\tau_\| = \sqrt{\frac{m_0}{m_\|}}\,\tau_\|, \tag{27}$$

$$\kappa_{\|,\perp} = \frac{\tau_{0\nu}}{\tau_{\|,\perp}} = \sqrt{\frac{m_0}{m_{\|,\perp}}}\,\frac{\tau_{0\nu}}{\tau_0} = \sqrt{\frac{m_0}{m_{\|,\perp}}}\,\frac{v_0}{v_{0\nu}}, \tag{28}$$

v_0 and $v_{0\nu}$ — respectively, characteristic velocities of charge carriers with and without taking into account the quantization of the energy spectrum of charge carriers, which are introduced as follows:

$$mv_0^2 = 4\Big(\frac{m_0}{h}\Big)^3 v_{z1}\,\frac{5}{3}\sum_{l=1}^{\infty}\iint V_l^2 f_l^{(0)} dv_x dv_y, \tag{29}$$

$$n_0 v_{0v}^2 = 2\Big(\frac{m_0}{h}\Big)^3 v_{z1}\,\frac{5}{3}\sum_{l=1}^{\infty}\iiint V^2 f_0 d^3v, \tag{30}$$

$$V_l^2 = \frac{(m_\| v_x^2 + m_\perp v_y^2 + m_\perp v_{zl}^2)}{m_0}, \tag{31}$$

$$V^2 = (m_\| v_x^2 + m_\perp v_y^2 + m_\perp v_z^2)/m_0. \tag{32}$$

Here n and n_v — respectively, the concentration of charge carriers with and without taking into account the quantization of the energy spectrum of charge carriers, determined in the papers [14,15].

Integrating expressions (29), (30), we obtain

$$v_{0\nu} = \left(\frac{10}{3}\,\frac{k_0T}{m}\,\frac{I_{3/2}}{I_{1/2}}\right)^{1/2}, \tag{33}$$

$$v_0 = \left(\frac{10}{3}\,\frac{k_0T}{m}\,\frac{K}{P}\right)^{1/2}, \tag{34}$$

$$I_s = \int_0^{\infty}\frac{u^s du}{\exp(u-u_\mu)+1}, \tag{35}$$

$$K = \sum_{l=1}^{\infty}\int_{u_{zl}}^{\infty}\frac{udu}{\exp(u-u_\mu)+1}, \tag{36}$$

$$P = \sum_{l=1}^{\infty}\ln\big(\exp(u_\mu - u_{zl})+1\big). \tag{37}$$

In case of a degenerate electron gas, v_0, $v_{0\nu}$ transform into the effective Fermi velocity $V_F = \sqrt{2\varepsilon_F/m_0}$, and in the case of a non-degenerate Fermi gas they are of the order of the average thermal velocity of charge carriers [14,15].

Taking into account the above-mentioned dimensionless parameters, the expressions for the functions $B_\|$ and $B_\perp$ take the form

$$B_{\|,\perp} = \frac{\rho y_p^2\sqrt{u_{0\nu}}}{4\cos\theta x_0 I_{1/2} z_{0\|,\perp}\Phi_{\|,\perp}(\gamma)} \times\sum_{l=1}^{\infty}\ln\big(\exp(u_\mu-u_{zl})+1\big)\left(1-\chi\left(\frac{2x_0^2 z_{0\|,\perp}\sqrt{\gamma}}{lx_\lambda\Phi_{\|,\perp}(\gamma)}\right)\right). \tag{38}$$

The following notations are introduced here

$$\Phi_\perp(\gamma) = \sqrt{\gamma},\quad \Phi_\|(\gamma) = \frac{1}{\gamma},\quad \frac{m_0 v_{0\nu}^2}{2k_0T}, \tag{39}$$

Limit cases

Let us review the case of a spherical band structure ($\gamma = 1$). In this situation, the results obtained taking into account the longitudinal and transverse orientations of the main axis of the constant energy ellipsoid coincide with each other. Setting $\gamma = 1$ in (38), we obtain

$$B_\| = B_\perp = \frac{\rho y_p^2\sqrt{u_{0\nu}}}{4\cos\theta x_0 I_{1/2} z_0}\sum_{l=1}^{\infty}\ln\big(\exp(u_\mu-u_{zl})+1\big) \times\left(1-\chi\left(\frac{2x_0^2 z_0}{lx_\lambda}\right)\right). \tag{40}$$

The obtained result coincides with the results of the paper [19].

Let us consider the case of a degenerate electron gas ($u_\mu \gg 1$), corresponding to high concentration, low effective mass of charge carriers and low temperature. The equilibrium function of distribution takes the form of the stepped approximation:

$$f_l^{(0)}(\varepsilon_l) = \begin{cases}1, & 0<\varepsilon_l<\varepsilon_F,\\ 0, & \varepsilon_l>\varepsilon_F,\end{cases} \tag{41}$$

where ε_F — Fermi energy.

The reflectances, the coefficients of transmission, absorption will be determined by the expressions (15)– (17), in

which the functions $B_{\parallel}$ and $B_{\perp}$ have the following form:

$$B_{\parallel,\perp} = \frac{3\rho y_p^2}{8x_\lambda z_{0\parallel,\perp}\cos\theta\Phi^2_{\parallel,\perp}(\gamma)} \times \sum_{l=1}^{N}\left(1-\frac{l^2}{4x_0^2}\right)\left(1-\chi\left(\frac{2x_0^2 z_{0\parallel,\perp}\sqrt{\gamma}}{x_\lambda l}\right)\right). \quad (42)$$

Let us note that the upper limit of summation in expression (42) is equal to the integer N, i.e. the ratio of the wave number of the charge carrier in the uppermost sub-band k_{zN} to the wave number of the charge carrier in the first sub-band k_{z1} [14,15]:

$$N = \frac{k_{zN}}{k_{z1}} = \left[\frac{k_F}{k_{z1}}\right] = [2x_0]. \quad (43)$$

Let us proceed to the case of a non-degenerate electron gas ($u_\mu \to -\infty$), corresponding to a low concentration, a large effective mass of charge carriers, and a high temperature. The equilibrium function of distribution transfers to the classical distribution of the Maxwell-Boltzmann.

$$f_l^{(0)}(\varepsilon_l) = \exp\big((\nu-\varepsilon_l)/k_0T\big). \quad (44)$$

The functions $B_{\parallel}$ and $B_{\perp}$ included in the expressions (15)–(17) are defined as follows:

$$B_{\parallel,\perp} = \frac{\rho y_p^2}{2\cos\theta x_\lambda z_{0\parallel,\perp}\Phi^2_{\parallel,\perp}(\gamma)}\sqrt{\frac{5}{2\pi}} \times \sum_{l=1}^{\infty}\exp\left(-\frac{5l^2}{8x_0^2}\right)\left(1-\chi\left(\frac{2x_0^2 z_{0\parallel,\perp}\sqrt{\gamma}}{x_\lambda l}\right)\right). \quad (45)$$

Analysis of results

Figure 1 shows the plotted dependences of the coefficients of absorption on the dimensionless thickness of the semiconductor nanolayer. There is a review of the cases of longitudinal (solid curves) and transverse (dashed curves) directions of the rotation axis of a constant energy ellipsoid. The absorption coefficient was calculated using formula (17) taking into account the expression for the functions $B_{\parallel}$ and $B_{\perp}$ (45) in the case of a non-degenerate electron gas.

The dependence of the absorption coefficient on thickness is non-monotonic. As the thickness decreases, the absorption coefficient increases, and at $x_0 < 1$ it decreases. This dependency behavior can be explained as follows. At large thicknesses, the nanolayer has a fairly high concentration of free charge carriers, which influence the formation of a secondary reflected wave. Almost all the energy of the incident wave is converted into reflected energy. As the thickness decreases, the concentration of free charge carriers entering the conduction band decreases, as a result of which part of the electromagnetic wave penetrates into the nanolayer and is absorbed by it, and the absorption coefficient increases. With a further decrease in thickness ($x_0 < 1$), the concentration of free charge carriers becomes insufficient for effective absorption of radiation; the absorption coefficient decreases and is practically equal to zero at $x_0 < 0.5$. There are oscillations in the dependences of optical coefficients on thickness, the reason and conditions for their occurrence are given in the work [18]. Figure 1 shows that the maximum absorption value in the case of a longitudinal orientation of the main axis of a constant energy ellipsoid is blurred and is half as much as the absorption maximum calculated taking into account the transverse orientation. At the diffuse maximum of the solid curve *1* there are small oscillations in contrast to the

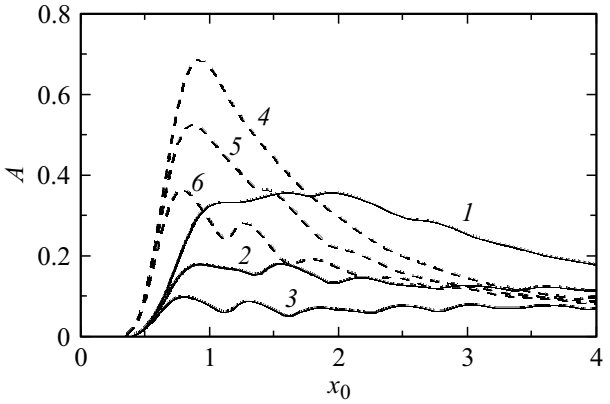

Figure 1. Dependences of the absorption coefficient A on the dimensionless thickness x_0 at values $g_1 = g_2 = 0.2$; $\rho = 0.005$; $y_p = 200$; $x_\lambda = 8$; $\varepsilon_\lambda = 7$; $\varepsilon_2 = 4$; $\gamma = 0.6$; $\theta = 48°$. *1, 4* — $y_0 = 10$; *2, 5* — $y_0 = 17$; *3, 6* — $y_0 = 25$. Solid curves *1–3* — the case of the longitudinal direction of the main axis of a constant energy ellipsoid, dashed curves *4–6* — the case of the transverse direction.

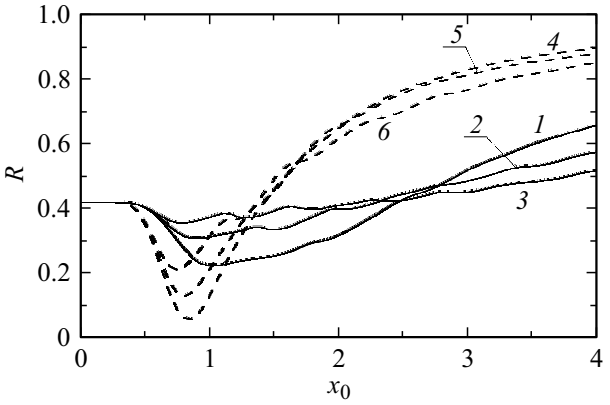

Figure 2. Dependences of the reflectance R on the dimensionless thickness x_0 at values $g_1 = g_2 = 0.2$; $\rho = 0.005$; $y_p = 200$; $x_\lambda = 8$; $\varepsilon_\lambda = 7$; $\varepsilon_2 = 4$; $\gamma = 0.6$; $\theta = 48°$. *1, 4* — $y_0 = 10$; *2, 5* — $y_0 = 17$; *3, 6* — $y_0 = 25$. Solid curves *1–3* — the case of the longitudinal direction of the main axis of a constant energy ellipsoid, dashed curves *4–6* — the case of the transverse direction.

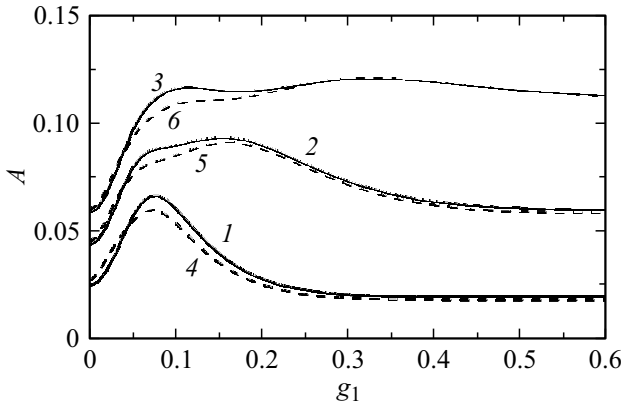

Figure 3. Dependences of the absorption coefficient A on the roughness parameter of the upper surface g_1 at values $y_0 = 4$; $\rho = 0.005$; $y_p = 200$; $g_2 = 0$; $x_\lambda = 50$; $\gamma = 0.7$; $\varepsilon_1 = 3$; $\varepsilon_2 = 5$; $\theta = 66^\circ$: curves *1, 4* — $x_0 = 1$; *2, 5* — $x_0 = 1.5$; *3, 6* — $x_0 = 2$. Solid curves *1–3* — the case of degenerate, dashed curves *4–6* — non-degenerate electron gas.

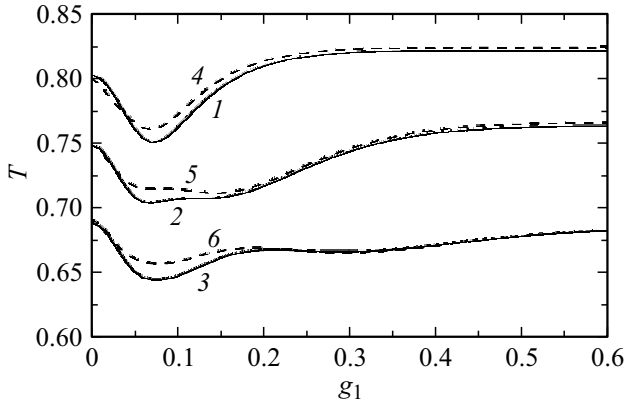

Figure 4. Dependences of the transmittance coefficient T on the roughness parameter of the upper surface g_1 at values $y_0 = 4$; $\rho = 0.005$; $y_p = 200$; $g_2 = 0$; $x_\lambda = 50$; $\gamma = 0.7$; $\varepsilon_1 = 3$; $\varepsilon_2 = 5$; $\theta = 66^\circ$: curves *1, 4* — $x_0 = 1$; *2, 5* — $x_0 = 1.5$; *3, 6* — $x_0 = 2$. Solid curves *1–3* — the case of degenerate, dashed curves *4–6* — non-degenerate electron gas.

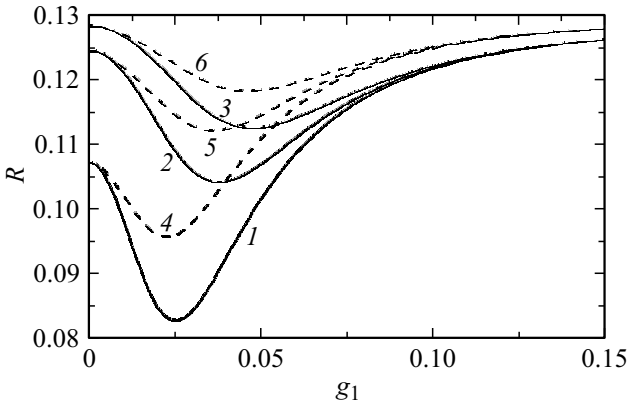

Figure 5. Dependences of the reflectance R on the roughness parameter of the upper surface g_1 at values $x_0 = 0.7$; $\rho = 0.005$; $y_p = 200$; $g_2 = 0$; $x_\lambda = 50$; $\gamma = 0.7$; $\varepsilon_1 = 3$; $\varepsilon_2 = 6$; $\theta = 37^\circ$: curves *1, 4* — $y_0 = 2$; *2, 5* — $y_0 = 4$; *3, 6* — $y_0 = 6$. Solid curves*1–3* — the case of degenerate, dashed curves *4–6* — non-degenerate electron gas.

curve *4*, i.e. in the case of a longitudinal orientation of the main axis of a constant energy ellipsoid, the oscillatory effect is observed at lower frequencies than in the case of a transverse orientation.

Figure 2 shows the dependence of the reflectance, calculated using formula (15) taking into account (45), on the dimensionless thickness of the semiconductor layer. From Fig. 2 it follows that at a certain thickness there is a minimum of reflection. A potential reason for the behavior of the dependence of the reflectance on thickness is as follows. As the thickness decreases (up to $x_0 = 0.8$), the reflectance decreases, since the concentration of free charge carriers forming the reflected wave decreases. At small thicknesses ($x_0 < 0.5$), another mechanism for the formation of a reflected wave operates, similar to the case of a dielectric layer: as a result of multiple reflection of radiation from the upper and lower surfaces of the nanolayer. The presence of a small amount of free carriers absorbing radiation prevents the formation of a reflected wave. There is a decrease of the reflectance at $0.5 < x_0 < 0.8$.

Figures 3 and 4 show the dependences of the absorption and transmittance coefficients on the roughness parameter of the upper surface, plotted in the case of the longitudinal direction of the main axis of a constant energy ellipsoid. The calculation was carried out using formulas (16) and (17) taking into account the expression for the function $B_\parallel$ (42) in the case of a degenerate electron gas and (45) in the case of a non-degenerate electron gas. In Figs. 3 and 4, there are absorption maxima and transmittance minima at certain roughness values. In Fig. 3 and 4 it is clear that curves *1, 4* have one absorption maximum (transmittance minimum), and curves *2, 3, 5, 6* — two maxima (minima). A potential reason for the non-monotonic behavior of the dependences of the absorption and transmittance coefficients on the roughness parameter is explained by the discrete structure of the energy bands of the semiconductor.

Figures 5 and 6 show the dependences of the reflectance calculated using formula (15) taking into account (42) (solid curves) and (45) (dashed curves) on the roughness parameter of the upper surface. The dependences are plotted in the case of the longitudinal direction of the main axis of a constant energy ellipsoid. Fig. 5 is constructed in the case when the dielectric constant of the upper insulating layer ε_1 is less than the dielectric constant of the lower layer ε_2, and Fig. 6 — vice versa. In Fig. 5 there are reflection minima, and in Fig. 6 there are maxima. With an increase in the frequency of the electromagnetic wave, the maxima (minima) decrease and shift towards higher surface roughness values.

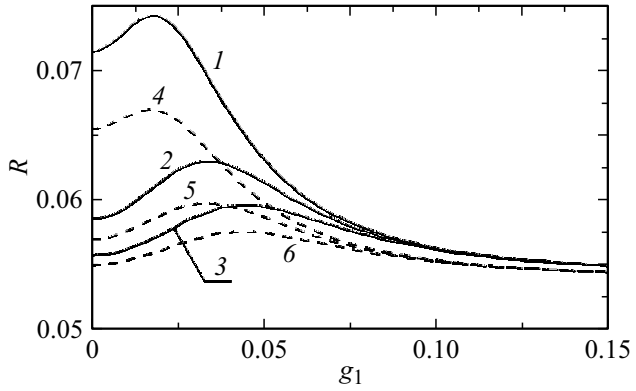

Figure 6. Dependences of the reflectance R on the roughness parameter of the upper surface g_1 at values $x_0 = 0.7$; $\rho = 0.005$; $y_p = 200$; $g_2 = 0$; $x_\lambda = 50$; $\gamma = 0.7$; $\varepsilon_1 = 6$; $\varepsilon_2 = 3$; $\theta = 37°$: curves *1, 4* — $y_0 = 2$; *2, 5* — $y_0 = 4$; *3, 6* — $y_0 = 6$. Solid curves *1–3* — the case of degenerate, dashed curves *4–6* — non-degenerate electron gas.

Conclusion

In this paper, as part of the quantum theory of transport phenomena, analytical expressions are obtained for the reflectance, transmittance and absorption coefficients of a layered nanostructure „dielectric-semiconductor-dielectric" taking into account the anisotropy of the band structure of the semiconductor.

It has been specified that in case of a transverse orientation of the main axis of a constant energy ellipsoid, the maximum value of the absorption coefficient is almost twice as high as the absorption coefficient calculated in the case of a longitudinal orientation. In case of the longitudinal direction of the rotation axis of the ellipsoid high-frequency oscillations in the dependences of the absorption coefficient on the thickness of the semiconductor layer can be observed at lower frequencies than in the case of the transverse direction.

A non-monotonic behavior of the dependences of the optical coefficients on the roughness parameters of the semiconductor nanolayer boundaries was discovered. At certain roughness values, there are absorption maxima and transmission minima, the appearance of which may be associated with quantization of the energy spectrum of the semiconductor.

Conflict of interest

The authors declare that they have no conflict of interest.

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