RESISTANCE OF POLYCRYSTALLINE MEDIA IN STRONG MAGNETIC FIELDS

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Submitted February 3, 1970; resubmitted April 10, 1970

Zh. Eksp. Teor. Fiz. 59, 510-515 (August, 1970)

The resistance of polycrystalline media is found as a function of the magnetic field in the case where closed electron trajectories on the Fermi surface are encountered much more frequently than open trajectories. The linear increase in the resistance (Kapitza's law) in the case of polycrystalline gold is explained.

 \mathbf{I}_{T} is known that the presence of open electron trajectories on the Fermi surface is responsible for the sharp anisotropy of the transverse resistance of many metals in strong magnetic fields.¹⁾ The theory of galvanomagnetic effects (see the review in^[1] and the references therein) enables us to find the asymptotic behavior of the components of the conductivity tensor of a single crystal as functions of r/l if we know the nature of the electron trajectories (i.e. depending on whether they are closed within a unit cell of the reciprocal lattice, or closed within the limits of a few cells, or open). However, the linear increase in the resistance of polycrystalline specimens with increasing magnetic field, which was first discovered by Kapitza^[2] and subsequently ob-served by Justi^[3] and Chambers^[4], has not been satis-factorily explained. Herring^[5] has investigated the various tensor characteristics of polycrystalline media but the method used by him demands that these parameters should vary very little from one crystallite to another. If the conductivity tensor of a single-crystal specimen is sharply anisotropic, which is the case for metals in strong magnetic fields, then strong texture is necessary for the method to succeed. Assuming that only the Hall components of σ_{ik} fluctuate, Herring derived a linear increase in the resistance but admitted himself that he exceeded the range of validity of his method. In fact, calculations based on the method employed by Lifshitz and Peschanskii^[6] to find the elastic constants of polycrystalline media do not lead in this case to a linear relation between the resistance and the magnetic field.²⁾ Moreover, the method employed in^[6] is mathematically more rigorous and physically more easily interpreted.

Lifshitz and Peschanskii^[7] obtained a linear increase for the resistance of a wire whose cross section contained a single crystallite. They assumed that the Fermi surface contained highly elongated trajectories (in particular, they considered the Fermi surface in the form of a corrugated cylinder). However, in the experiments of Chambers^[4] all the linear dimensions of the

specimens were much greater than the size of an individual crystallite and, therefore, the conclusions reported in^[7] do not apply to this case. The method of calculation put forward in^[7] cannot be generalized because the boundary conditions $j_{\perp} = 0$ (no current through the lateral surface of each crystallite) which, in practice, allow us to complete the calculation do not apply in the general case of an infinite polycrystalline medium. Ziman^[8] obtained a linear increase in the resistance, assuming that the Fermi surface was a right cylinder. He did not introduce the effective conductivity tensor Σ_{ik} (see below) but simply took an average over the conductivity-tensor components of a single crystal with respect to the angles (with the reservation that this procedure can be justified by the final results). This can be done only for a thin plate whose cross section contains a single crystallite (but d \gg l) and one must then take an average not of each component of σ_{ik} but of the scalar conductivity $\sigma_{ik}n_in_k$ $(n_i = E_i/|E|)$.³⁾

In this paper we shall consider the resistance of a polycrystalline medium which extends in all directions and is located in a strong magnetic field, assuming that the fraction of crystallites in which there are open electron trajectories is small. We shall allow for the fact that the asymptotic behavior of the components of σ_{ik} is different for open and closed trajectories. We shall introduce certain additional assumptions which are satisfied, for example, in the case of gold, and we shall obtain a linear increase in the resistance with magnetic field, which is in good agreement with existing experimental data.^[3,4]

We shall assume that the mean linear size d of a crystallite is much greater than the mean free path l, so that each crystallite has its own conductivity tensor and we can use the macroscopic equations with the conductivity tensor taken from the solution of the kinetic problem. Consider the effective conductivity tensor

$$\langle \sigma_{ik} \nabla_{k} \varphi \rangle = \Sigma_{ik} \langle \nabla_{k} \varphi \rangle, \qquad (1)$$

where the potential φ satisfies the equation div $\mathbf{j} = 0$:

$$\nabla_i(\sigma_{ik}\nabla_k\phi) = 0, \qquad (2)$$

and the mean field $\langle \nabla_h \varphi \rangle$ is given. Equation (2) is a second-order elliptic differential equation with variable coefficients which are random functions of the coordinates. If we demand the invariance under rotations about

¹⁾Magnetic fields will be regarded as strong if the Larmor radius $r = cp_F/eH$ is much less than the mean free path *l*; however, if the field is too high the Landau level separation μH will not be much smaller than the Fermi energy ϵ_F and energy quantization will have to be taken into account.

 $^{^{2)}\}mbox{If all the trajectories are closed the asymptotic behavior of <math display="inline">\Sigma_{ik}$ is unaffected.

³⁾The quantity $\rho_{ik}m_im_k = R$, $m_i = f_i/|j|$ was averaged in [⁷].

the Z axis, which will always be parallel to the magnetic field, we obtain

$$\Sigma_{ik} = \begin{pmatrix} \sigma_1 & \sigma_2 & 0 \\ -\sigma_2 & \sigma_1 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix}$$

In zero magnetic field the conductivity tensor will depend on the coordinates as follows:

$$\sigma_{ik}(\mathbf{r}) = (\alpha_{il}\alpha_{km})(\mathbf{r})\sigma_{lm}^{\circ};$$

where $\alpha_{ik}(\mathbf{r})$ is a unitary rotation matrix which describes the random orientation of the crystallographic axis of the crystallites and σ_{lm}^0 is the conductivity tensor of a given crystallite.

The situation becomes more complicated when the magnetic field is not zero. It is $known^{(7,9)}$ that the conductivity tensor of a single crystal when the electron trajectory on the Fermi surface is closed is of the form

$$\sigma_{ik} = \sigma_0 \begin{pmatrix} a_{11}\gamma^2 & a_{12}\gamma & a_{13}\gamma \\ a_{21}\gamma & a_{22}\gamma^2 & a_{23}\gamma \\ a_{31}\gamma & a_{32}\gamma & a_{33} \end{pmatrix}, \quad a_{ik} = -a_{ki} \text{ for } i \neq k.$$

In this expression $\sigma_0 = ne^2 l/p_F$ is the conductivity of the metal in zero magnetic field, $\gamma = H_0/H$, $cp_F/eH_0 = l$, and all the a_{ik} are of the order of unity. If the trajectory is open the symmetric part of σ_{ik} will contain, in addition to σ_{33} , further terms which do not vanish for $\gamma \rightarrow 0$. Consequently, on the stereographic projection of the magnetic field there will be two types of region, corresponding to closed and open trajectories, respectively. Assuming that the crystallites are randomly oriented, we can introduce the concentrations of crystallites corresponding to these two types as ratios of the corresponding solid angles to 4π .

Let us begin by considering the situation where the concentration of crystallites with open trajectories is much less than unity. For the sake of simplicity, we shall ignore effects which are longitudinal with respect to the magnetic field, i.e., all the $\sigma_{3\nu} = \sigma_{\mu_3} = 0$ when μ and $\nu = 1, 2$. We shall also assume that crystallites belonging to a given type have the same conductivity tensor because rotations within a given type do not affect the order of magnitude of the components of σ_{ik} . This means that we are ignoring the weak anisotropy which is due to changes in the matrix aik when the crystallites are rotated, and take into account only the strong anisotropy which is connected with different powers of γ in the conductivity tensors of the individual crystallites. This can be done because we are interested only in the dependence of resistance on the magnetic field.

In view of the above assumptions we can write the conductivity tensor for crystallites belonging to the first type in the form

$$\sigma_{ik}^{out} = \sigma_0 \begin{pmatrix} \gamma^2 & \gamma & 0 \\ -\gamma & \gamma^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

whereas for crystallites of the second type we have

$$\sigma_{ik}^{in} = \sigma_0 \begin{pmatrix} 1 & \gamma & 0 \\ -\gamma & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(The conductivity tensor is of this form if, for example, the plane perpendicular to the magnetic field contains two orthogonal directions of the open trajectories.)

two orthogonal directions of the open trajectories.) The conductivity tensors σ_{ik}^{in} and σ_{ik}^{out} have equal Hall

components. This is introduced in order to simplify the analysis because equal antisymmetric parts of conductivity tensors can be omitted during the intermediate calculations and then substituted into the final results (see Appendix).

We shall assume, for the sake of simplicity, that crystallites of the second type, whose concentration is low, are spherical in shape. Consider, to begin with, a single sphere in an infinite medium. Outside the sphere, Eq. (2) becomes

$$\gamma^2 \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \right) + \frac{\partial^2 \varphi}{\partial z^2} = 0.$$
 (3)

Inside the sphere, the potential φ satisfies the Laplace equation. The usual boundary conditions should be satisfied on the surface of the sphere, i.e., the potential and the normal component of the current density must be continuous across the boundary. The field at infinity E_i^{∞} must also be specified. It will become clear later that it is sufficient for our purpose to know the field inside the sphere. Let us transform the coordinates so that

$$x_1 = \frac{x}{\gamma}, \quad y_1 = \frac{y}{\gamma}, \quad z_1 = z,$$

and Eq. (3) takes the form of a Laplace equation, whereas the sphere of radius r_0 becomes the ellipsoid of revolution $\gamma^2(x_1^2 + y_1^2) + z_1^2 = r_0^2$ inside which the potential satisfies the equation

$$\frac{1}{\gamma^2}\left(\frac{\partial^2\varphi}{\partial x_1^2}+\frac{\partial^2\varphi}{\partial y_1^2}\right)+\frac{\partial^2\varphi}{\partial z_1^2}=0.$$

It is shown in^[10] that the field inside the ellipsoid (and hence inside the sphere) is uniform, and to find it we need not carry out a direct solution of Eq. (2) or (3). It is readily verified that Eq. (8.10) in^[10] can be generalized to our case as follows:

$$E_{i^{in}} = [\sigma_{ik}^{out} + n_{im}(\sigma_{mk}^{in} - \sigma_{mk}^{out})]^{-1} \sigma_{kl}^{out} E_{l^{\infty}}.$$
 (4)

In this expression n_{im} is the depolarization tensor of the ellipsoid whose principal values are determined only by the geometry of the ellipsoid, i.e. in our case, by the tensor σ_{ik}^{out} in the final analysis. In our case, these values are as follows:^[10]

$$n_{zz} = \frac{1+e^2}{e^3} (e - \operatorname{arctg} e), \quad n_{xx} = n_{yy} = \frac{1}{2} (1-n_{zz}),$$
$$e = \sqrt{\frac{1}{\gamma^2} - 1}.$$

When $\gamma \ll 1$ we have $n_{ZZ} = 1 - \frac{1}{2}\pi |\gamma|$, $n_{ZZ} = n_{yy} = \frac{1}{4}\pi |\gamma|$.

To find Σ_{ik} we shall use the artificial device employed in^[10]. Consider the integral

$$\lim_{V\to\infty}\frac{1}{V}\int dV(j_i-\sigma_{ik}^{out}E_k).$$

This is equal to $(\Sigma_{ik} - \sigma_{ik}^{out})\langle E_k \rangle$. The integrand is nonzero only inside the inclusions and, therefore, the integral is proportional to the concentration of these inclusions. Substituting Eq. (4) into the integral, we obtain

$$\lim_{V \to \infty} \frac{1}{V} \int dV (\sigma_{ik}^{in} E_k^{in} - \sigma_{ik}^{out} E_k^{in})$$

$$= k \left\{ (\sigma_{ik}^{in} - \sigma_{ik}^{out}) \left[\sigma_{kl}^{out} + n_{km} (\sigma_{ml}^{in} - \sigma_{ml}^{out}) \right]^{-1} \sigma_{ln}^{out} \right\} E_n^{\infty}.$$
(5)

It is readily shown (we shall not do this here) that if we take the difference between E_k^∞ and $\langle E_k\rangle$ into account we obtain corrections to Σ_{ik} which are the second-order

in the concentration. Therefore

 $\Sigma_{ik} = \sigma_{ik}^{out} + k \{\ldots\}_{ik}.$

If we perform the necessary operations and add the antisymmetric part we obtain

$$\Sigma_{ik} = \sigma_0 \begin{pmatrix} \gamma^2 + \frac{4}{\pi} k |\gamma| & \gamma & 0 \\ -\gamma & \gamma^2 + \frac{4}{\pi} k |\gamma| & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$
 (6)

Suppose that $k \to k_0 \neq 0$ as $\gamma \to 0$. If we also demand that $j_v = 0$ we obtain

$$E_x = \frac{j_x}{\sigma_0} \left(1 + \frac{4}{\pi} k_0 \frac{1}{|\gamma|} \right). \tag{7}$$

It is clear that the second term in the parentheses increases linearly with the magnetic field. If we plot $\rho(H)/\rho_0$ as a function of H/H_0 we obtain a straight line of slope $4k_0/\pi$. Gaidukov^[11] has given the stereographic projection of special directions for the Fermi surface of gold, using measured resistances for single-crystal specimens. The value of k₀ calculated from this projection is ~ 0.03 . This agrees to within an order of magnitude with experimental results^[3,4] for polycrystalline specimens. The linear increase in the resistance of polycrystalline gold specimens can thus be explained on the basis of the general properties of the conductivity tensor for single crystals and a minimal amount of information about the Fermi surface (the Fermi surface need not be constructed and it is sufficient to know the area of the corresponding regions).

Our method can be used even when the Fermi surface is in the form of a corrugated cylinder. In this case, $k \sim \gamma^{(7)}$ and σ_{ik}^{in} must be taken in the form

$$\sigma_{ik}^{in} = (\alpha_{il}\alpha_{km})(\theta) \, \sigma_{lm}^{'}, \quad \sigma_{lm}^{'} = \sigma_0 \begin{pmatrix} 1 & \gamma & 0 \\ -\gamma & \gamma^2 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

where $\alpha_{il}(\theta)$ is the matrix representing rotation through the angle θ about the Z axis, and at the end of the calculation we must average with respect to θ within the interval $(0, 2\pi)$. The necessity for this procedure is also a consequence of the results given in^{[7],4)} We obtain

$$\Sigma_{ik} = \sigma_0 \begin{pmatrix} (1+\delta)\gamma^2 & \gamma & 0 \\ -\gamma & (1+\delta)\gamma^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad \delta \sim 1.$$

In contrast to a wire, a specimen which extends in all directions behaves as if all the electron trajectories were closed.

We note in conclusion that the results reported by Stachowiak^[12,13] are in conflict with our own. In our view, this is connected with an incorrect averaging procedure. Stachowiak obtained by direct calculation a special case of Eq. (4)^[12] and identified in it E_i^{∞} with $\langle E_i \rangle$, σ_{ik}^{out} with Σ_{ik} , and σ_{ik}^{in} with the conductivity tensor at a given point in the polycrystalline specimen (and not just within the crystallites whose concentration was small, as in our case). He then obtained in^[13] the self-consistent equation for Σ_{ik}

$$k \langle E_i^{in} \rangle_{\text{w.r.t. angles}} + (1-k) \langle E_i^{out} \rangle_{\text{w.r.t. angles}} = \langle E_i \rangle_{ki}$$

The first of these assumptions is valid only for low concentrations of the inclusions, whereas the second and third are valid if the polycrystalline specimen is weakly inhomogeneous. In this way, Stachowiak obtained a number of results which were not correct. In particular, in the case mentioned above, when only the Hall components of σ_{ik} fluctuated and all the trajectories were closed, he found that $R \sim H$ and $R \sim H^{2/3}$. In the case of a Fermi surface in the form of a corrugated cylinder, he found $R \sim H$. Stachowiak tried to justify the assumptions we have mentioned but introduced a number of new errors as a result.

APPENDIX

Identical antisymmetric parts of the conductivity tensor in the inclusions and in the medium can be omitted from Σ_{ik} during the derivation and then substituted directly into the final result. Let us prove this. Suppose σ_{ik} is a symmetric tensor and

$$\nabla_i (\sigma_{ik} \nabla_k \varphi_1) = 0, \quad \langle \sigma_{ik} \nabla_k \varphi_1 \rangle = \sigma_{ik}^{\text{eff}} \langle \nabla_k \varphi_1 \rangle,$$

Let us add to σ_{ik} the constant antisymmetric part Λ_{ik} so that the electric field will also change. Equation (2) assumes the form

$$\nabla_{i}[(\sigma_{ik} + \Lambda_{ik}) \nabla_{k}(\varphi_{1} + \varphi_{2})] = 0 \quad \text{or} \quad \nabla_{i}(\sigma_{ik} \nabla_{k} \varphi_{2}) = 0,$$

since the contraction of the symmetric tensor $\nabla_i \nabla_k$ with the antisymmetric Λ_{ik} yields zero. Since φ_2 satisfies the same differential equation as φ_1 , we have

$$\begin{split} \langle (\sigma_{ik} + \Lambda_{ik}) \nabla_k (\varphi_1 + \varphi_2) \rangle &= \sigma_{ik}^{\text{eff}} \langle \nabla_k \varphi_1 \rangle + \Lambda_{ik} \langle \nabla_k \varphi_1 \rangle \\ + \sigma_{ik}^{\text{eff}} \langle \nabla_k \varphi_2 \rangle + \Lambda_{ik} \langle \nabla_k \varphi_2 \rangle &= (\sigma_{ik}^{\text{eff}} + \Lambda_{ik}) \langle \nabla_k (\varphi_1 + \varphi_2) \rangle. \end{split}$$

This is readily generalized to the case when σ_{ik} (but not Λ_{ik} !) is a discontinuous function of coordinates.

The author is indebted to V. G. Peschanskiĭ for suggesting this problem and for his constant interest in this research.

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⁴⁾We note that this procedure is not connected with the fact that $k \sim \gamma$ since for such rotations the direction of the magnetic field does not leave the open region. σ_{ik}^{in} can be taken in this form with subsequent averaging with respect to θ right from the beginning, in which case the factor $4/\pi$ in Eqs. (6) and (7) is replaced by another factor of the order of unity.