

WHY MATTHEIJSSEN'S RULE OF THE THEORY OF METALS MAY BE BROKEN: BY ARRAYING DEFECTS INTO PLANES

BEŽÁK V.,¹⁾ BRATISLAVA

Geometrically simple bicrystalline and polycrystalline metallic samples with layer-like grains are considered. Taking all grains identical, we calculate the zero-temperature longitudinal electrical conductivity using the Boltzmann kinetic equation for the conduction electrons. We assume that there are only two types of point defects on which the conduction electrons are liable to scatter: one type for the bulk of the grains, another for the interface(s) between the grains. Defining the average (volume) densities of the defects, we ask whether it is actually justified to use, at least approximately, the usual Matthiessen rule in the transport theory of metallic samples with internal interfaces. In general, our answer is negative. (Even in the case of bicrystalline samples when the outer surfaces are taken as perfectly smooth.) Some numerical results obtained by machine integrations are presented in two tables.

I. INTRODUCTION

Planar arrays of defects in solids are not rare. We can readily call to mind facets which form interfaces between grains in polycrystals. As a rule, the interfaces are locations where atomic bonds are weakened and can therefore play a role of "attractors" for various defects (e.g. impurity atoms). For simplicity, let all interface defects be of one sort; if we consider this situation in a metallic polycrystal, we may regard each point defect "stuck" to the interface as a certain, uniquely definable, cross-section in the scattering theory of a conduction electrons. Ascertaining in any way the total number of the interface defects, dividing it by the volume Ω of the polycrystal and defining thus the average volume density of the interface defects, we can — employing the standard quasi-classical kinetic theory [1] — define some relaxation time characterizing the electron scattering on the interface defects. Analogically, we can obtain the relaxation time corresponding to the scattering (again separately) on the bulk defects. Now we pose the question: may we combine these two

¹⁾ Department of Solid State Physics, Comenius University, 84215 BRATISLAVA, Czechoslovakia

relaxation times in the same way as in the case of a single-crystalline metal in order to obtain the total relaxation time τ for the conduction electrons? To give the proper answer — and it is the aim of the present paper — we will refrain from any geometrical intricacies typical for common "metallurgical" polycrystals. Instead we shall first consider a bicrystal and afterwards a superlattice equivalent to it. We define the superlattice as a "homosubstructure": our superlattice arises by inserting equidistant, exactly planar, interfaces into some single-crystalline metallic matrix.

In Section II, we present a general discussion of how the solid-state physicists usually understand the notion "Matthiessen's rule". We suggest that the very simple formula for the electrical conductivity offered by the formal application of Matthiessen's rule has to be subject to some serious criticism. For this purpose, we scrutinize the problem in Sections III—V within the framework of the consistent quasi-classical transport theory. We prove the statement conveyed by the title of this paper. (Sometimes the breach may be neglected but many times not.) Section VI is reserved for conclusions.

II. GENERAL FORMULATION OF THE PROBLEM

Let us first consider a single-crystalline metallic plate of length L_x , width L_y and thickness a at zero temperature. We write $A = L_x L_y$, $\Omega = aA$. We assume that $L_x \gg a$, $L_y \gg a$ and that the surfaces of the plate, located at $z = \pm \frac{1}{2} a$, are perfectly smooth. The conduction electrons are taken as non-interacting particles with some scalar (effective) mass $m > 0$ and with density n . The Fermi energy E_F and Fermi velocity v_F are given by the well-known expressions:

$$E_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}, \quad v_F = \frac{\hbar}{m} (3\pi^2 n)^{1/3}.$$

Moreover, we assume that point scatterers of two types are present inside the plate; let their average numbers per unit surface area be N_1 , N_2 ; for the corresponding average bulk densities we introduce the denotation $n_a = N_a/a$; then $AN_a = \Omega n_a$, $a = 1, 2$.

If the position $r_i^{(j)}$, $r_j^{(i)}$ ($i = 1, 2, \dots, AN_i$; $j = 1, 2, \dots, AN_2$) of the scatterers are distributed at random in the bulk, we may respectively use two relaxation times, τ_1 and τ_2 , to characterize the scattering of the electrons on the defects. (The relaxation times may be taken with the constant electron energy $E = E_F$.) The value τ_1 (value τ_2) equals the relaxation time when defects of type 2 (type 1) are absent. If the defects of both types are mixed together in a non-correlated way, the total relaxation time τ is determined by the formula

$$\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} \quad (1)$$

For the electron mobility $\mu = e\tau/m$, we might then write the relation

$$\frac{1}{\mu} = \frac{1}{\mu_1} + \frac{1}{\mu_2} \quad (2)$$

where $\mu_a = e\tau_a/m$ ($a = 1, 2$). (We shall take $e > 0$, the elementary charge.) Relations (1) and (2) represent what is called Matthiessen's rule. In the case of metals, Matthiessen's rule may directly concern the conductivities $\sigma_{(a)}$:

$$\frac{1}{\sigma} = \frac{1}{\sigma_1} + \frac{1}{\sigma_2} \quad (3)$$

as $\sigma_{(a)} = e^2 n \tau_{(a)} / m$.

The theoretical derivation of relation (1) is based on the formula

$$\frac{1}{\tau} = \sum_{\mathbf{k}} W(\mathbf{k}, \mathbf{k}') (1 - \cos \vartheta), \quad \mathbf{k} = |\mathbf{k}| = |\mathbf{k}'|, \quad \cos \vartheta = \frac{\mathbf{k} \cdot \mathbf{k}'}{k^2} \quad (4)$$

(The sum runs over the first Brillouin zone and $W(\mathbf{k}, \mathbf{k}') \equiv W(\mathbf{k}', \mathbf{k})$ means the probability for the transition $|\mathbf{k}\rangle \rightarrow |\mathbf{k}'\rangle$ per unit time. We use the denotation $|\mathbf{k}\rangle = (1/\sqrt{\Omega}) \exp(i\mathbf{k} \cdot \mathbf{r})$; the reciprocal lattice vectors \mathbf{k} are taken discrete.) The transition probability $W(\mathbf{k}, \mathbf{k}')$ (for the elastic scattering) is given by the "Golden Rule":

$$W(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2 \delta(E(\mathbf{k}') - E(\mathbf{k})). \quad (5)$$

($E(\mathbf{k}) = \hbar^2 k^2 / (2m)$). When substituting the potential energy

$$V(\mathbf{r}) = \sum_{i=1}^{\Omega n_1} v_1(\mathbf{r} - \mathbf{r}_i^{(1)}) + \sum_{j=1}^{\Omega n_2} v_2(\mathbf{r} - \mathbf{r}_j^{(2)}) \quad (6)$$

into formula (5) and taking into account only short-range potentials $v_1(\mathbf{r} - \mathbf{r}_i^{(1)})$, $v_2(\mathbf{r} - \mathbf{r}_j^{(2)})$ of the scatterers (so that we may neglect any overlap between them), we obtain the formula

$$W(\mathbf{k}, \mathbf{k}') = \Omega [n_1 w_1(\mathbf{k}, \mathbf{k}') + n_2 w_2(\mathbf{k}, \mathbf{k}')], \quad (7)$$

where

$$w_a(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | v_a | \mathbf{k} \rangle|^2 \delta(E(\mathbf{k}') - E(\mathbf{k})). \quad (8)$$

Thus, by choosing the potentials $v_a(\mathbf{r})$ central symmetric we obtain, after stating that

$$\frac{1}{\tau_a} = \Omega n_a \sum_{\mathbf{k}} w_a(\mathbf{k}, \mathbf{k}') (1 - \cos \vartheta), \quad (9)$$

relation (1).

This proof has involved one important prerequisite: the Poissonian bulk randomness of the points $\mathbf{r}_i^{(1)}$, $\mathbf{r}_j^{(2)}$. (Actually, we have utilized its consequence: the randomness of the phases in the matrix elements $\langle \mathbf{k}' | v_a | \mathbf{k} \rangle$ owing to which many terms cancelled out after we had put expression (6) into formula (5).) Nevertheless, the dissemination of defects in real crystals may indeed be correlated: the defects are apt to form clusters. We argue that essentially the very clustering of the defects in metal can bring about some remarkable breach of the Matthiessen rule. To exemplify this statement, we shall consider all defects uniformly around (in the bulk of the plate). Even with this partitioning, we retain the Poissonian distributions for all the defects: we realize both the Poissonian bulk randomness for the defects of type 1 and simultaneously some independent Poissonian surface randomness for the defects of type 2. Then we shall label the quantities related to the defects of type 1 by the subscript b (indicating "bulk") and the quantities related to the defects of type 2 by the subscript p (indicating "plane").

In accordance with the above, only two relaxation times are considered: τ_b and τ_p — the first being the true relaxation time due to the bulk defects and the second representing an effective relaxation time which corresponds to some fictitious bulk density $n_p = N_p/a$. With the values $\tau_1 \equiv \tau_b$ and $\tau_2 \equiv \tau_p$, we can then define, according to formula (3), the effective conductivity

$$\sigma_M = \left(\frac{1}{\sigma_b} + \frac{1}{\sigma_p} \right)^{-1} = \sigma_b \left(1 + \frac{\tau_b}{\tau_p} \right)^{-1} \quad (10)$$

Obviously, if we take $a \rightarrow \infty$, keeping N_p constant, we obtain $\sigma \rightarrow \sigma_b$.

We call the central plane $z = 0$ an interface, although we do not consider two differently oriented lattices in contact but one single crystal with specially distributed defects; despite this, we call our sample a bicrystal. The very presence of the interface makes clear two attributes of the electrical conductivity σ which otherwise would be either absent or hidden. First, the conductivity depends on the direction of the driving electric field \mathbf{E} . To avoid complications, we shall calculate the longitudinal conductivity when $\mathbf{E} \equiv (E_x, 0, 0)$. Secondly, the conductivity σ is a non-local quantity. Its non-locality may become signifi-

cant if one considers the thicknesses a less than, or comparable to, the relaxation length

$$l_b = v_F \tau_b. \quad (11)$$

The internal electrical field E_x is taken as independent of the coordinates x and y (because of the statistical uniformity of our problem in the directions x, y). The Maxwell equation $\text{rot } \mathbf{E} = 0$ implies that $\partial E_x / \partial z = 0$, hence we may take $E_x = \text{const}$. On the other hand, the electrical current density j_x may depend on z . We define therefore the conductivity σ by the integral formula

$$\sigma E_x = -\frac{1}{a} \int_{-\frac{1}{2}a}^{\frac{1}{2}a} dz j_x(z). \quad (12)$$

As we take the thickness a comparable with the value l_b , our problem turns out to be a topic of the theory of the so-called classical size effects [1—6]. In calculating the conductivity σ we could well take advantage of our previous experience with calculations of longitudinal transport coefficients of our previous films [7, 8], see also [9, 10]). But there are two aspects in which our present problem differs from (and is, we may say, simpler than) the former. First, now we do not consider a heterojunction and this implies that there is no refraction of the conduction electrons on the plane $z = 0$; besides, we may even neglect their reflection on this plane (see our discussion below, related to the quantity ϵ , formula (29)). Secondly, now our stochastic definition of the interface does not involve any concept of roughness.

It is excusable (and usual) to model $v_a(r)$ by simple functions. The simplest reasonable choice are the pseudopotentials

$$v_a(r) = U_a \delta(r) \quad (13)$$

with constant real values U_a . Then formula (8) yields the perfectly isotropic scattering:

$$w_a(k, \mathbf{k}) = \frac{2\pi U_a^2}{\hbar \Omega^2} \delta(E(\mathbf{k}) - E(\mathbf{k})) = \frac{2\pi m U_a^2}{\hbar^3 \Omega^2 k} \delta(k' - k) \quad (14)$$

($k = |\mathbf{k}|$). After inserting expression (14) into formula (9) and taking into account the customary replacement

$$\sum_{\mathbf{k}} \rightarrow \frac{\Omega}{(2\pi)^3} \int d^3 k',$$

we obtain the result

$$\frac{1}{\tau_a} = \gamma_a n_a, \quad (15)$$

$$\gamma_a = \frac{m U_a^2}{\pi \hbar^3} k \quad (16)$$

(cf., e.g., [6]). (The term with $\cos \vartheta$ has vanished.) As we are dealing with the conduction electrons in a metal at $T = 0$, we may take

$$k \rightarrow k_F = (3\pi^2 n)^{1/3}.$$

If this case, if the defects of both types were uniformly mixed in the bulk with the densities n_b and n_p , Matthiessen's rule would give the formula

$$\frac{1}{\tau} = \frac{m(3\pi^2 n)^{1/3}}{\pi \hbar^3} (U_b^2 n_b + U_p^2 n_p) = \gamma_b n_b + \gamma_p n_p. \quad (17)$$

So, for the corresponding conductivity $\sigma_M = e^2 n \tau / m$, we could obtain the simple expression

$$\sigma_M = \sigma_b \left(1 + \frac{\gamma_p N_p}{\alpha \gamma_b n_b} \right)^{-1}. \quad (18)$$

Thus, we are to calculate the longitudinal electrical conductivity σ of a metallic single-crystalline plate of thickness a taking the potential energy of the conduction electrons in the form

$$V(r) = U_b \sum_{i=1}^{2n_b} \delta(r - r_b^{(i)}) + U_p \delta(z) \sum_{j=1}^{2n_p} \delta(\varrho - \varrho_p^{(j)}), \quad -\frac{1}{2}a < z < \frac{1}{2}a,$$

where the points $r_b^{(i)}$ and $\varrho_p^{(j)}$ are distributed randomly in the bulk and on the plane $z = 0$, respectively, in the Poissonian way. (We use both three-dimensional and two-dimensional radiusvectors: $\mathbf{r} \equiv (x, y, z)$, $\varrho \equiv (x, y)$.) Secondly, we are to ascertain to which extent the value σ differs from the value σ_M given by formula (18) (where γ_b, γ_p are related to U_b, U_p by formula (16)).

III. KINETIC EQUATION AND BOUNDARY CONDITIONS OF THE PROBLEM

We write the distribution function of the conduction electrons in the form

$$f(z, \mathbf{k}) = f_0(E) + g(z, \mathbf{k}), \quad (19)$$

where $f_0(E)$ is the equilibrium (Fermi-Dirac) function. (Note that

$f_0(E) = \mathcal{Q}(E_F - E)$ for $T = 0$). We assume that electrical field E_x is weak. Then we may use the "linearized" Boltzmann kinetic equation

$$v_z \frac{\partial g}{\partial z} + \frac{g}{\tau_b} = e E_x v_x \frac{\partial f_0}{\partial E}, \quad (20)$$

where $v = \hbar k/m$. ($-e < 0$ is the charge of the electron.) The relaxation time τ_b is given by formula (15) ($\alpha = b$, $k = k_F$).

Before formulating the boundary conditions for the solution g of equation (20), we write

$$g = \begin{cases} g_{\beta}^{\geq} & \text{if } v_z > 0 \\ g_{\beta}^{\leq} & \text{if } v_z < 0 \end{cases} \quad \beta = \begin{cases} 1 & \text{if } -\frac{1}{2}a < z < 0 \\ 2 & \text{if } 0 < z < \frac{1}{2}a \end{cases} \quad (21)$$

We use this denotation for f as well: f_{β}^{\geq} , f_{β}^{\leq} . For f_0 , however, the subscripts $\beta = 1, 2$ and the superscripts $>$, $<$ are irrelevant. Let χ be the angle between the vector \mathbf{k} and the z -axis. We take first $k_z > 0$ (i.e. $0 < \chi < \frac{1}{2}\pi$). We consider some unit area on the plane $z = 0$ with N_p defects. For every second, we record (discrete) wavevector \mathbf{k} . A fraction of them will pass the plane $z = 0$ without striking a defect; the probability of such an event will be denoted as Q . We say that Q is the free-transit probability of the impacting electrons. Then, if $Q \neq 0$, $1 - Q$ is the probability that the electrons undergo the diffuse (i.e. isotropic) scattering on the interface $z = 0$. (Pay attention, however, to our later discussion of the possibility that the electrons may also be specularly reflected from the plane $z = 0$ if $Q = 0$.) As the electrons are fermions, we must respect the Pauli exclusion principle. (The significance of the exclusion principle for the coefficients occurring in boundary conditions relating interfaces between grains was first recognized by Grendel [11].)

When considering transitions from $|\mathbf{k}\rangle$ to $|\mathbf{k}'\rangle$ (with some given spin) we must take into account on the one hand the probability $f(\mathbf{k})$ for the state $|\mathbf{k}\rangle$ and on the other the probabilities $1 - f(\mathbf{k}')$ for the states $|\mathbf{k}'\rangle$ — otherwise the transitions are forbidden. Thus we can write the balance identity

$$v \cos \chi f_1^{\geq}(0, \mathbf{k}) = \Omega N_p \sum_{\mathbf{k} > 0} w_p(\mathbf{k}, \mathbf{k}') f_1^{\geq}(0, \mathbf{k}') [1 - f_2^{\geq}(0, \mathbf{k}')] + \Omega N_p \sum_{\mathbf{k} < 0} w_p(\mathbf{k}, \mathbf{k}') f_1^{\geq}(0, \mathbf{k}') [1 - f_1^{\leq}(0, \mathbf{k}')] + Q v \cos \chi f_1^{\geq}(0, \mathbf{k}), \quad (22)$$

from which we get at the relation

$$1 - Q = \frac{\Omega N_p}{v \cos \chi} \left\{ \sum_{\mathbf{k} > 0} w_p(\mathbf{k}, \mathbf{k}') [1 - f_2^{\geq}(0, \mathbf{k}')] + \sum_{\mathbf{k} < 0} w_p(\mathbf{k}, \mathbf{k}') [1 - f_1^{\leq}(0, \mathbf{k}')] \right\}. \quad (23)$$

The sums can be simplified. We make substitution (19) and notice that the function $g(z, \mathbf{k})$ changes its sign if k_x is replaced by $-k_x$ but remains unchanged if k_y is replaced by $-k_y$. (Such statements follow directly from equation (20).) Moreover, $w_p(\mathbf{k}, \mathbf{k}') \equiv w_p(\mathbf{k}, -\mathbf{k}')$ (cf. formula (14)). With respect to these relations, it is easy to see that

$$\begin{aligned} & \sum_{\mathbf{k} > 0} w_p(\mathbf{k}, \mathbf{k}') g_2^{\geq}(0, \mathbf{k}') + \sum_{\mathbf{k} < 0} w_p(\mathbf{k}, \mathbf{k}') g_1^{\leq}(0, \mathbf{k}') = \\ & = \sum_{\mathbf{k} > 0} w_p(\mathbf{k}, \mathbf{k}') [g_2^{\geq}(0, \mathbf{k}') + g_1^{\leq}(0, -\mathbf{k}')] = \\ & = \sum_{\mathbf{k} > 0} w_p(\mathbf{k}, \mathbf{k}') [g_1^{\leq}(0, k'_x, k'_y, -k'_z) + g_1^{\leq}(0, -k'_x, k'_y, -k'_z)] = 0. \end{aligned}$$

The last equality proves that we may simply replace the functions $f_2^{\geq}(0, \mathbf{k}')$, $f_1^{\leq}(0, \mathbf{k}')$ in formula (23) by the equilibrium function $f_0(E(\mathbf{k}'))$. Owing to the delta function in the formula for w_p , we may put the factor $1 - f_0(E)$ in front of the sum. With w_p given by formula (14), we arrive at the result

$$1 - Q = \frac{\gamma_p N_p [1 - f_0(E)]}{v |\cos \chi|} = \frac{m^2 U^2 N_p [1 - f_0(E)]}{\pi \hbar^4 |\cos \chi|}. \quad (24)$$

(We have utilized that $\Omega \Sigma w_p(\mathbf{k}, \mathbf{k}') = \gamma_p$, cf. formula (15).) (Of course, the formula for Q has equally to be valid if $k_z < 0$; that is why we have written $|\cos \chi|$.)

The asymmetry in the energy dependence of Q (near the Fermi energies E_F) due to the factor $1 - f_0(E)$ may be felt like a formal disadvantage. We can remove it, since we may interpret the states $|\mathbf{k}\rangle$ as the "Landau electrons" if $E > E_F$ and as the "Landau holes" if $E < E_F$. (Taking the energies E on the "electron scale", we must measure the "hole energies" downwards: $E_h = E_F - E$.) In this way we obtain the probability

$$Q_F = \begin{cases} Q & \text{if } E > E_F \\ Q^{(h)} & \text{if } E < E_F \end{cases} \quad (25)$$

In our particular case when take $T = 0$, Q_F is entirely energy-independent.

The right-hand side of the formula for $1 - Q$ given above has always to be less than unity. If this requirement is not satisfied, we are forced to define Q equal to zero. Thus, after introducing the dimensionless parameter

$$\eta = \frac{\chi_p N_p}{v} = \frac{m^2 U_p^2 N_p}{\pi k^4}, \quad (26)$$

we can write the full angular dependence of Q_F in the form:

i) if $0 \leq \eta \leq 1$, then

$$Q_F(\chi) = 1 - \frac{\eta}{|\cos \chi|} \quad \text{for } 0 \leq \chi < \chi_m \text{ and for } \pi - \chi_m < \chi \leq \pi,$$

$$Q_F(\chi) = 0 \quad \text{for } \chi_m < \chi < \pi - \chi_m, \quad (27.1)$$

where

$$\chi_m = \arccos \eta; \quad (27.2)$$

ii) if $1 < \eta$, then

$$Q_F(\chi) = 0 \quad \text{for all angles } \chi. \quad (27.4)$$

We can explain relations (27) as follows. The "Golden Rule" used in our calculation of the probability $W_p(\mathbf{k}, \mathbf{K})$ (formula (5)) corresponds to the first case) for $\eta \ll 1$. If $\eta \rightarrow 1$, and particularly if $\eta > 1$, the "Golden Rule" ceases to apply: a higher order perturbation theory should be employed. Nevertheless, we regard the function $Q_F(\chi)$ defined by formula (27) as a simplification whose departure from reality is not serious.

If the interface scatterers are weak (i.e. if $U_p \rightarrow 0$) and/or if their density is small (i.e. if $N_p \rightarrow 0$) so that $\eta \ll 1$, we obtain the approximate value

$$\frac{1}{2} \pi - \chi_m = \frac{m^2 U_p^2 N_p}{\pi k^4} = \eta \ll 1. \quad (28)$$

The width $2 \left(\frac{1}{2} \pi - \chi_m \right)$ of the interval for which $Q_F = 0$ (according to formula (27.2)) is then small; but for $\eta \geq 1$, this interval spans all angles χ (from 0 to π).

If $Q_F = 0$, then we must admit that there exists a narrow interval I_ε of the angles of incidence χ , $I_\varepsilon \equiv \left(\frac{1}{2} \pi - \varepsilon, \frac{1}{2} \pi + \varepsilon \right)$, with the half-width

$$\varepsilon = 2 \frac{N_p^{1/2}}{n^{1/3}}, \quad (29)$$

in which the specular reflection of the electrons from the interface might take place. We can explain this possibility by returning to formula (5) and inserting

$$Y(\mathbf{r}) \approx U_p \delta(z) \sum_{j=1}^{N_p} \delta(\theta - \theta_p^{(j)})$$

into it. The state $|\mathbf{k}\rangle$ represents a coherent de Broglie plane wave. Let \mathbf{k} be parallel with the plane $y = 0$. The average distance between the points $\theta_p^{(j)}$ is $\sim N_p^{-1/2}$. Take two points, $\theta_p^{(1)}$ and $\theta_p^{(2)}$, such that

$$|x_p^{(1)} - x_p^{(2)}| \approx N_p^{-1/2}, \quad y_p^{(1)} = y_p^{(2)} = 0.$$

The front of the wave $|\mathbf{k}\rangle$ reaches the point $\theta_p^{(2)}$ with the phase delay

$$\overline{\Delta\varphi} \approx k_F N_p^{-1/2} |\cos \chi|$$

against the point $\theta_p^{(1)}$. If $\overline{\Delta\varphi} > 2\pi$, we may take

$$W_p(\mathbf{k}, \mathbf{K}) \doteq AN_p W_p(\mathbf{k}, \mathbf{k}'),$$

i.e. we may accept the averaging procedure with respect to the random positions $\theta_p^{(j)}$ that was used in the reduction of formula (5) to formula (7) as well-established. But then, in the case when $\Delta\varphi \lesssim 2\pi$, i.e. when

$$\cos \chi \lesssim 2 \frac{N_p^{1/2}}{n^{1/3}}$$

(here we have omitted the numerical factor $\pi/(3\pi^2)^{1/3}$ that is approximately equal to unity), the averaging procedure, contrary to the former case, will not entirely suppress the delta-function term $\sim \delta(k_x' - k_x) \delta(k_y' - k_y) \delta(k_z' + k_z)$ in the probability $W_p(\mathbf{k}, \mathbf{K})$; and just such a term corresponds to the specular reflection.

From now on, we assume that the quantity ε is sufficiently small so that the phenomenon of the specular reflection may be neglected.

We write our boundary conditions in the form of two linear relations coupling the values of $g_\beta^>$ and $g_\beta^<$ on the upper and lower side of the plane $z = 0$:

$$g_2^>(0, \mathbf{k}) = Q_F g_1^>(0, \mathbf{k}), \quad k_z > 0, \quad (30.1)$$

$$g_1^<(0, \mathbf{k}) = Q_F g_2^<(0, \mathbf{k}), \quad k_z < 0, \quad (30.2)$$

Conditions (30) represent a special case of more general conditions originally formulated for heterojunctions [7]; mathematically taken, the present specification of the conditions consists in the zero values of the specularly parameters for the plane $z = 0$: $P_{12} = P_{21} = 0$ (cf. also [1], §91).

A comment is required here. We would like to emphasize that relation (19) is not a mere formal mathematical substitution: we may interpret it as a "decomposition" as well, with which the "Landau electrons" and the "Landau holes" (excited by the electrical field E_x) can be detached (in a "Gedankenexperiment", naturally) from the sea of the equilibrium electrons. This is what a priori explains, we believe, why conditions (30) — where we have taken into account the above probability meaning of the quantity Q_r — have to concern just the functions g_{β}^{\rightarrow} , g_{β}^{\leftarrow} , and not the primary distribution functions f_{β}^{\rightarrow} , f_{β}^{\leftarrow} .

It remains to formulate boundary conditions for the functions g_{β}^{\rightarrow} , g_{β}^{\leftarrow} on the free surfaces $z = \pm \frac{1}{2}a$. This is not a point at which it would be worth while to complicate our calculations in the present paper. We choose, therefore, the conditions

$$\begin{aligned} g_1^{\rightarrow} \left(-\frac{1}{2}a, \mathbf{k} \right) &= g_1^{\leftarrow} \left(-\frac{1}{2}a, k_x, k_y, -k_z \right), & k_z > 0, \\ g_2^{\leftarrow} \left(\frac{1}{2}a, \mathbf{k} \right) &= g_2^{\rightarrow} \left(\frac{1}{2}a, k_x, k_y, -k_z \right), & k_z < 0, \end{aligned} \quad (31.1)$$

in agreement with the assumption that the surfaces $z = \pm \frac{1}{2}a$ are perfectly smooth. We can easily invent a situation where the identities (31) are quite obvious: if we consider, instead of the plate of thickness a (Fig. 1a), a macroscopic ("infinite") single-crystalline metallic piece and instead of one plane dotted with N_{β} defects per unit area a large set of such planes (all with statistically identical densities of the defects) located equidistantly in the bulk (Fig. 1b). In the latter case, we have got a periodic problem whose elementary cell is defined by the interval $-\frac{1}{2}a < z < \frac{1}{2}a$. Conditions (31) then follow directly from the symmetry of the problem.

IV. SOLUTION OF THE PROBLEM

The general solution of equation (20) has the form

$$g(z, k) = eE_x \tau_{\beta} v_x \frac{\partial f_0}{\partial E} \left[1 + C(k) \exp \left(-\frac{z}{\tau_{\beta} v_x} \right) \right], \quad (32)$$

where $C(\mathbf{k})$ is an arbitrary function of \mathbf{k} not depending on z ($\partial C/\partial z = 0$). For g_{β}^{\rightarrow} , g_{β}^{\leftarrow} , we denote $C(\mathbf{k})$ as $C_{\beta}^{\rightarrow}(\mathbf{k})$, $C_{\beta}^{\leftarrow}(\mathbf{k})$, respectively. We assume that $k_z > 0$,

$k_z = -k_z < 0$ and $k_x' = k_x$, $k_y' = k_y$. (We shall show, however, that $C_{\beta}^{\rightarrow}(\mathbf{k})$, $C_{\beta}^{\leftarrow}(\mathbf{k})$ do not depend on k_x , k_y at all.) Conditions (30), (31) give us four variables $C_{\beta}^{\rightarrow}(\mathbf{k})$, $C_{\beta}^{\leftarrow}(\mathbf{k})$ ($\beta = 1, 2$). Let us consider a "Landau electron" flying through some point \mathbf{r} with the velocity $\mathbf{v} = \hbar \mathbf{k}/m$; we can construct — neglecting any scattering except the reflections on the surfaces $z = \pm \frac{1}{2}a$ — the complete

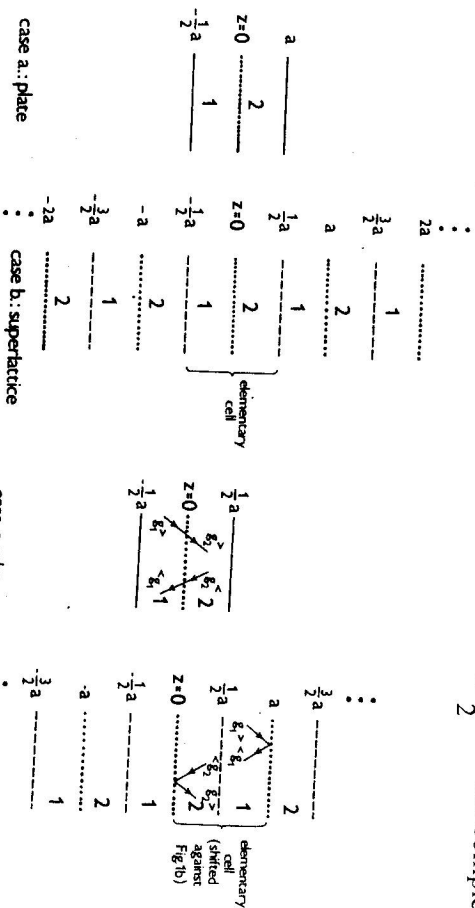


Fig. 1. a. A metallic plate of thickness a with perfectly smooth surfaces (full lines) with one interface (dotted line) in the middle.

b. A metallic superlattice formed by the periodic arrangement of the interfaces (dotted lines) with the lattice constant a . The space between the neighbouring dashed lines corresponds to one elementary cell.

deterministic trajectory. It is a broken straight line (if E_x is approximated as zero) along which the values k_x , k_y and $|k_z|$ are conserved. We expect, therefore, that C_{β}^{\rightarrow} , C_{β}^{\leftarrow} are functions of $|k_z|$; even in order to avoid formal errors, we prefer to write v_z in formula (32) by means of the absolute value $|v_z|$ (i.e. $v_z = |v_z|$ if $v_z > 0$ but $v_z = -|v_z|$ if $v_z < 0$). Then we put the functions g_{β}^{\rightarrow} , g_{β}^{\leftarrow} given by formula (32) into the relations (30), (31). After solving the equations implied by conditions (30), (31), we obtain the values:

$$\begin{aligned} C_1^{\leftarrow} &= -(1-Q) \left[1 - Q \exp \left(-\frac{a}{\tau_{\beta} |v_z|} \right) \right]^{-1} \\ &= -(1-Q) \sum_{s=0}^{\infty} Q^s \exp \left(-\frac{as}{\tau_{\beta} |v_z|} \right), \end{aligned} \quad (33.1)$$

$$C_2^> = C_1^<$$

$$C_1^> = C_1^< \exp\left(-\frac{a}{\tau_b |v_z|}\right), \quad (33.2)$$

$$C_2^< = C_1^>. \quad (34.1)$$

With these values the functions $g_{\beta}^>(z, \mathbf{k})$, $g_{\beta}^<(z, \mathbf{k})$ are determined uniquely. We can then calculate the local current density $j_x(z)$ and, eventually, the averaged current density \bar{j}_x (cf. formula (12)).

We prefer, however, an alternative way of calculating \bar{j}_x . Compare Figs. 1a and 1b. It is clear that the value \bar{j}_x , when calculated for the periodic problem (Fig. 1b), must be conserved if the centre of the elementary cell is arbitrarily shifted. Fig. 2b shows the situation when the shift is $\frac{1}{2}a$. Let $g_{\beta}^>$, $g_{\beta}^<$ be the values of the corresponding functions g at the interface $z = 0$ drawn in Fig. 1a. We symbolize them by the four arrows in Fig. 2a. The two pairs of the arrows symmetry of the problem, we can conclude that $g_1^> = g_2^<$ and $g_1^< = g_2^>$. Therefore, if we take the elementary cell as in Fig. 2b, we may equivalently consider "reflections" on the boundaries of the cell instead of the transitions suggested in Fig. 2a; the probability of the specular transitions (i.e. the reflections) indicated by the broken lines with the arrows in Fig. 2b is, of course, equal to Q_F , since $g_1^< = Q_F g_1^>$ and $g_2^> = Q_F g_2^<$.

But if the value \bar{j}_x (or the longitudinal conductivity σ) were calculated for a metallic film of thickness a (Fig. 3), with surfaces corresponding to the dotted lines of Fig. 2b and with the Fuchs specularly parameter [2] equal to Q_F , the result should ultimately be the same as for the periodical problem (Figs. 1b, 2b), and then also for the original problem of the plate with the central interface (Figs. 1a, 1b).

Having shown that our double-layer problem may be solved without any loss in accuracy as the equivalent single-film problem, we may omit the subscript β . (Therefore, g in Fig. 3 is denoted as $g^>$ if $k_z > 0$ and as $g^<$ if $k_z < 0$; clearly, if the elementary cell of the periodical problem is chosen according to Fig. 2b, its

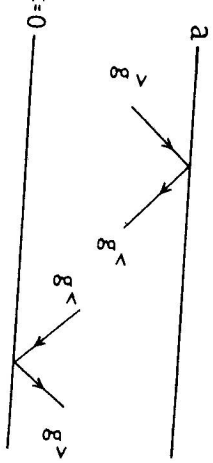


Fig. 3. The equivalent Fuchs problem (for a single thin film of thickness a).

central dashed line may be deleted.) Thus, now we have only two boundary conditions for $g^>(z, \mathbf{k})$, $g^<(z, \mathbf{k})$:

$$g^>(0, \mathbf{k}) = Q_F g^<(0, \mathbf{k}'), \quad (35)$$

$$g^<(a, \mathbf{k}') = Q_F g^>(a, \mathbf{k}), \quad (36)$$

where $\mathbf{k}' = (k_x, k_y, -k_z)$. They result in the values:

$$C^> = -(1 - Q_F) \left[1 - Q_F \exp\left(\frac{as}{\tau_b |v_z|}\right) \right]^{-1}, \quad (37)$$

$$C^< = \exp\left(-\frac{a}{\tau_b |v_z|}\right) C^>. \quad (38)$$

We write

$$g^>(z, \mathbf{k}) = g_b(\mathbf{k}) \left[1 + C^> \exp\left(-\frac{z}{\tau_b |v_z|}\right) \right], \quad (39)$$

$$g^<(z, \mathbf{k}) = g_b(\mathbf{k}) \left[1 + C^> \exp\left(-\frac{a-z}{\tau_b |v_z|}\right) \right], \quad (40)$$

where

$$g_b(\mathbf{k}) = g_b(\mathbf{k}') = e E_x \tau_b v_x \frac{\partial f_0}{\partial E}. \quad (41)$$

As $g^>(z, \mathbf{k}) = g^<(a-z, \mathbf{k}')$, both functions $g^>(z, \mathbf{k})$, $g^<(z, \mathbf{k}')$ contribute equally to the value \bar{j}_x . Hence we may express \bar{j}_x as the integral

$$\begin{aligned} \bar{j}_x &= -\frac{e}{4\pi^3 a} \int_0^a dz \int d^3 k v_x g(z, \mathbf{k}) = \\ &= -\frac{e}{2\pi^3 a} \int_0^a dz \int_{-\infty}^{\infty} dk_x dk_y v_x \int_0^{\infty} dk_z g^>(z, \mathbf{k}). \end{aligned}$$

The integration with respect to z is easy and gives the result:

$$\bar{j}_x = -\frac{e}{2\pi^3} \iint_{-\infty}^{\infty} dk_x dk_y v_x \int_0^{\infty} dk_z g_b \left\{ 1 + C^> \frac{\tau_b v_z}{a} \left[1 - \exp\left(-\frac{a}{\tau_b v_z}\right) \right] \right\}. \quad (42)$$

This formula is essentially correct even in the case when $f_0(E)$ does not relate strongly degenerate fermions (for $T > 0$); we must only assume that the energy bands of the electrons are flat.

It is convenient to introduce the spherical angles:

$$k_x = k \cos \varphi \sin \chi, \quad k_y = k \sin \varphi \sin \chi, \quad k_z = k \cos \chi. \quad (43)$$

If we take into account that $-\partial f_0/\partial E = \delta(E - E_F)$, we may replace v_x by $v_F \cos \chi$ and v_y by $v_F \cos \varphi \sin \chi$. We define the dimensionless quantity

$$K = \frac{a}{l_b} \quad (44)$$

(cf. definition (11) and assumption (13)). For the longitudinal electrical conductivity σ (given by the relation $\bar{j}_x = \sigma E_x$, cf. definition (12)), we obtain the result

$$\sigma = \sigma_0 \left\{ 1 + \frac{3}{2K} \int_0^{\frac{1}{2}\pi} d\chi \sin^3 \chi \cos \chi C_F^2(\eta, \chi) \left[1 - \exp\left(-\frac{K}{\cos \chi}\right) \right] \right\}, \quad (45)$$

where

$$\sigma_0 = \frac{e^2 \tau_0 n}{m} = \frac{e^2 l_b n}{m v_F}. \quad (46)$$

We have used the denotation $C_F^2(\eta, \chi)$ for $C^2(\chi)$ if $E = E_F$:

$$C_F^2(\eta, \chi) = -|1 - Q_F(\eta, \chi)| |1 - Q_F(\eta, \chi) \exp\left(-\frac{K}{\cos \chi}\right)|^{-1};$$

here $Q_F(\eta, \chi) \equiv Q_F(x)$ (given by formulae (27)).

Formula (45) shows that the ratio σ/σ_0 depends on two positive parameters: η and K . Note that if $\eta = 0$, then $Q_F = 1$ (according to formulae (27)) and hence $\sigma = \sigma_0$. On the other hand, if $\eta \geq 1$, then $Q_F = 0$ so that $C_F^2 = -1$; this is the special case for which the conductivity σ is equal to the Fuchs conductivity of a single metallic film of thickness $a = Kl_b$ with the total diffuse (surface) scattering of the conduction electrons:

$$\sigma_{\text{Fuchs}} = \sigma_0 \left\{ 1 - \frac{3}{2K} \int_0^{\frac{1}{2}\pi} d\chi \sin^3 \chi \cos \chi \left[1 - \exp\left(-\frac{K}{\cos \chi}\right) \right] \right\}, \quad (48)$$

$\sigma = \sigma_{\text{Fuchs}}$ if $\eta \geq 1$.

The quantity $\eta = \gamma_b N_p / v_F$ characterizes some cumulative strength of the

scattering of conduction electrons on the defects located on the interface $z = 0$. In the special case when $0 \leq \eta \leq 1$, we can give η a probabilistic meaning: it is the probability of the diffuse scattering for the perpendicular incidence (of a "Landau electron" or a "Landau hole") upon the interface, i.e.

$$\eta = 1 - Q_F(0) \quad (50)$$

according to formula (27.1)). (Of course, formula (50) does not concern the case when $\eta > 1$, since then $Q_F(0) = 0$.)

V. SPECIAL RESULTS

In order to obtain the values

$$\frac{\sigma}{\sigma_0} = F(\eta, K) \quad (51)$$

we must apply the integration required by formula (45). Our aim is to compare the values $F(\eta, K)$ with the "Mathiessen-type values"

$$\frac{\sigma_M}{\sigma_0} = F_M(\eta, K) = \frac{1}{1 + \eta/K}. \quad (52)$$

Notice that η/K is the ratio of the relaxation lengths l_b, l_p :

$$\frac{\eta}{K} = \frac{l_b}{l_p}. \quad (53)$$

(Recall formula (18) and the definitions $l_b = v_F/(\gamma_b n_b)$, $l_p = a v_F/(\gamma_p N_p)$.)

When fixing K for a moment, we can conclude that $F(\eta, K)$ behaves analytically as a function of the variable η near the point $\eta = 0$ (i.e. this point is not a pole); obviously, the analyticity proceeds along the whole positive semi-axis $\eta > 0$. For $\eta = 0$, we obtain the value

$$F(0, K) = 1 \quad (54)$$

for all (reduced) thicknesses $K = a/l_b > 0$. (In other words, if $\eta = 0$, then $\sigma = \sigma_0$; however, remember that this conclusion has resulted from our boundary conditions on the outer surfaces on the plate — conditions (31). Were there through even some slight deterioration in the reflectivity of the electrons on the outer surfaces, the values $F(0, K)$ would become less than unity.) On the other hand, when taking $F(\eta, K)$ as a function of the variable K , we can at once see that $\sigma \rightarrow \sigma_0$ if $K \rightarrow \infty$, i.e.

$$F(\eta, \infty) = 1 \quad (55)$$

for all values $\eta \geq 0$. Formula (52) implies that conditions (54), (55) are equally satisfied by Mathiessen-type function:

$$F_M(0, K) = F_M(\eta, \infty) = 1.$$

Moreover, we can prove that

$$\left. \frac{\partial F(\eta, K)}{\partial \eta} \right|_{\eta=0} = \left. \frac{\partial F_M(\eta, K)}{\partial \eta} \right|_{\eta=0} = -\frac{1}{K}. \quad (56)$$

(The proof relies on the direct differentiation of formula (45) with respect to η , with fixed K .) Hence, we may state that

$$F(\eta, K) = F_M(\eta, K) + O(\eta^2) = 1 - \frac{\eta}{K} + O(\eta^2) \quad (57)$$

in $\eta \ll K$. Thus, so far we have only proved that Matthiessen's rule holds under the condition that the density of the defects on the interface, N_p , is sufficiently low against the value an_b of the bulk defects, i.e. if

$$N_p \ll \left(\frac{\gamma b}{\gamma'}\right) an_b. \quad (58)$$

Apparently this case is not so very interesting since the relative deviation of the conductivity σ from the value σ_0 is small (given by the value η/K).

Now we will give our attention to the opposite condition, when $0 < K \ll \eta$. In this case, as it is derived by some lengthy calculations in the Appendix, the function $F(\eta, K)$ is approximated by the function $F_1(\eta, K)$,

$$F(\eta, K) = F_1(\eta, K) + O(K), \quad (59.1)$$

$$F_1(\eta, K) = -\frac{3}{4} K \ln\left(\frac{K}{\eta}\right) + \left[1 - \frac{3}{4}(\gamma - \ln \eta)\eta - \frac{1}{4}\eta^3\right] \frac{K}{\eta}, \quad (60.1)$$

or more precisely by the function $F_2(\eta, K)$,

$$F(\eta, K) = F_2(\eta, K) + O(K^2), \quad (59.2)$$

$$F_2(\eta, K) = F_1(\eta, K) - \left[1 - \left(1 - \frac{3}{2} \ln \eta\right)\eta - \frac{1}{2}\eta^3\right] \frac{K^2}{\eta^2}. \quad (60.2)$$

(In formula (60.1), γ means the Euler number — see the Appendix, formula (A.11).)

Clearly, when taking the limit $K \rightarrow +0$ (from the right), we obtain, for all positive values η , the result

$$F(\eta, +0) = 0, \quad (61)$$

$$F_M(\eta, +0) = 0$$

in full agreement with the result expected from formula (52). Notwithstanding this, here the parallel between the functions $F(\eta, K)$ and $F_M(\eta, K)$ ends: if we juxtapose, for small values of K , the derivatives $\partial F(\eta, K)/\partial K$, $\partial F_M(\eta, K)/\partial K$, we find very different values. Moreover, $\partial F/\partial K$ diverges for $K \rightarrow +0$,

$$\frac{\partial F}{\partial K} = -\frac{3}{4} \eta \ln\left(\frac{K}{\eta}\right) + 1 - \frac{3}{4}(1 + \gamma - \ln \eta)\eta - \frac{1}{4}\eta^3 + O(K), \quad (62)$$

whilst the Matthiessen-type function F_M behaves regularly:

$$\frac{\partial F_M}{\partial K} = 1 + O(K). \quad (63)$$

If neither the condition $0 < K \ll \eta$ nor the condition $0 < \eta \ll K$ is fulfilled, then any further formal adaptation of integral (45) appears to be more or less superfluous and some numerical integration is needed for obtaining the values $F(\eta, K)$. Fortunately, there exists one exception — concerning the value $\eta = 1$: in this case, we may use the Fuchs result [1—3, 12]. We write

$$F_{\text{Fuchs}}(K) = F(1, K). \quad (64)$$

Note that, according to our definition,

$$F(\eta, K) = F(1, K) \quad \text{for } \eta > 1 \quad (65)$$

as well. Using the substitution $u = 1/\cos \chi$ in formula (48) and the definition of the function $E_n(x)$ (formula (A.5) of the Appendix) we can bring $F_{\text{Fuchs}}(K)$ to the form

$$F_{\text{Fuchs}}(K) = 1 - \frac{3}{8K} (1 + e^{-K}) + \frac{3}{2K} E_3(K) + \frac{3}{8} E_4(K). \quad (66)$$

We have utilized the relation

$$E_5(K) = \frac{1}{4}[e^{-K} - K E_4(K)].$$

Values (66) can easily be computed since there are tables of the functions $E_3(K)$, $E_4(K)$ in an accessible handbook [13]. ($E_5(K)$ was not tabulated in [13].) Some results of our numerical computations are presented in two Tables.

Table I

Asymptotic functions $F_1(\eta, K)$ and $F_2(\eta, K)$ for $K \ll \eta$, with $K = 0.01$; their comparison with the Matthiessen-type function $F_M(\eta, K)$; $\tau_2 = 100 (F_2 - F_M)/F_M$.

$\eta =$	0.1	2	.3	.4	.5	.6	.7	.8	.9	1.0
F_1	.0956	.0560	.0453	.0411	.0392	.0383	.0379	.0378	.0377	.0377
F_2	.0899	.0551	.0451	.0410	.0392	.0384	.0380	.0378	.0378	.0378
F_M	.0909	.0476	.0323	.0244	.0196	.0164	.0141	.0123	.0110	.0100
$[\%]\tau_2$	-1.11	+15.72	39.68	68.23	99.96	133.96	169.572	207.32	243.66	281.37
$F =$.0904	F_2								

In Table I, the parameter K is kept constant ($K = 0.01$) and ten values of η are chosen such that $K \leq \eta$. The first two rows present the values of the asymptotic functions $F_1(\eta, K)$, $F_2(\eta, K)$ (formulae (60)). Looking at this Table, we may state that the improvement offered by the function F_2 in comparison with the function F_1 is not significant unless for a narrow interval of the values η , such that $10 < \eta/K < 30$. (For $\eta/K < 10$, the function F_2 ceases to suffice at all and higher-order approximations have to be adopted. For $\eta/K > 30$, the I presents the Matthiessen-type values $F_M(\eta, K)$. Finally, the fourth row of Table how much (per cent) the values $F_2(\eta, K)$ deviate from the values $F_M(\eta, K)$. As it is seen, the deviation

$$\frac{r}{100} = \frac{F - F_M}{F_M} + O(K^2) \quad (67)$$

becomes considerable for $\eta/K > 20$. Note that, for small values of K , we may write

$$\begin{aligned} \frac{r}{100} &= \frac{r_1}{100} + O(K) = \frac{F_1 - F_M}{F_M} + O(K), \text{ i.e.} \\ \frac{r}{100} &= -\frac{3}{4} \eta \ln\left(\frac{K}{\eta}\right) - \frac{3}{4} (\gamma - \ln \eta) \eta - \frac{1}{4} \eta^3 + O(K). \end{aligned} \quad (68)$$

If $K \rightarrow +0$, the first term, being positive, prevails over the remaining negative terms and thus the relative deviation of $F(\eta, K)$ against $F_M(\eta, K)$ is positive. (Naturally, this is not contradicted by the negative value of $r = r_2$ for $\eta = 0.1$ in Table I. Namely, in this case, the value $K = 0.01$ to which Table I relates must not be considered as sufficiently low for the confirmation of the statement yet.)

Table II demonstrates similar data, but for some fixed value η . We have chosen $\eta = 1$; then $F = F_{\text{facts}}(K)$. The values of $F_{\text{facts}}(K)$ were computed from formula (66) and independently, with equal success, from formula (48) without the use of the functions $E_n(K)$. (Integral (48) was first computed numerically with the aid of the Simpson method [14]. We did the numerical integration in order to have tested the suitability of the Czechoslovak 8-bit microcomputer PMD-85-2 for this purpose; when the integration interval $(0, \frac{1}{2}\pi)$ was divided into 100 subintervals, the computation of one value $F_{\text{facts}}(K)$ took about 45 seconds of the machine time. Secondly, we have also checked the numerical integration with the aid of another scheme: we have taken the integral

$$z(x) = \int_0^x dy(t) \text{ as the solution of the differential equation } dz/dx = y(x) \text{ with}$$

the Cauchy "initial condition", $z(0) = 0$. Then, after having defined $\Delta = \pi/$

(2N), $N = 100$, we employed the iteration scheme $z(x + \Delta) = z(x - \Delta) + 2\Delta y(x)$ for $x = \Delta, 3\Delta, 5\Delta, \dots, \frac{1}{2}\pi - \Delta$ ($z(-\Delta) = 0$); so we have obtained the resulting value $z(\frac{1}{2}\pi)$ in full concordance with the result

Table II

Comparison of the function $F_{\text{facts}}(K)$ with the Matthiessen-type function $F_M(1, K)$; their relative deviation is $r = 100(F_{\text{facts}} - F_M)/F_M$ (per cent, $\eta = 1$); for $K \leq 1$, the asymptotic functions $F_1(1, K)$, $F_2(1, K)$ are also given.

K	F_1	F_2	F_{facts}	F_M	[%] r
0.01	0.0377		0.0378	0.0099	281.5
.02	.0650		.0652	.0196	232.6
.03	.0884		.0889	.0291	205.1
.04	.109		.110	.0385	186.1
.05	.128		.129	.0476	171.1
.06	.146		.147	.0566	160.3
.07	.162		.164	.0654	150.9
.08	.177		.180	.0741	142.9
.09	.191		.195	.0826	136.1
.1	.204		.209	.0909	130.0
.2	.305	.325	.323	.167	93.8
.3	.366	.411	.406	.231	75.7
.4	.402	.482	.470	.286	64.4
.5	.418	.543	.522	.333	56.6
.6	.420	.600	.565	.375	50.7
.7	.409	.654	.602	.412	46.1
.8	.388	.708	.633	.444	42.4
.9	.356	.761	.660	.474	39.4
1.0	.317	.817	.684	.5	36.8
1.2			.723	.545	32.6
1.4			.755	.583	29.4
1.6		not defined	.780	.615	26.8
1.8			.801	.643	24.7
2.0			.819	.667	22.9
4			.906	.8	13.3
6			.938	.857	9.4
8			.953	.889	7.2
10			.962	.909	5.9
20			.981	.952	3.0
50			.992	.980	1.2
100			.996	.990	0.6

from the Simpson integration.) The comparison of the values F_1 and F_2 with the values $F_{\text{incls}}(K)$ enables us to see to which extent the first-order (F_1) and second-order (F_2) asymptotic approximations are reliable for $K < \eta$. The last column in Table II shows very convincingly the failure of Matthiessen's rule for K comparable to, and especially for K much less than, η . For $K \rightarrow +0$, the relative deviation

$$\frac{r(1, K)}{100} = \frac{F_{\text{incls}}(K)}{F_M(1, K)} - 1$$

becomes very high indeed! And it becomes still higher if η is chosen greater than unity: define

$$\frac{r(\eta, K)}{100} = \frac{F_{\text{incls}}(K)}{F_M(\eta, K)} - 1; \quad (69)$$

it is a matter of some elementary mathematics to verify that

$$\frac{r(\eta, K)}{100} = \frac{\eta + K \left[\frac{r(1, K)}{100} + 1 \right] - 1}{1 + K \left[\frac{r(1, K)}{100} + 1 \right] - 1} \quad \text{for } \eta > 1. \quad (70)$$

VI. CONCLUSIONS

A brief summarization of our results reads as follows. We have put forward a quasi-classical theory of the longitudinal electrical conductivity (at $T = 0$) of the metallic samples corresponding to Fig. 1. The samples may be realized either as a) plates (or layers) of thickness a with ideal outer surfaces, the central interface formed of some uniform random array of defects with some planar density N_p , or as b) superlattices, i.e. periodic structures where the interfaces are located equidistantly apart. The space between the surfaces and the central interface in case a., or between the interfaces in case b., is defined as a "background" with some bulk density n_b of possibly other defects. (The interface defects and the bulk defects may differ in the strengths γ_p , γ_b of their potentials.) If the interface(s) were absent, the conductivity would equal some value σ_0 proportional to the relaxation length l_b of the conduction electrons. (l_b is proportional to the bulk relaxation time τ_b of the conduction electrons. (l_b is $l_b = \tau_b v_F$, where v_F is the Fermi velocity.) Otherwise, under the assumption of the presence of the interface(s), we have shown that $\sigma = F\sigma_0 < \sigma_0$ and derived the dependence of the dimensionless factor F ($0 < F < 1$) upon two dimensionless parameters: $\eta = \gamma_p N_p / v_F$ and $K = a/l_b$. With these parameters, Matthiessen's rule would require that $\sigma \approx F_M \sigma_0$, where $F_M = K/(\eta + K)$, but we have shown that such a simple relationship would only apply under the condition $\eta \ll K$. Hence our main conclusion is that Matthiessen's rule is not validated if $K \lesssim \eta$.

However, it should be emphasized here that the results of the present paper should certainly be modified if extremely small (reduced) thicknesses K were treated (i.e. in the limiting case when $K \rightarrow +0$). Namely, then our calculations should be replaced by more demanding ones, well, beyond those of the quasi-classical theory. To suggest why the theory must be modified if the values K are small, let us discuss the extreme situation when the density n_b of the bulk defects vanishes, i.e. when all defects are located on the interface(s). Then, according to our assumptions, $\sigma_b \rightarrow \infty$ (since $l_b \rightarrow \infty$, the so-called Bloch superconductor), although $\sigma_0 K$ tends to some finite non-zero constant. Nevertheless, the leading term in the function F (see the asymptotic formula (60.1)) is of the form $\sim -K \ln K$ and hence $\sigma \sim \sigma_0 (-K \ln K)$ diverges logarithmically if $K \rightarrow +0$. This result is, of course, physically incorrect and has to be considered as a consequence of the quasi-classical approximation.

A rigorous application of the quantum mechanics should moderate the deviation between the functions $F(\eta, K)$ and $F_M(\eta, K)$ (see Tables I, II); the deviation is, according to the quasi-classical theory, very high just for $K \ll \eta$ (the relative deviation $r/100 = (F - F_M)/F_M \sim -\ln K$, cf. formula (68)).

The quantum mechanical revision of the problem would surely be interesting in view of some submicrometer microelectronic structures, and especially semiconductor superlattices "tailormade" for high-mobility devices (such as the so-called HEMTs, MODFETs, etc.). To describe exactly the (possible) functioning of such devices, theory must cope with many further difficulties. (The ballistic transport employed in these devices may concern warm, or even hot, electrons so that the inter-electronic interactions may be important enough, the driving electric field may be high so that the linear transport theory may become insufficient, quantum-mechanical surface states may arise as a new vital factor, etc.) Physical problems due to these devices are certainly challenging not only for researchers trying to invent new microelectronic applications but also for contemporary solid-state theorists eager to better understand new phenomena related to two-dimensional electron gases.

APPENDIX

We will derive a formula for $\sigma/\sigma_0 = F(\eta, K)$ under the assumption that

$$0 < K/\eta \ll 1. \quad (\text{A.1})$$

Here η may be arbitrary but such that $0 < \eta < 1$. We dissect the integration interval $\left(0, \frac{1}{2}\pi\right)$ in formula (45) into two subintervals: 1. the right-hand subinterval $I_1 \equiv \left(\chi_m, \frac{1}{2}\pi\right)$, and 2. the left-hand subinterval $I_2 \equiv \left(0, \chi_m\right)$, where

$\cos \chi_m = \eta$. We use the denotation

$$F = 1 + \Delta F, \tag{A.2}$$

where

$$\Delta F = (\Delta F)_I + (\Delta F)_{I'}, \tag{A.3}$$

$(\Delta F)_I, (\Delta F)_{I'}$ being the contributions due to the subintervals I, I' .

Contribution due to I ,

$$(\Delta F)_I = -\frac{3}{2K} \int_{\chi_m}^{\frac{1}{2}\pi} dx \sin^3 \chi \cos \chi \left[1 - \exp\left(-\frac{K}{\cos \chi}\right) \right]. \tag{A.4}$$

The substitution $u = \eta/\cos \chi$ gives the interval

$$(\Delta F)_I = -\frac{3\eta^2}{2K} \int_1^\infty du \left(\frac{1}{u^3} - \frac{\eta^2}{u^5} \right) \left[1 - \exp\left(-\frac{Ku}{\eta}\right) \right].$$

We can rewrite it, using the definition of the integral exponential functions

$$E_n(x) = \int_1^\infty dt \frac{e^{-xt}}{t^n} \quad (n = 0, 1, 2, \dots) \tag{A.5}$$

for $x > 0$ (cf. [13]), in the form

$$(\Delta F)_I = -\frac{3\eta^2}{4K} \left(1 - \frac{\eta^2}{2} \right) + \frac{3\eta^2}{2K} E_3\left(\frac{K}{\eta}\right) - \eta^2 E_5\left(\frac{K}{\eta}\right). \tag{A.6}$$

Formula (A.6) holds for arbitrary positive values of K . When taking condition (A.1) into account, we may utilize the asymptotic formulae for $E_3(x), E_5(x)$ ($0 < x \ll 1$):

$$\begin{aligned} E_3(x) &= \frac{1}{2} - x - \frac{1}{2} x^2 \ln x + \frac{1}{2} \psi(3) x^2 + \frac{1}{6} x^3 - \frac{1}{48} x^4 + O(x^5), \\ E_5(x) &= \frac{1}{4} - \frac{1}{3} x + \frac{1}{4} x^2 - \frac{1}{6} x^3 - \frac{1}{24} x^4 \ln x + \frac{1}{24} \psi(5) x^4 + O(x^5), \end{aligned}$$

where

$$\psi(n) = \sum_{m=1}^{n-1} \frac{1}{m} - \gamma \quad (\text{for } n > 1),$$

with γ equaling the well-known Euler number (see below). Hence

$$\begin{aligned} (\Delta F)_I &= -\frac{3}{2} \eta \left(1 - \frac{1}{3} \eta^2 \right) - \frac{3}{4} K \ln\left(\frac{K}{\eta}\right) + \frac{3}{4} \left[\psi(3) - \frac{1}{2} \eta^2 \right] K + \\ &+ \frac{1}{4} \frac{1 + \eta^2}{\eta} K^2 + O(-K^3 \ln K). \end{aligned} \tag{A.7}$$

Contribution due to I' ,

$$(\Delta F)_{I'} = \frac{3}{2K} \int_0^{\chi_m} dx \sin^3 \chi \cos \chi C_F^2(\eta, \chi) \left[1 - \exp\left(-\frac{K}{\cos \chi}\right) \right], \tag{A.8}$$

where C_F^2 is given by formula (47) with $Q_F = 1 - \eta/\cos \chi$ (formula (27.1)). We can show that $(\Delta F)_{I'}$ is analytic in K (including the point $K = 0$) for $K \geq 0$; we may develop the functions C_F^2 and $1 - \exp(-K/\cos \chi)$ into the Maclaurin series with respect to K :

$$\begin{aligned} C_F^2 &= -1 + \left(1 - \frac{\eta}{\cos \chi} \right) \frac{K}{\eta} + \left(-1 + \frac{3}{2} \frac{\eta}{\cos \chi} - \frac{1}{2} \frac{\eta^2}{\cos^2 \chi} \right) \frac{K^2}{\eta^2} + O(K^3), \\ 1 - \exp\left(-\frac{K}{\cos \chi}\right) &= \frac{K}{\cos \chi} \left(1 - \frac{1}{2} \frac{K}{\cos \chi} \right) + O(K^3). \end{aligned}$$

Then we have to calculate the integral

$$\begin{aligned} (\Delta F)_{I'} &= -\frac{3}{2} \int_0^{\chi_m} dx \sin^3 \chi \left[1 - \left(1 - \frac{1}{2} \frac{\eta}{\cos \chi} \right) \frac{K}{\eta} + \right. \\ &\left. + \left(1 - \frac{\eta}{\cos \chi} + \frac{1}{6} \frac{\eta^2}{\cos^2 \chi} \right) \right] \frac{K^2}{\eta^2} + O(K^3). \end{aligned} \tag{A.9}$$

The integration is easy and gives the result:

$$\begin{aligned} (\Delta F)_{I'} &= -1 + \frac{3}{2} \eta \left(1 - \frac{1}{3} \eta^2 \right) + \left(1 + \frac{3}{4} \eta \ln \eta - \frac{9}{8} \eta + \frac{1}{8} \eta^3 \right) \frac{K}{\eta} - \\ &- \left[1 - \frac{1}{2} \eta (1 - 3 \ln \eta + \eta) \right] \frac{K^2}{\eta^2} + O(K^3). \end{aligned} \tag{A.10}$$

Complete asymptotic formula for $\Delta F (K \rightarrow 0)$

Putting contributions (A.7) and (A.10) together, we obtain the final result:

$$\Delta F = -1 - \frac{3}{4} K \ln \left(\frac{K}{\eta} \right) + \left[1 - \frac{3}{4} \eta (\gamma - \ln \eta) - \frac{1}{4} \eta^3 \right] \frac{K}{\eta} - \left[1 - \frac{3}{4} \eta (1 - 2 \ln \eta) - \frac{\eta^2}{2} \left(1 + \frac{1}{2} \eta \right) \right] \frac{K^2}{\eta^2} + O(K^3). \quad (A.11)$$

Note that $\gamma = 0.5772156649$.

REFERENCES

- [1] Hrivnák, L., Bezák, V., Follin, J., Ožvold, M.: *Teória tuhých látok (Theory of Solids, in Slovak)*, Veda, Bratislava 1985.
- [2] Fuchs, K.: Proc. Cambridge Phil. Soc. 34 (1938), 100.
- [3] Ziman, J. M.: *Electrons and Phonons*. University Press, Oxford 1960 (Russian translation: Moscow 1962).
- [4] Lišić, I. M., Azbel, M. J., Kaganov, M. J.: *Elektromagnitna teorija metallov*. Nauka, Moskva 1971.
- [5] Abrikosov, A. A.: *Uvedenie v teoriju normalnykh metallov*. Nauka, Moskva 1972.
- [6] Askeroov, B. M.: *Elektromagnitnaja ianuljija perezosa v poluprovodnikach*. Nauka, Moskva 1985.
- [7] Bezák, V., Kempaský, J.: *Czech. J. Phys. B18* (1968), 1264.
- [8] Bezák, V., Kedro, M., Revala, A.: *Thin Solid Films* 23 (1974), 305.
- [9] Khater, F.: *Acta Phys. Slov. 33* (1983), 43.
- [10] Khater, F., Seoud, : *Acta Phys. Slov. 38* (1988), 38.
- [11] Grendel, M.: *Czech. J. Phys. B31* (1981), 416.
- [12] Ilkovič, V.: *Ubrnité problémy z teorie tuhých látok (Selected Problems of the Solid State Theory, in Slovak)*, Veda, Bratislava 1984.
- [13] Abramowitz, M., Stegun, I.: *Handbook of Mathematical Functions*, Nat. Bureau of Standards 1967 (Russian translation: Nauka, Moskva 1978).
- [14] Rektorys, K., et al.: *Prehled užité matematiky (Handbook of Applied Mathematics, in Czech)* SNTL, Praha 1981.

Received March 28th, 1988

Revised version received May 23rd, 1988

Accepted for publication May 31st, 1988

ПОЧЕМУ ПРАВИЛО МАТТИССЕНА ТЕОРИИ МЕТАЛЛОВ МОЖЕТ УТРАТИТЬ СИЛУ? — ИЗ-ЗА РАЗМЕЩЕНИЯ ДЕФЕКТОВ В ПЛОСКОСТЯХ

В статье учтены геометрически простые бикристаллические и поликристаллические металлические плиты с зернами в форме равных слоев. Тема статьи — теория их продольной электрической проводимости и предположение, что электроны сталкиваются с дефектами

двух типов: одного типа — в объеме зерн, другого — на границах между зернами. Определены средние (объемные) плотности этих дефектов, автор на самом деле ставит вопрос о том, оправдано ли, хотя бы приблизительно, в теории проводимости металлов с внутренними границами правило Маттиссена. В общем случае ответ отрицательный (даже если в случае бикристаллов внешние поверхности взяты как совершенно гладкие). Некоторые численные результаты автора получены машинным интегрированием; они приведены в двух таблицах. В основе теории — кинетическое уравнение Больцмана для электронов проводимости.