Relaxation type Kinetic equation for electrons in polycrystalline metal

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Abstract. The kinetic equation for electrons in a polycrystalline metal is considered. A kinetic equation is written that describes in a unified manner the scattering of conduction electrons both by impurities or phonons and by grain boundaries. This kinetic equation takes into account the scattering of electrons at the boundaries of crystallites of a polycrystalline metal. An expression is obtained for the bulk conductivity in the general case. Let us analyze the effect of electron scattering at grain boundaries on its electrical properties.

1. Introduction

In the granular conductor electron scattering at grain boundaries leads to that they are scattered mainly backward. Thus, some of the electrons acquire the velocity the opposite original one.

Up to now this was considered by a formal summation of the contribution to the electrical resistance of the conductor caused by electron scattering on the surface and by lattice defects (and phonons) and the contribution due to electron scattering at the grain boundaries [1]. Such an approach would not be quite satisfactory. It is obvious that the contributions of these processes in the electrical resistance of the conductor are not independent.

For correct accounting of contributions of these processes is necessary to use the unified kinetic approach to the problem. This approach must account for all phenomena in a unified way. Up to now such a kinetic approach was absent.

Scattered at the interface between the grains, the electrons will have a speed mainly directed in the opposite direction from the initial velocity. Therefore, the equilibrium electron velocity after the collision will be nonzero, because of the scattering on impurities and defects. And the sign of the average speed of the electrons after the collision with the grain boundaries will be the opposite of the original average speed of electrons.

2. Kinetic equation

Kinetic equation with the relaxation type collision integral for electrons will be as follows [2]— [4]

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{r}} + e\mathbf{E} \frac{\partial f}{\partial \mathbf{p}} = \nu (f_{eq} - f).$$

(1)

where \( \mathbf{v}, e \) — the velocity and charge of electrons, \( \mathbf{E} \) — Electric field strength, \( \nu \) — the rate of collision of electrons, the function \( f_{eq} \) - the equilibrium Fermi distribution for electrons in a solid plasma:
\[ f_{eq} = \left[ 1 + \exp \frac{\mathcal{E} - \mu}{k_B T} \right]^{-1}, \quad (2) \]

here \( \mathcal{E} \) – equilibrium electron energy after scattering, \( \mu \) – chemical potential, \( T \) – temperature, \( k_B \) – Boltzmann’s constant.

We assume that the conducting medium has a spherical symmetry. In this case for energy of electrons \( \mathcal{E}_0 \) we have:

\[ \mathcal{E}_0 = \frac{mv^2}{2}. \]

Here \( m \) — the effective mass of the electron.

However, in general, after scattering, the average speed of the electron will be nonzero. That is, the electron will “remember” the velocity, which had before the scattering. In the case when the electron–electron scattering is dominant, electron after scattering partially retains the original velocity.

The average speed of the electrons after scattering, we denote \( u \). We assume that the magnitude of \( u \) is connected to the average electron velocity \( u_0 \) by the following relation:

\[ u = \alpha u_0. \]

The value of \( \alpha \) took into account the fact that the scattering electrons partially retain their memory of their velocity before scattering. In this approach, the value of \( \alpha \) is an empirical coefficient.

Then we get the following relationship:

\[ \mathcal{E} = \frac{m(v - u)^2}{2}. \quad (3) \]

A similar approach was previously used to take into account electron-electron collisions [5] — [7]. In the case of electron-electron collisions, the value of \( \alpha \) is positive, since the scattering of electrons occurs predominantly forward. In the case of electron scattering at the crystallite boundary of a polycrystalline metal, the value of \( \alpha \) is negative, that is, \( \alpha < 0 \). This is due to the fact that in this case the scattering of electrons occurs mainly in the direction opposite to the direction of the initial motion of electrons.

We assume that the velocity \( u \) is much less than the thermal velocity of electrons (or Fermi velocity for the case of degenerate Fermi–gas). Then the value of \( \mathcal{E} \) (3) can be linearized:

\[ \mathcal{E} \approx \frac{mv^2}{2} - mvu = \mathcal{E}_0 - mvu. \]

Through appropriate linearization for the locally equilibrium functions \( f_{eq} \), we obtain the following expression:

\[ f_{eq} = f_0 - \frac{\partial f_0}{\partial \mathcal{E}} mvu, \quad (4) \]

Similarly, in the linear case, the term with the electric field in the kinetic equation (1) takes the following form:

\[ eE \frac{\partial f}{\partial p} \approx eEv \frac{\partial f_0}{\partial \mathcal{E}}, \quad (5) \]

where \( p = mv \) – electron momentum.

The magnitude of \( u_0 \) is defined through the distribution function:

\[ u_0 = \frac{1}{n} \int f v \frac{d^3p}{(2\pi\hbar)^3}. \]

Here \( n \) – concentration of electrons:

\[ n = \int f \frac{d^3p}{(2\pi\hbar)^3}. \]

Note that the current density \( f \) can be represented in the form:

\[ f = neu_0. \]

The linearized distribution function has the form [2]:

\[ f = f_0 + f_1. \]
For a function $f_1$ in the works [5] — [7] has been proposed model equation taking into account the contribution of electron-electron collisions in the kinetic processes. For a degenerate Fermi gas of electrons this equation has the following form:

$$\frac{\partial f_1}{\partial t} + \mathbf{v} \cdot \nabla f_1 + e\mathbf{E} \cdot \mathbf{v} \frac{\partial f_0}{\partial \mathbf{E}} = -\nu \left( \frac{3ma}{4\pi n^2 f} \mathbf{v} \frac{\partial f_0}{\partial \mathbf{E}} \int \mathbf{v}' f_1 d^3v' + f_1 \right).$$

Here $\nu = \frac{1}{\tau}, \tau$ - the average time between two successive collisions of an electron. The integral term corresponds to the taking into account the value $u_0$. $\mathbf{E}$ - Fermi velocity, $E_F = \frac{mv_F^2}{2}$.

In this case

$$u_0 = \frac{1}{n} \int f_1 v \frac{2d^3p}{(2\pi \hbar)^3}.$$

We have the following relation $p_F^2/m = E_F$. Then

$$u_0 = \frac{1}{n} \int f_1 v \frac{2d^3p}{(2\pi \hbar)^3} = \frac{3(2\pi)^3}{8\pi p_F^3} \int f_1 v \frac{2d^3p}{(2\pi \hbar)^3} = \frac{3}{4\pi n^2 f} \int f_1 v d^3v.$$

We introduce a new function $h$ by using the relation:

$$\psi = \frac{m v_y v_F h}{n}.$$

We assume that the field $\mathbf{E} \sim \exp(-i\omega t)$. Then $\psi \sim \exp(-i\omega t)$. Taking into account the relations (4), (5) and (6), the kinetic equation (1) can be written as follows for the function $\psi$ [2]:

$$-i \omega \psi + \mathbf{v} \frac{\partial \psi}{\partial \mathbf{r}} - e\mathbf{E} \mathbf{v} = -\nu(\mathbf{v} \cdot \mathbf{u}_0) - \psi.$$

The value $u$ is related to the average velocity of the electron before collision. In the case of electron-electron collisions the electrons partially retain the initial impulse and the initial velocity. In this case, the coefficient $\alpha$ is positive, $\alpha > 0$. In the case of scattering by grain boundaries the situation is the opposite. Thus, the electrons after scattering by the grain boundaries have a velocity opposite to the initial one. Therefore, the sign $\alpha$ in the equation (8) is negative. Equation (8) can be rewritten in the following form:

$$-i \omega \psi + \mathbf{v} \frac{\partial \psi}{\partial \mathbf{r}} + v \psi = \mathbf{v}(e\mathbf{E} + v \alpha \mathbf{u}_0).$$

Consider the one-dimensional problem, when the function $\psi$ depends only on the spatial variable $x$. Axis $y$ will direct along a direction of the electric field $E$. Thus, $\mathbf{E} = E_y \exp(-i\omega t)$. Then the equation (9) will be of the form:

$$-i \omega \psi + v_x \frac{\partial \psi}{\partial x} + \psi = v_y (eE_y + v \alpha \mathbf{u}_0).$$

We introduce a new function $h$ by using the relation:

$$\psi = \frac{m v_y v_F h}{n}.$$
The function $h$ is dimensionless.

We calculate the value $\mathbf{u}_0 y$:

$$\mathbf{u}_0 y = \frac{3}{4\pi\nu_F^3} \int f_i v_j d^3v = \frac{3}{4\pi\nu_F^3} \int \delta(\mathcal{E} - \mathcal{E}_F) \psi v_j d^3v = -\frac{3}{4\pi\nu_F^3} \int \delta(\mathcal{E} - \mathcal{E}_F) mv_j v_F d^3v = \frac{3m}{4\pi\nu_F^3} \int \delta(\mathcal{E} - \mathcal{E}_F) v_F^3 h d^3v.$$ But

$$\delta(\mathcal{E} - \mathcal{E}_F) = \frac{\delta}{(\mathcal{E} - \mathcal{E}_F)} = \frac{1}{\nu_F} \delta(v - v_F).$$

Then

$$\mathbf{u}_0 y = \frac{3m}{4\pi\nu_F^3} \int \frac{1}{\nu_F^3} \delta(v - v_F) v_F^3 h d^3v = \frac{3}{4\pi\nu_F^3} \int \delta(v - v_F) v_F^3 h d^3v.$$ Let’s go over to a spherical frame of reference in the velocity space:

$$v_x = v \cos \theta, \quad v_y = v \sin \theta \cos x, \quad v_y^2 = v^2 \sin^2 \theta \cos^2 x.$$ Let’s introduce the designation:

$$\mu = \cos \theta,$$

then

$$v_x = v \mu, \quad v_y^2 = v^2(1 - \mu^2) \cos^2 \phi, \quad d^3v = v^2 \sin \theta dv d\theta d\phi = -v^2 d\mu d\phi.$$

In this case:

$$\mathbf{u}_0 y = \frac{3}{4\pi\nu_F^3} \int \delta(v - v_F) v_F^3 h d^3v = -\frac{3}{4\pi\nu_F^3} \int \left[ 0 \int_{\frac{1}{\mu^2}}^{\frac{1}{\mu^2}} \int_{-1}^{1} \int_{-1}^{1} d\phi d\mu \right] d\mu.$$ It is convenient to introduce the following dimensionless variables:

$$z_0 = \frac{\alpha (v - \omega)}{v_F}, \quad \mu' = \frac{v_x}{v_F}, \quad x' = \frac{x}{a}.$$ Then the kinetic equation takes the form:

$$\mu \frac{\partial h}{\partial x'} + z_0 h(x', \mu') = E_0 + \frac{3}{4} \beta \int_{-1}^{1} (1 - \mu^2) h(x', \mu') d\mu.$$ Here

$$E_0 = \frac{eE_y a}{mv_F^3}, \quad \beta = \frac{aa \mu}{v_F}.$$ In the future, the variable $x'$ will be written without dash for short.

3. Calculation of the conductivity coefficient

Let’s calculate the current density $j_y$:

$$j_y = n e \mathbf{u}_0 y = \frac{3v_F n e}{4} \int_{-1}^{1} (1 - \mu^2) h d\mu.$$ Consider the case of not varying in space electric field. Then $\frac{\partial h}{\partial x'} = 0$. Then the function $h(x, \mu')$ is a constant. We denote this using a constant $H$, i.e. $h(x, \mu') = H$. From equation (10) we find this constant:
\[ z_0 H = E_0 + \frac{3}{4} \beta \int_{-1}^{1} (1 - \mu^2) H \, d\mu. \]

Or

\[ z_0 H = E_0 + \beta H. \]

Therefore

\[ H = \frac{E_0}{z_0 - \beta}. \]

Calculate the current density \( j_y \):

\[ j_y = \frac{3 \nu_F ne}{4} \int_{-1}^{1} (1 - \mu^2) \, d\mu = \frac{\nu_F ne E_0}{z_0 - \beta}. \]

The expression for the electrical conductivity \( \sigma \) has the following form:

\[ \sigma = \frac{j_y}{E_y} = \frac{\nu_F ne E_0}{z_0 - \beta E_y} = \frac{\nu_F ne}{a \nu F} \frac{E_y}{E_y} = \frac{ne^2}{m (\nu - \omega - \alpha \nu)}. \]

When \( \omega = 0, \alpha = 0 \) we get the classical expression for static conductivity:

\[ \sigma_0 = \frac{ne^2}{m \nu}. \]

In the general case for the electrical conductivity we have:

\[ \sigma = \frac{\sigma_0}{1 - \alpha - \omega \mu / \nu}. \]

When \( \omega = 0, \alpha \to 1 \), the value \( \sigma \to \infty \). This case corresponds to the fact that in the scattering of electrons their momentum is conserved. So the friction of the electron gas on a lattice is missing.

When \( \alpha \to -\infty \), we get \( \sigma \to 0 \). That is, in this case scattering at grain boundaries dominates. Moreover, the grain boundaries become impermeable for the electrons.

4. Conclusion
We have considered the kinetic equation for electrons in polycrystalline conductor (metal). The influence of scattering electrons at the boundaries of the crystallites on the kinetic the processes have been analyzed. We showed how these processes affect the value of electric conductivity. The considered kinetic equation can be used to study the electrical conductivity of thin metal polycrystalline films. It is possible to use this kinetic equation for the analysis of skin–effect in polycrystalline metal.

References

[1] Chawla J S, F Gstrein, O’Brien K P, Clarke J S and Gall D 2011 Electron scattering at surfaces and grain boundaries in Cu thin films and wires (Physical Review B vol 84) p 235423.

[2] Abrikosov A A 1998 Fundamentals of the Theory of Metals (North–Holland, Amsterdam) p 380.

[3] Sondheimer E H 2001 The mean free path of electrons in metals (Advances in Physics vol 50), chapter 6 pp 499-537.

[4] Lifshitz E M and Pitaevskii L P 1981 Physical Kinetics: Volume 10 (Butterworth-Heinemann), p 466.

[5] Borchi E and De Gennaro S 1980 On the low–temperature electrical resistivity of copper and gold (J. Phys. F vol 10) pp 271–274.

[6] De Gennaro S and Retorry A 1984 The low–temperature electrical resistivity of potassium: size effects and the role of normal electron–electron scattering (J. Phys. F vol 14) pp 237–242.

[7] De Gennaro S and Retorry A 1985 Normal electron–electron contribution to the anomalous surface impedance (J. Phys. F vol 15) pp 227–230.