Relaxation type Kinetic equation for electrons in polycrystalline metal

Lam Thi Nhung[1] and Alexander Yushkanov[2]
Moscow Region State University
141014 Mytishi, Russia
[1] nhunglam279@gmail.com, [2] yushkanov@inbox.ru

***Abstract*—The kinetic equation for electrons in polycrystalline metal has been considered. This kinetic equation takes into account, along with collisions of electrons with impurities the collisions of electrons with the boundaries of the grains. We analyze the influence of a scattering of electrons on the boundaries of the grains on his electric properties.**

***Index Terms*—kinetic, grains, boundaries, electrons**

I. 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.

Kinetic equation

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

$$\frac{\partial f}{\partial t}+\mathbf{v}\frac{\partial f}{\partial \mathbf{r}}+e\mathbf{E}\,\frac{\partial f}{\partial \mathbf{p}}=\nu(f_0-f), \tag{1}$$

where f_{eq} - the equilibrium Fermi distribution for electrons in a solid plasma.

$$f_0=\Big[1+\exp\frac{\mathcal{E}_0-\mu}{k_BT}\Big]^{-1}.$$

Here $\mathcal{E}_0$ — equilibrium electron energy after scattering, μ — chemical potential, T – temperature, k_B – Boltzmann's constant, e – the charge of the electron. The value $\nu=1/\tau$ – the rate of collision of electrons, τ – the average time between two successive collisions of an electron.

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

$$\mathcal{E}_0=\frac{m\mathbf{v}^2}{2}.$$

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 $\mathbf{u}$. We assume that the magnitude of $\mathbf{u}$ is connected to the average electron velocity $\mathbf{u}_0$ by the following relation

$$\mathbf{u}=\alpha\mathbf{u}_0. \tag{2}$$

Here α — some coefficient.

Then we get the following relationship

$$\mathcal{E}_{eq}=\frac{m(\mathbf{v}-\mathbf{u})^2}{2}. \tag{3}$$

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

$$\mathcal{E}_{eq}\simeq\frac{m\mathbf{v}^2}{2}-m\mathbf{v}\mathbf{u}=\mathcal{E}_0-m\mathbf{v}\mathbf{u}.$$

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

$$f_{eq}=f_0-\frac{\partial f_0}{\partial\mathcal{E}}m\mathbf{v}\mathbf{u}. \tag{4}$$

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

$$e\mathbf{E}\,\frac{\partial f}{\partial \mathbf{p}}\simeq e\mathbf{E}\mathbf{v}\frac{\partial f_0}{\partial\mathcal{E}}. \tag{5}$$

The magnitude of $\mathbf{u}_0$ is defined through the distribution function

$$\mathbf{u}_0 = \frac{1}{n}\int f\mathbf{v}d^3p\frac{2d^3p}{(2\pi\hbar)^3}.$$

Here n — concentration of electrons.

$$n = \int fd^3p\frac{2d^3p}{(2\pi\hbar)^3}.$$

Note that the current density $\mathbf{j}$ can be represented in the form

$$\mathbf{j} = ne\mathbf{u}_0.$$

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

$$\frac{\partial f_1}{\partial t} + \mathbf{v}\,\mathrm{grad}\, f_1 + e\mathbf{v}\mathbf{E}\frac{\partial f_0}{\partial \varepsilon}$$
$$= -\nu\left(\frac{3m\alpha}{4\pi v_F^3}\mathbf{v}\frac{\partial f_0}{\partial \varepsilon}\int \mathbf{v}' f_1\, d^3v' + f_1\right).$$

The integral term corresponds to the taking into account the value $\mathbf{u}_0$.

Here v_F – the Fermi velocity, $v_F = p_F/m$, p_F – the Fermi momentum.

The function f_1 comfortably search in the form

$$f_1 = -\frac{\partial f_0}{\partial \mathcal{E}}\psi. \tag{6}$$

Here ψ is a new unknown function. For an electron degenerate Fermi gas we have

$$\frac{\partial f_0}{\partial \mathcal{E}} = -\delta(\mathcal{E} - \mathcal{E}_F),$$
$$f_1 = \delta(\mathcal{E} - \mathcal{E}_F)\psi.$$

Here $\delta(x)$ – the Dirac Delta function $\mathcal{E}_F$ – Fermi energy, $\mathcal{E}_F = mv_F^2/2$.

In this case

$$\mathbf{u}_0 = \frac{1}{n}\int f_1\mathbf{v}d^3p\frac{2d^3p}{(2\pi\hbar)^3},$$

$$n = \int f_0 d^3p\frac{2d^3p}{(2\pi\hbar)^3}.$$

Or

$$n = \int f_0\frac{2d^3p}{(2\pi\hbar)^3} = \frac{8\pi}{(2\pi\hbar)^3}\int\limits_0^{p_F} p^2dp.$$

Therefore

$$n = \frac{8\pi p_F^3}{3(2\pi\hbar)^3}.$$

We have the following relation

$$p_F^2/m = \mathcal{E}_F = \mu_0.$$

Then

$$\mathbf{u}_0 = \frac{1}{n}\int f_1\mathbf{v}\frac{2d^3p}{(2\pi\hbar)^3} = \frac{3(2\pi\hbar)^3}{8\pi p_F^3}\int f_1\mathbf{v}\frac{2d^3p}{(2\pi\hbar)^3}$$
$$= \frac{3}{4\pi v_F^3}\int f_1\mathbf{v}d^3v. \tag{7}$$

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 ψ [2]

$$-i\omega\psi + \mathbf{v}\frac{\partial\psi}{\partial\mathbf{r}} - e\mathbf{v}\mathbf{E} = \nu(\alpha m\mathbf{v}\mathbf{u}_0 - \psi). \tag{8}$$

The value $\mathbf{u}$ 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 α 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 α in the equation (8) is negative.

Equation (8) can be rewritten in the following form

$$-i\omega\psi + \mathbf{v}\frac{\partial\psi}{\partial\mathbf{r}} + \nu\psi = \mathbf{v}(e\mathbf{E} + \nu\alpha m\mathbf{u}_0). \tag{9}$$

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

$$-i\omega\psi + v_x\frac{\partial\psi}{\partial x} + \nu\psi = v_y(eE_y + \nu\alpha m u_0). \tag{10}$$

We introduce a new function h by using the relation

$$\psi = mv_yv_Fh. \tag{11}$$

The function h is dimensionless.

Let's introduce the designation

$$\mu = \cos\theta.$$

It is convenient to introduce the following dimensionless variables

$$z_0 = \tau(\nu - i\omega)v_F.$$
$$\mu = \frac{v_x}{v_F}, \quad x' = \frac{x}{\tau v_F}.$$

Then the kinetic equation takes the form

$$\mu\frac{\partial h}{\partial x'}+z_0h(x',\mu)=E_0+\frac{3}{4}\alpha\int\limits_{-1}^{1}(1-\mu'^2)h(x',\mu')\,d\mu'. \quad (12)$$

Here

$$E_0=\frac{eE_y\tau}{mv_F}.$$

In the future, the variable x' will be written without dash for short.

Let's calculate the current density j_y

$$j_y=neu_{0x}=\frac{3v_Fne}{4}\int\limits_{-1}^{1}(1-\mu^2)hd\mu.$$

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 (1.10) we find this constant

$$z_0H=E_0+\frac{3}{4}\alpha\int\limits_{-1}^{1}(1-\mu'^2)H\,d\mu'.$$

Or

$$z_0H=E_0+\alpha H.$$

Therefore

$$H=\frac{E_0}{z_0-\alpha}.$$

Calculate the current density j_y

$$j_y=\frac{3v_Fne}{4}\int\limits_{-1}^{1}(1-\mu^2)hd\mu=\frac{v_FneE_0}{z_0-\alpha}.$$

The expression for the electrical conductivity σ has the following form

$$\sigma=\frac{j_y}{E_y}=\frac{ne^2}{m(\nu-i\omega-\alpha\nu)}.$$

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

$$\sigma=\frac{\sigma_0}{1-\alpha-i\omega/\nu}.$$

When $\omega=0$, $\alpha\to1$ 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 $\sigma\to0$. That is, in this case scattering at grain boundaries dominates. Moreover, the grain boundaries become impermeable for the electrons.

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] J. S. Chawla, Gstrein F., K. P. O'Brien, J. S. Clarke and D. Gall, "Electron scattering at surfaces and grain boundaries in Cu thin films and wires," Physical Review B, Vol. 84, p. 235423, 2011.

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

[3] E.H. Sondheimer, "The mean free path of electrons in metals Advances in Physics", 2001, Vol. 50, no. 6, pp. 499-537.

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

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

[6] S. De Gennaro and A. Rettory, "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, 1984.

[7] De Gennaro S. and Rettory A., "Normal electron–electron contribution to the anomalous surface impedance," J. Phys. F., Vol. 15, pp. 227–230, 1985.