

Boundary condition for the distribution function of electrons interacting with phonons

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The boundary condition is derived for the kinetic equation for the distribution function of electrons interacting with Rayleigh and bulk phonons. Both the change of the phonon field as a result of the presence of the sample surface and the vibration of the surface itself are taken into account. The problem is solved with the aid of Keldysh's technique by determining the electron and phonon Green functions for the half-space. The condition found ensures the absence of current through the surface and is fulfilled identically in the equilibrium state. The result obtained can also be used for the case of the interaction of electrons with impurities in the layer adjacent to the surface. The transition to the Fuchs condition, with the diffusivity coefficient depending on the glancing angle and energy of the electrons, is discussed.

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1. INTRODUCTION

In solving problems that take into account the effect of the boundary of the sample on the kinetic properties it is necessary to know the boundary condition satisfied by the distribution function. In the theory of metals the boundary condition for the electron distribution function is of greatest interest, since in many cases the phonons can be assumed to be in equilibrium. For electrons one usually uses the Fuchs boundary condition, which introduces a phenomenological parameter—the diffusivity coefficient.

Recently a number of papers have appeared in which the boundary condition is derived taking into account a particular mechanism of interaction of the electrons with a nonideal surface (cf., e.g., Ref. 1). The simplest interaction leading to diffuse scattering is scattering by surface roughness. A boundary condition that takes this scattering into account was obtained in a paper by the author (Ref. 2). In a paper by Okulov and Ustinov³ the same problem was considered with allowance for the finite height of the potential barrier at the boundary of the metal with the vacuum. We note that, in principle, the effect of surface scattering is important even at the atomic scale of roughness, inasmuch as information about the properties of the surface is carried away by the reflected electrons over a mean free path.

Scattering by static surface irregularities occurs with conservation of the energy of the electrons, and only their momentum distribution is changed. As the temperature is raised the role of the interaction of the electrons with thermal vibrations of the surface increases. This interaction gives rise to relaxation of the electrons in both momentum and energy, and is the course of the temperature-dependent diffusivity.

In a semi-infinite metal the independent acoustic modes are the surface Rayleigh phonons and the bulk phonons, which, in the presence of the surface, even in an isotropic substance, cannot be completely divided into longitudinal and transverse phonons.

As will be shown below, at large distances from the

surface (large compared with the normal component λ_x of the wavelength of the phonons and electrons), the kinetic equation has the same form as for an infinite metal. The contribution of shorter distances (the effect here of the surface and bulk phonons, and also of the boundary condition on the electron wave function) is written in the form of a boundary condition. Of course, this can be done only if all the macroscopic parameters (the sample thickness d , mean free path l , and skin depth δ) are large compared with the characteristic wavelength λ_x . Since we are not in a position to consider distances of the order of interatomic distances, it is necessary that the length λ_x be large compared with these. This implies that, strictly, the result obtained below can be applied only in the situation of the anomalous skin effect: $l \gg \delta$ or $l \gg d$, when the decisive contribution is that of glancing electrons with large wavelength λ_x .

In the case when these conditions are fulfilled, we can assume that a boundary condition is specified at the surface of the metal, and, moreover, in deriving it we can disregard the external electromagnetic field and neglect collisions with phonons in the bulk. The latter statement requires some explanation.

There are two independent mechanisms of the effect of phonons on the boundary condition for the electrons. First, there is the direct electron-phonon interaction, describable by the coupling constant g . Because of the presence of the Rayleigh phonons, in the layer adjacent to the surface this interaction differs from its bulk value. The interaction with the bulk phonons is taken into account by the kinetic equation itself, and in the surface layer it is of little importance because of the condition $l \gg \lambda_x$. Thus, only the Rayleigh contribution should be kept in this case. Secondly, vibrations of the sample surface lead to the result that the initial boundary condition for the electron wavefunction is fulfilled on the actual moving surface. Since the displacement of the surface is determined by both Rayleigh and bulk phonons, here it is necessary to take both types of phonons into account.

2. THE COLLISION INTEGRAL

We shall show that, far from the surface, at distances large compared with the electron and phonon wavelengths, the collision integral for the half-space is written in the same form as for an unbounded metal. We shall assume that the surface barrier for the electrons is infinite, i.e., the wave functions of the electrons can be chosen in the form

$$\psi_p(xst) \sim \sin p_x x \exp[i(p_x s - e_p t)], \quad (1)$$

and we shall assume the phonons to be equilibrium phonons (actually, it is sufficient that their distribution function depend only on the energy); the x axis is chosen along the normal to the surface, and s is a two-dimensional vector in the plane of the surface; for simplicity we consider an isotropic medium with a quadratic electron spectrum.

At large distances from the surface there are only bulk phonons. The associated displacement of the medium is

$$u_\alpha^i(xst) \sim \exp[i(ks - \omega t)] \left\{ e_\alpha^i \exp(-ik_\gamma x) + \sum_{\gamma'} e_\alpha^i R_{\gamma'} \exp(ik_\gamma x) \right\}, \quad (2)$$

which is specified by the frequency ω , the two-dimensional vector k parallel to the surface, and the polarization γ of the incident wave; the normal component $k_\gamma = (\omega^2/c_\gamma^2 - k^2)^{1/2}$ of the wave vector is positive in the reflected wave for $|\omega| > c_\gamma k$; $c_\gamma = c_l, c_t$ are the longitudinal and transverse sound velocities, α is a three-dimensional vector index, and the e_α^i are unit vectors depending on the direction of propagation. The reflection coefficients $R_{\gamma'}$ are found in the familiar way from the condition for the absence of surface forces. For a wave polarized in the plane of incidence,

$$\begin{aligned} R_{ll} &= [4k^2 k_l k_t - (k^2 - k_t^2)^2] / \Delta, \\ R_{lt} &= 4k k_t (k^2 - k_t^2) c_l / c_t \Delta, \\ R_{tl} &= 4k k_l (k_t^2 - k^2) c_l / c_t \Delta, \\ R_{tt} &= R_{ll}, \\ \Delta &= (k^2 - k_t^2)^2 + 4k^2 k_l k_t. \end{aligned} \quad (3)$$

For a wave polarized at right angles to the plane of incidence, $R_{tt} = 1$ and $R_{lt} = 0$. In the collision integral the square of the modulus of the matrix element

$$g \int d^3r \bar{\psi}_p \frac{\partial u_\alpha^i}{\partial t_\alpha} \psi_p$$

is multiplied by the occupation numbers of the electrons and phonons and integrated over p'_x and k and positive p'_x and k_γ . As the volume of integration tends to infinity the square of the integral over s gives, as usual, the product of the surface area with the δ -function of the tangential components of the momentum. The square of the integral over x is a sum of products of integrals, each of which contains an incident or a reflected wave. A product of integrals of which one contains an incident wave and the other a reflected wave does not give a factor proportional to the size L_x of the sample. Only for a product of integrals with waves of the same polarization is this statement not entirely obvious. In this case there arises the expression

$$\left[\int_0^{L_x} dx \sin p'_x x \sin p_x x \exp(-ik_\gamma x) \right]^2,$$

which contains the dangerous form

$$I(\alpha) = \alpha^{-2} \sin^2 \frac{\alpha L_x}{2} \exp(i\alpha L_x),$$

where $\alpha = p'_x - p_x - k_\gamma$. However, on subsequent integration over p'_x (i.e., over α) of a product of the quantity $I(\alpha)$ with an arbitrary function, in the limit of large L_x there appears the integral

$$\int_{-\infty}^{+\infty} d\alpha \alpha^{-2} \sin^2 \alpha \exp(2i\alpha),$$

which is equal to zero.

The square of the matrix element containing only the reflected wave makes the following contribution to the collision integral:

$$\int d^3p'_x d^3p_x d^3k d^3k' \sum_{\gamma, \gamma'} k'_\alpha e_\alpha^i k'_\beta e_\beta^i R_{\gamma'} R_{\gamma'} \times \delta(k + p_x - p'_x) \delta(k_\gamma + p_x - p'_x) \delta(\omega + e_p - e_{p'}) n_p (1 - n_{p'}) (N_\alpha + 1); \quad (4)$$

the summation indices α, β take the values x, y, z , where, for $\alpha, \beta = x$, in accordance with our notation, $k'_x = k_\gamma$. We do not write out the terms that differ from (4) in the signs in front of p_x, p'_x , and k_γ in the arguments of the δ -functions.

We make the change of variable $k_\gamma \rightarrow k'_\gamma$ and sum over the initial polarization γ , making use of the relation

$$\sum_{\gamma} R_{\gamma'} R_{\gamma'} \frac{c_l^2 k'_\gamma}{c_t^2 k_\gamma} = \delta_{\gamma' \gamma' \gamma},$$

which expresses the conservation of the energy flux in the sound wave. We obtain an expression which, when combined with the contribution of the incident wave, coincides in form with the collision integral corresponding to an infinite space.

3. ELECTRON AND PHONON GREEN FUNCTIONS FOR THE HALF-SPACE

We shall relate the distribution function for electrons flying from the surface to its value for electrons flying toward the surface, at distances large compared with the normal component of the electron and phonon wavelengths but small compared with all the macroscopic parameters l, δ , and d . At such distances we can neglect the effect of the electromagnetic field, expanding the Green functions of the noninteracting electrons and phonons in the wavefunctions in the absence of the field. Here we must assume the occupation numbers of the electrons to be arbitrary, and those of the phonons, as we stipulated earlier, to be equilibrium occupation numbers.

To solve the problem formulated we shall make use of the Keldysh technique,⁴ in which, with the aid of the Green function

$$G^+(rt, r't') = i \langle \psi^+(r't') \psi(r, t) \rangle,$$

we can determine the electron distribution function

$$n(p_{r,t}) = \frac{1}{2\pi i} \int de dt_- dr_- G^+(rt, r't') \times \exp[-i(p_{r-} - et_-)], \quad (5)$$

where $r \mp r' = r_{\mp}, t \mp t' = t_{\mp}$.

The Dyson equation for G^+ has the form

$$G^+ = G_0^+ + ig^2(G_0^+ \Sigma^+ G^+ + G_0^+ \Sigma^+ G^0 + G_0^+ \Sigma^- G^+ + G_0^+ \Sigma^+ G^0 + G_0^+ \Sigma^+ G^0). \quad (6)$$

Here G^0 is the causal function, \tilde{G}^0 contains ordering in the inverse time, G^- differs from G^+ in the order of the operators, and the Σ are the self-energy parts.

The Green functions with subscript zero should satisfy the appropriate boundary condition on the vibrating surface of the metal. In second order in the phonon displacements the surface vibrations can be treated in the same way as surface roughness was investigated in Ref. 2. We shall write out the corresponding contribution later; for now we shall neglect the surface vibration and require that the boundary conditions for the Green functions be fulfilled at $x=0$.

In the derivation of the kinetic equation it is assumed that the collision frequency is small compared with the characteristic energy of the particles. Therefore, in the same approximation, in the right-hand side of Eq. (6) we must substitute Green functions that are of zeroth order in the phonon displacements but correspond to a certain arbitrary distribution of occupation numbers, determined by the kinetic equation.

The retarded and advanced functions, which do not depend on the occupation numbers for a semi-infinite metal with an infinite potential barrier at the boundary at $x=0$, are obtained from the corresponding functions for the unbounded metal. For example, for the Fourier component in the difference $s-s'$ and $t-t'$ of the retarded function we have

$$G_0^R(x'p, \epsilon) = G_{\infty}^R(x-x', p, \epsilon) - G_{\infty}^R(x+x', p, \epsilon). \quad (7)$$

Performing the integration in the well known expression for the retarded function of the unbounded metal

$$G_{\infty}^R(xp, \epsilon) = \frac{1}{2\pi} \int \frac{dp_x}{\epsilon - \epsilon_p + i\delta} \exp(ip_x x), \quad (8)$$

we obtain

$$G_0^R(x'p, \epsilon) = -\frac{im}{p_1} \{ \exp(ip_1|x-x'|) - \exp[ip_1(x+x')] \}, \quad (9)$$

where $p_1 = [2m(\epsilon + i\delta) - p_s^2]^{1/2}$. The advanced function is found analogously:

$$G_0^A(x'p, \epsilon) = \frac{im}{p_1} \{ \exp[-ip_1|x-x'|] - \exp[-ip_1(x+x')] \}. \quad (10)$$

With the aid of the standard expansion in the eigenfunctions (1) of the half-space the function G_0^+ is expressed in terms of the occupation numbers:

$$G_0^+(x'p, \epsilon) = \frac{4im}{p_1} n^<(p_s, \epsilon) \sin p_1 x \sin p_1 x'. \quad (11)$$

We shall see below that the quantity $n^<(p_s, \epsilon)$ is the distribution function for the electrons incident on the surface.

Knowing the functions G^R , G^A , and G^+ , we find the causal functions from the general formulas of Ref. 4:

$$G^0 = G^+ + G^R, \quad \tilde{G}^0 = G^+ - G^A. \quad (12)$$

We turn to the determination of the phonon functions. The boundary condition for them—the absence of ex-

ternal forces acting on the surface—can be written in the form

$$\hat{\Pi}_{\alpha\beta} \mathcal{D}_{\beta\alpha}(xx'k\omega) |_{x=0} = 0; \quad (13)$$

here,

$$\hat{\Pi}_{\alpha\beta} = \delta_{\alpha\beta} \hat{k}_x + \delta_{\alpha\beta} \hat{k}_x + \left(\frac{c_t^2}{c_l^2} - 2 \right) \delta_{\alpha\beta} \hat{k}_y,$$

in which $\hat{k}_\alpha = -i\partial/\partial x$ for $\alpha = x$, while for $\alpha = y, z$ the operator \hat{k}_α reduces to multiplication by the corresponding component of the two-dimensional vector \mathbf{k} .

The retarded phonon Green function

$$\mathcal{D}_{\alpha\beta}^R(rt, r't') = -i\theta(t-t') \langle [u_\alpha(rt), u_\beta(r't')]_- \rangle$$

in an unbounded substance is obtained by means of the usual expansion in longitudinal and transverse waves. Its Fourier component in the difference $s-s'$ and $t-t'$ is equal to

$$\mathcal{D}_{\alpha\beta}^R(xk\omega) = \sum_{\gamma} \int \frac{dk_x}{2\pi\rho} \frac{e_{\alpha\gamma}(k_x k) e_{\beta\gamma}(k_x k)}{(\omega + i\delta)^2 - \omega_{\gamma}^2(k_x k)} e^{ik_x x}, \quad (14)$$

where ρ is the density of the substance and ω_{γ} are the frequencies of the longitudinal and transverse sound.

The Green function of the semi-infinite medium satisfies for $x, x' > 0$ the same elasticity-theory equation as the function (14), and the boundary condition (13). It has the form

$$\mathcal{D}^R(xx'k\omega) = \mathcal{D}_{\infty}^R(x-x', k\omega) - \mathcal{D}_{\infty}^R(x, k\omega) [\hat{\Pi} \mathcal{D}_{\infty}^R(0, k\omega)]^{-1} \hat{\Pi} \mathcal{D}_{\infty}^R(-x', k\omega). \quad (15)$$

The operator $\hat{\Pi}$ in the last term in (15) acts on the variable x , which then tends to zero from the right:

$$\hat{\Pi} \mathcal{D}_{\infty}^R(-x', k\omega) = \lim_{x \rightarrow 0^+} \hat{\Pi} \mathcal{D}_{\infty}^R(x-x', k\omega).$$

The indication of the direction of $x \rightarrow 0^+$ is essential for $x' = 0$. Owing to the difference in the limit values from right and left, the product of the last two factors in (15) for $x' = 0$ is not equal to unity.

It is easy to verify directly, by acting on the right-hand side of (15) with the operator $\hat{\Pi}$, that the function (15) satisfies the boundary condition (13).

We give the necessary expressions for \mathcal{D}_{xx}^R and $D^R(rt, r't') = \partial^2 \mathcal{D}_{\alpha\beta}^R(rt, r't') / \partial r_x \partial r'_\beta$:

$$\mathcal{D}_{xx}^R(0k\omega) = \frac{-i}{2\omega^2\rho} \left\{ k_l + \frac{k^2}{k_l} - \left[\frac{k^2}{k_l} (k_l^2 - k^2 - 2k_l k_l) \right]^2 - k_l (k_l^2 + k^2)^2 \right\} \Delta^{-1}, \quad (16)$$

$$D^R(xx'k\omega) = \frac{-i\omega^2}{2\rho c_l^2 k_l} \left\{ e^{ik_l(x-x')} - [(k^2 - k_l^2)^2 - 4k^2 k_l k_l] \Delta^{-1} e^{ik_l(x+x')} \right\}; \quad (17)$$

the definition of Δ is contained in (3), and the root $k_{\gamma} = \{ [(\omega + i\delta)/c_{\gamma}]^2 - k^2 \}^{1/2}$ is assumed to be positive for real positive values of the expression under the root.

The advanced function \mathcal{D}^A is obtained by changing the sign of the infinitesimal imaginary part of the frequency in the formulas (14)–(17):

$$\mathcal{D}^A(xx'k\omega) = \mathcal{D}^R(xx'k, -\omega).$$

Green functions containing the phonon occupation numbers can be obtained for the equilibrium state with the aid of Landau's theorem. Usually, this theorem is written for the Fourier components of Green functions that depend only on the difference of the space and time variables. It is possible to see that in the case of an inhomogeneous medium the difference consists entirely in the replacement of the real and imaginary parts [cf. (17.13) in the book⁵] by the half-sum and half-difference of the Green functions \mathcal{D}^R and \mathcal{D}^A :

$$\mathcal{D}^c(r, r', \omega) = \frac{1}{2}(\mathcal{D}^R + \mathcal{D}^A) + \frac{1}{2}(\mathcal{D}^R - \mathcal{D}^A) \operatorname{cth} \frac{\omega}{2T}.$$

Thus, for the functions \mathcal{D}^\pm we find

$$\mathcal{D}^\pm = \frac{\mathcal{D}^R - \mathcal{D}^A}{2} \left(\operatorname{cth} \frac{\omega}{2T} \mp 1 \right),$$

$$\mathcal{D}^+(x, x', k, \omega) = \mathcal{D}^-(x, x', k, -\omega). \quad (18)$$

We shall discuss the formulas obtained. The last term in (15)–(17) takes account of the difference of the Green function from its value for the unbounded substance. This term describes the mutual transformation of the sound waves on reflection from the surface, and also the propagation of the surface Rayleigh waves. The quantity Δ , proportional to $\det \Pi \mathcal{D}_\infty^R(0, k, \omega)$, vanishes on the spectrum of the Rayleigh waves. For the Rayleigh waves, $|\omega| < c_\gamma k$. In this region the integration contour in (14) can be closed in the complex k_x -plane without attention to $i\delta$, which must be retained only in the pole determinant in (15) (i.e., in Δ) and in (16) and (17). For this reason, for $|\omega| < c_\gamma k$ the difference

$$\mathcal{D}^R - \mathcal{D}^A \sim \left(\frac{\partial \Delta}{\partial \omega^2} \right)^{-1} \{ [(\omega + i\delta)^2 - \omega_s^2]^{-1} - c.c. \}$$

$$= \frac{-i\pi}{\omega_s} \left(\frac{\partial \Delta}{\partial \omega^2} \right)^{-1} [\delta(\omega - \omega_s) - \delta(\omega + \omega_s)],$$

where $\omega_s = \xi c_\gamma k$ is the spectrum of the Rayleigh waves, ξ being a number that depends on the ratio c_γ/c_t (see, e.g., Ref. 6).

With the aid of formula (18) we see that, in the region $|\omega| < c_\gamma k$, the functions

$$\mathcal{D}^\pm \sim \frac{-i\pi}{\omega_s} \left(\frac{\partial \Delta}{\partial \omega^2} \right)^{-1} [N_{\omega_s} \delta(\omega \mp \omega_s) + (N_{\omega_s} + 1) \delta(\omega \pm \omega_s)] \quad (19)$$

contain the usual factors, which depend in the given case on the Bose numbers of the Rayleigh phonons.

4. THE BOUNDARY CONDITION

We shall complete the derivation of the boundary condition. In accordance with what was said earlier, by replacing G by G_0 in the right-hand side of (6) we find for each term an expression of the form

$$\int dx_1 dx_2 G_0(x, x_1, p, \varepsilon) \Sigma(x_1, x_2, p, \varepsilon) G_0(x_2, x', p, \varepsilon). \quad (20)$$

With the aid of the formulas (12), and also the identity $\Sigma^c + \bar{\Sigma}^c + \Sigma^+ + \Sigma^- = 0$, we can transform the sum of the terms containing the interaction:

$$G_0^c \Sigma^c G_0^c + G_0^c \Sigma^+ \bar{G}_0^c + G_0^c \Sigma^- G_0^c + G_0^c \Sigma^c \bar{G}_0^c = G_0^c (\Sigma^c + \Sigma^-) G_0^c + G_0^c \Sigma^+ (\Sigma^c + \Sigma^+) G_0^c - G_0^c \Sigma^- G_0^c. \quad (21)$$

This expression can be further simplified if we note the following. As already mentioned, here we should take

into account only the contribution of the Rayleigh phonons. In (21) this contribution falls off in the variables x_1 and x_2 over the phonon wavelength. The integration over x_1 and x_2 is conveniently carried out using the representation (8) of the functions G_0 . After this there still remains the integral over the variables p_x and p'_x , on which two functions depend, e.g., G_0^R and G_0^A in the last term in (21). Closing the contour of integration over p_x in the upper half of the complex plane, so that the integrand falls off for $x > 0$ and $\operatorname{Im} p_x \rightarrow +\infty$, we see that the two poles of the integrand introduce terms of different characters. The first—the pole of the Green function (8)—gives a term that is slowly decreasing in x (thanks entirely to the extra part $i\delta$). The second, which arose after the integration over x_1 , gives a term that decreases in x over a phonon wavelength. The latter term must be omitted, since the boundary condition is written for a distance from the boundary that is large compared with a wavelength. Only the first term is obtained if, in the integral (20), for the first factor, e.g., $G_0^R(x, x_1, p_s, \varepsilon)$, we use from the outset the expression (9) with $x - x_1 > 0$ and integrate over x_1 between 0 and ∞ . Everything that has been said also applies to the last factor in (20).

Thus, the prescription reduces to the following: for the functions G_0 , in the entire region of integration over x_1 and x_2 in (20), it is necessary to use the expressions (9) and (10) for $x - x_1 > 0$ for the first factor and for $x_2 - x' < 0$ for the last factor. If, in addition, we omit terms that depend only on $x + x'$ and do not give a contribution to the Fourier component in $x - x'$ with $p_x \neq 0$, we obtain the following expression:

$$G(x, x', p, \varepsilon) = G_0(x, x', p, \varepsilon) + i \left(\frac{2mg}{p_1} \right)^2$$

$$\times \exp[ip_1(x - x')] \int_0^\infty dx_1 dx_2 \sin p_x x_1 \sin p_x x_2$$

$$\times \left\{ [n^<(p, \varepsilon) - 1] \Sigma_{sur}^+(x_1, x_2, p, \varepsilon) - n^<(p, \varepsilon) \Sigma_{sur}^-(x_1, x_2, p, \varepsilon) \right\}, \quad (22)$$

where the subscript *sur* shows that only the Rayleigh term need be kept.

The self-energy parts Σ^\pm are equal to

$$\Sigma^\pm(rt, r't') = -G^\pm(rt, r't') D^\mp(r't', rt).$$

To find the distribution function at large distances from the surface it is necessary, in accordance with (5), to integrate G^+ (22) over $x_- = x - x'$ between $-2x_+$ and $2x_+$ under the condition $|x_+ p_x| \gg 1$. For the incident wave, i.e., for $p_x < 0$, a contribution proportional to $\delta(p_x + p_1)$ arises only from G_0^+ (11). Integrating next over ε , we obtain for $p_x < 0$

$$n(p_x p_1) = n^<(p_1, \varepsilon = (p_x^2 + p_1^2)/2m). \quad (23)$$

For the reflected wave ($p_x > 0$), using (18) we find

$$n(p_x p_1) = n(-p_x p_1) - i \frac{2m^2 g^2}{\pi^3} \int d^2 p' d\varepsilon'$$

$$\times \int_0^\infty \frac{dx_1 dx_2}{p_x p_x'} \sin p_x x_1 \sin p_x x_2$$

$$\times \sin p_x' x_1 \sin p_x' x_2 \{ [n(-p_x p_1) - 1] n(-p_x' p_1') - D_{sur}^-(x_2, x_1, p_1' - p_1, \varepsilon' - \varepsilon) - (p_x \varepsilon \mp p_1' \varepsilon') \}, \quad (24)$$

where

$$p_x' = [2m\varepsilon' - p_x'^2]^{1/2}.$$

The calculation of the integral over x_1 and x_2 is elementary—the dependence of D^- on these variables is given by the formulas (17)–(19).

We write the boundary condition thus obtained in the form

$$n(p_x p_s) = n(-p_x p_s) + \int d^2 p_s' d\varepsilon' \times \{n(-p_x' p_s') [1 - n(-p_x p_s)] [W_1(p_s \varepsilon, p_s' \varepsilon') + W_2(p_s \varepsilon, p_s' \varepsilon')] - (p_s \varepsilon \rightleftharpoons p_s' \varepsilon')\}, \quad p_x > 0. \quad (25)$$

The integral term in this formula describes the departure from specular reflection. The function W_1 is determined by formula (24) and depends on the coupling constant with the phonons:

$$W_1(p_s \varepsilon, p_s' \varepsilon') = [(N_{\omega_s} + 1) \delta(\varepsilon' - \varepsilon - \omega_s) + N_{\omega_s} \delta(\varepsilon' - \varepsilon + \omega_s)] F(p_s \varepsilon, p_s' \varepsilon'), \quad (26)$$

where we have introduced the following notation:

$$F = \frac{(8gmc)^2 \kappa_1 \omega_s p_x p_x'}{\pi^2 \rho c_i^2 [(p_x^2 + p_x'^2 + \kappa_1^2)^2 - 4p_x^2 p_x'^2] f},$$

$$f = [4k^4 (c_i^2 \kappa_1^2 + c_i^2 \kappa_1^2) - c_i^2 (k^2 + \kappa_1^2)^2] k^{-1} \kappa_1^{-2} \kappa_1^{-2},$$

$$\kappa_1 = (k^2 - \omega^2 / c_i^2)^{1/2}, \quad k = p_s' - p_s,$$

$$\omega = \varepsilon' - \varepsilon, \quad p_x = (2m\varepsilon - p_x^2)^{1/2},$$

$$p_x' = (2m\varepsilon' - p_x'^2)^{1/2}, \quad \omega_s = \xi c_i k,$$

In (25), the function W_2 , which does not depend on the coupling constant, takes into account the contribution of the surface vibrations to the boundary condition. This term can be calculated by the same method by which the static surface roughness was treated earlier²:

$$W_2(p_s \varepsilon, p_s' \varepsilon') = \frac{i p_x p_x'}{2\pi^3} \mathcal{D}_{xx}^-(0, p_s' - p_s, \varepsilon' - \varepsilon). \quad (27)$$

The function \mathcal{D}_{xx}^- can be represented by means of the relations (16), (18), and (19) as follows:

$$i\mathcal{D}_{xx}^-(0k\omega) = \frac{\omega|\omega|}{\rho c_i^4} \left(\operatorname{cth} \frac{\omega}{2T} + 1 \right) \quad (28)$$

$$\times \begin{cases} k_i/\Delta, & |\omega| > c_i k, \\ 4k^2 \kappa_1 \kappa_1' [(k^2 - k_i^2)^{-1} + (4k^2 \kappa_1 k_i)^{-2}], & c_i k > |\omega| > c_i k, \end{cases} \quad (29)$$

$$i\mathcal{D}_{xx}^-(0k\omega) = \frac{8\pi(\kappa_1 - \kappa_1') c_i^2 c_i^2}{\rho \omega_s^3 f} [(N_{\omega_s} + 1) \delta(\omega - \omega_s) + N_{\omega_s} \delta(\omega + \omega_s)], \quad |\omega| < c_i k. \quad (30)$$

5. CONCLUSION

We shall discuss the boundary condition (25). It is easy to see that the boundary condition ensures the absence of current through the surface, irrespective of the concrete form of the distribution function. In fact, the normal component of the current is equal to

$$j_x = \frac{e}{4\pi^3} \int v_x n(p) d^3 p = \frac{e}{4\pi^3} \int d^2 p_s d\varepsilon [n(p_x p_s) - n(-p_x p_s)].$$

The difference $n(p_x p_s) - n(-p_x p_s)$ at the surface of the sample is found by means of the formulas (25)–(27). The integral that arises is equal to zero, since the integrand is odd under the change of variables $p_s \varepsilon \rightleftharpoons p_s' \varepsilon'$.

The regions (28) and (29) describe the contribution of the bulk phonons to the vibration of the sample surface; in the region (29) the longitudinal wave arising in the reflection of the incident transverse wave attenuates over a wavelength. The formulas (28) and (29) can be

represented in the form of integrals over k_x of a product of Bose occupation numbers with a δ -function expressing energy conservation in the excitation of the longitudinal and transverse phonons.

The condition (25) is fulfilled identically for an equilibrium system of electrons. In this case the integral in (25) vanishes, as can easily be seen directly using the Fermi distribution function for the electrons and energy conservation.

A quantitative estimate of the influence of phonons on the reflection of electrons from the surface requires calculation of the electrical conductivity with the aid of the boundary condition (25). Nevertheless, it is clear that since the formulas (26) and (27) contain the density of the substance in the denominator, the diffusivity of the surface has a small factor $(m/M)^{1/2}$, where M is the lattice-ion mass and m is the electron mass. Even so, the phonons can have an appreciable effect on the temperature dependence of, e.g., the resistivity of a thin plate, since the "surface" contribution taken into account by formula (25) is proportional to a lower power of the temperature than the volume contribution, which is proportional to T^5 at low temperatures. We note also that the diffusivity increases substantially in the case of a long mean free path, when an electron has time to collide many times with the surfaces of a small sample during the mean free time.

We shall discuss how the condition (25) goes over into the Fuchs boundary condition. In the approximation linear to the deviation from equilibrium the integral (25) breaks down into a sum of two terms, in which the non-equilibrium correction n_1 to the electron distribution function is contained in different forms. In one, n_1 depends on the integration variables p_s' and ε' , while in the other it depends on the external variables p_s and ε . The first of these terms can be neglected in comparison with the second in the case when the distribution function varies sufficiently rapidly in a region comparable with the characteristic momenta and frequencies of the phonons. It is then that a condition of the Fuchs type is obtained. However, the diffusivity coefficient in this case is a rapidly varying function of the glancing angle of the electrons, and also, possibly, of their energy.

We note that the formulas (24) and (27) enable us to consider surface scattering of electrons that is not associated with phonons. For example, the expression (27) also describes the scattering of electrons by a random surface $x = \xi(s)$. In this case the function \mathcal{D}_{xx}^- is related to the correlator of the irregularities:

$$i\mathcal{D}_{xx}^-(0, s-s', \omega) = \langle \xi(s) \xi(s') \rangle 2\pi \delta(\omega)$$

and we arrive at the boundary condition obtained in Ref. 2.

Another example is the scattering of electrons by impurities located randomly in the layer adjacent to the surface. If we describe the interaction with such impurities by the Hamiltonian

$$g \sum_j V(r-r_j),$$

the boundary condition will be determined by the formu-

la (24), in which the function $D_{s_{ur}}^-$ is expressed in terms of the correlator

$$iD_{s_{ur}}^-(rt, r't') = \left\langle \sum_{j,j'} V(r-r_j) V(r'-r_{j'}) \right\rangle,$$

which contains averaging over the configurations of the impurities r_j .

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Interaction of Bloch walls with dislocations in garnet films possessing a cylindrical domain structure

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The dislocation and domain structures of monocrystalline films of $(YBi)_3(FeGa)_5O_{12}$, grown on gadolinium-gallium garnet plates, are investigated by an optical polarization method and by selective chemical etching. The interaction with dislocations is studied for walls of stripe domains in a labyrinth structure and of cylindrical magnetic domains. For the first time, a direct experimental investigation is carried out of the potential contours for the motion of a 180° Bloch wall in the microstress field of an individual dislocation. The forces exerted by the dislocation on individual elements of the domain wall are measured. A theoretical calculation is made of the potential and forces of magnetoelastic interaction of various sections of the domain wall with the internal-stress field of the dislocation. The experimental data are compared with the calculation and with the predictions of current theories. The comparison reveals some peculiarities not considered earlier in the kinetics of the surmounting by a wall of potential barriers due to dislocations.

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INTRODUCTION

Study of the role of defects of the crystal lattice of a ferromagnetic material in the formation of its domain structure and in the kinetics of change of that structure is necessary for creation of a systematic theory of the magnetization of real magnetically ordered materials. Special interest attaches to the explanation of the nature of the interaction of domain walls with dislocations, the longest-range sources of internal stresses. Use of an optical polarization method for solution of this problem made it possible for the first time to carry out direct experimental investigation of the influence of individual dislocations on elementary events of the magnetization process^{1,2} in the example of monocrystals of yttrium-iron garnet. Comparison of experimental data with the predictions of current theories revealed basic contradictions between them. In particular, it was found that in a real crystal the interaction of a Bloch wall with a dislocation begins at distances far exceeding the thickness of the wall. During the process of their inter-

action, new domains originate in the dislocation-microstress field and at the wall. These data were obtained on a many-axis ferrimagnet, characterized by appreciable anisotropy of the energy of a Bloch wall,³ under conditions of motion of several walls through the specimen and presence of surface closure domains. It might be supposed that the regularities observed were characteristic solely of crystals whose magnetic structure allows formation of new domains magnetized in a direction not coinciding with the magnetization of the main domains. In order to elucidate the reasons for the disagreement between experimental data and theory, it was of interest to investigate also the anisotropy of the interaction of dislocations with a Bloch wall under conditions when its energy is independent of the direction of its normal to the plane perpendicular to the wall.

The present communication presents the results of a study of the regularities of the motion of a 180° domain wall in the elastic field of an individual dislocation in magnetically uniaxial, epitaxial films of $(YBi)_3(FeGa)_5O_{12}$.