Residual resistivity due to wedge disclination dipoles in metals with rotational plasticity

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Abstract

The residual resistivity ρ in metals caused by wedge disclination dipoles is studied in the framework of the Drude formula. It is shown that $\rho \sim L^{-p}$ with $p = 3$ for biaxial and $p = 2$ for uniaxial dipoles (L is a size of dipole arm).

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The effect of dislocations on electric transport in metals has been studied for many decades [1,2,3]. Dislocations serve as effective scattering centers for conducting electrons primarily due to their elastic strain fields. This scattering is essential in the region of the residual resistivity at low temperatures when all other scattering mechanisms are suppressed. However, the problem of disclination-induced charge scattering is not yet investigated in details, despite the fact that these linear defects can play an important role in nanocrystalline [4] and highly deformed metals [5]. Such defects, combined in dipole configurations, have been proposed as primary carries of the rotational plastic deformation in granular materials (see e.g. [6] and references therein) and observed recently in nanocrystalline Fe [7] using the high-resolution transmission electron microscopy. For metallic glasses the concept of disclinations has been worked out in [8] and much earlier for complex alloys in [9].

Theoretically, for the first time, the behaviour of the residual resistivity as a function of the density of defects in simple metals caused by *isolated* wedge disclinations has been studied in [10]. The analysis has been carried out with the assumption that there exist two mechanisms of scattering: due to deformation fields of wedge disclinations and Aharonov-Bohm-like scattering generated by topological nature of disclinations [11]. The deviation from the linear law of the disclination-induced residual resistivity on the concentration of the defects was found.

In this Letter we study the behaviour of the residual resistivity in metals containing wedge disclination dipoles (WDD). Our goal is to find the dependence of the residual resistivity on the value of the dipole arm L. In fact, keeping in mind the models where disclinations are settled in the triple junctions of inter grain boundaries [12,13] or form borders of misorientation band area [14,15], we study how residual resistivity depends on a grain size or a width of misorientation band.

On the other hand, it was found (see e.g. [16,17]) that strain fields caused by WDD are the same as for a finite wall of edge dislocations at large distances from the wall. Hence, the obtained here results can be considered in application to the materials containing dislocation arrays and small-angle grain boundaries. In our picture the dipoles in equilibrium with a mean dipole arm L and strength $\pm\omega$ are placed in xy-plane (disclination lines are oriented along the z-axis). Notice that a disordered distribution of disclination lines only modify the absolute value of a electron mean free path in our calculations. The axes of the rotations can be shifted relative to their lines by arbitrary distances l_1 and l_2. When $l_1 - l_2 = L$ or $l_1 = -l_2$ one gets the uniaxial and symmetrical uniaxial WDD, respectively. In the case when $l_1 \neq l_2 \neq 0$, we have biaxial WDD with shifted axes of rotation (see, e.g., [17,18]).

The effective perturbation energy of electron due to the WDD deformations E_{AB}

is [18]

$$U(x,y) = -G_d Sp E_{AB}(r) =$$

$$-\frac{G_d(1-2\sigma)\omega}{(1-\sigma)4\pi}\left(\ln\frac{(x+L/2)^2+y^2}{(x-L/2)^2+y^2} - l_1\frac{x+L/2}{(x+L/2)^2+y^2} + l_2\frac{x-L/2}{(x-L/2)^2+y^2}\right), \tag{1}$$

where G_d is the deformation-potential constant, σ is the Poisson ratio. For simplicity, in Eq.(1) we have considered only isotropic component of the deformation-potential constant, which is related to the Fermi energy as $(2/3)E_F$ [2]. In this context, in further calculations we use the typical meaning of $G_d = 3.7$eV. It is seen from the Eq.(1) that the WDD strain fields are located in xy-plane. It means that only normal to disclination line component of electron wave vector $\mathbf{k}_\perp$ are involved in scattering process. As a result, the problem reduces to the two-dimensional scattering where the matrix element which determines the transition of electron from Fermi state with wave vector $\mathbf{k}_F = \mathbf{k}_\perp + \mathbf{k_z}$ to state $\mathbf{k}'$ can be written as [2,18]

$$\langle \mathbf{k}_F | U(\rho,\phi) | \mathbf{k}' \rangle = \frac{1}{S}\int d^2\rho \exp[i(k_F - k')\rho\cos(\phi-\alpha)]U(\rho,\phi). \tag{2}$$

Here, S is the projected area, $U(\rho,\phi)$ is perturbation energy given by Eq.(1) in polar coordinates (ρ,ϕ), α is the angle between $\mathbf{q} = \mathbf{k}_F - \mathbf{k}'$ and x-axis.

Using Eqs.(1) and (2) with the general formula for the two-dimensional mean free path

$$l^{-1} = \frac{n_d k_F S^2}{2\pi\hbar^2 v_F^2} \int_0^{2\pi} (1 - \cos\theta) \overline{|\langle \mathbf{k}_F | U(x,y) | \mathbf{k}' \rangle|^2} d\theta, \tag{3}$$

after integration over scattering angle θ, we find the explicit expression for the mean free path as

$$l^{-1} = \frac{B^2 L^2 n_d \pi^2}{4 k_F \hbar^2 v_F^2} \left\{ z^2 \left(\frac{1}{2} + J_0^2(k_F L) \right) + \left(8 - \frac{z(z+8)}{2} \right) (J_0^2(k_F L) \right.$$
$$\left. + J_1^2(k_F L)) - \frac{8}{k_F L} J_0(k_F L) J_1(k_F L) \right\}, \tag{4}$$

where $z = 2(l_1 - l_2)/L$, $B = G_d \omega (1 - 2\sigma)/(1 - \sigma)2\pi$, v_F is the Fermi velocity, $J_n(t)$ are the Bessel functions. In Eqs.(3) and (4) n_d is the areal density of the dipoles, and the bar in Eq.(3) denotes the averaging over α.

Evidently, n_d is a function of the dipole arm L. To determine the relation between n_d and L, notice, that for two dimensional elastically isotropic medium n_d is inversely proportional to the square of the mean distance d between dipoles. In the framework of the dislocation-disclination model of misorientation band [15] the dependence of d on L at the state of equilibrium can be found from the relation

$$qb = \omega d \ln \left(\frac{L^2}{d^2} + 1 \right), \tag{5}$$

where b is the absolute value of a misorientation band Burgers vector, $q \geq 1$ is a dimensionless parameter which account the presence of "statistically-stored" dislocations. For the case when $d > L$ we have $d \approx \omega L^2/qb$, and $n_d \approx 1/d^2 = (qb/\omega L^2)^2$

Our analysis shows that for the mean free path given by Eq.(4) the condition $k_F l \gg 1$ is valid and the classical Drude formula to estimate the residual resistivity can be applied

$$\rho = \left(\frac{mv_F}{ne^2}\right) l^{-1}, \tag{6}$$

where m and n denote mass and electron density, respectively, e is the electron charge.

Thus, the L-dependence of the residual resistivity ρ can be defined numerically on the basis of the Eqs.(4)-(6). The results of the calculations are shown in Fig.1 for all types of WDD with strength $\omega = 36°$.

As is seen from the plot the least contribution to ρ is caused by WDD with $z = 0$, (i.e. $l_1 = l_2$ that corresponds to the symmetrical biaxial dipole), and ρ increases with z increasing. For $z = 2$ (uniaxial WDD) the contribution to ρ is the largest. This noticeable increase of $\rho(z = 2)$ relative to $\rho(z = 0)$ is due to the specific nature of the uniaxial WDD deformation fields. Uniaxial WDD can be simulated by a finite wall of edge dislocations complemented by two additional edge dislocations at both ends of the wall [17]. These two dislocations are represented in Eq.(1) by the second and third terms. Obviously, the residual resistivity due to a uniaxial WDD has a larger value due to the presence of this dislocation part which is absent for

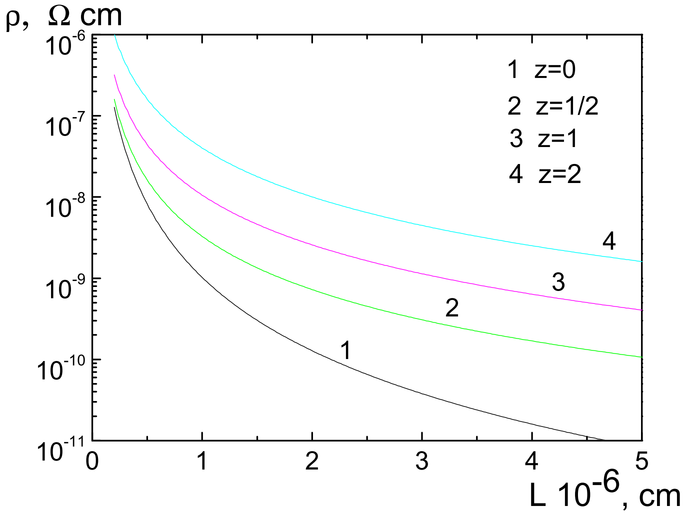

Figure 1: The residual resistivity as a function of the dipole arm of size L for symmetrical biaxial disclination dipole ($z = 0$); biaxial dipole with shifted axes of rotation ($z = 1/2$, $z = 1$); uniaxial dipole ($z = 2$). The curves have been plotted according to Eq.(4) and Eq.(6) with the set of the parameters: $B = 0.1$eV, $v_F \approx 1.2 \times 10^8$cm c^{-1}, $n = 5 \times 10^{22}$cm^{-3}, $m = 0.5 \times 10^6$eV

biaxial WDD. It should be noted that the functional L-dependence of ρ is different for biaxial and uniaxial dipoles. Indeed, $l^{-1} \sim Ln_d$ for Eq.(4) in the limit $k_F l \gg 1$ when $z = 0$. Taking into account the relation $n_d \sim L^{-4}$, we find for biaxial dipole $\rho(z = 0) \sim l^{-1} \sim L^{-3}$. In the case of the uniaxial dipoles $l^{-1} \sim L^2 n_d$, and, hence $\rho(z = 2) \sim l^{-1} \sim L^{-2}$.

The important result of our consideration here is that the residual resistivity increases when L (or,equivalently, granular size) decreases. It is easily understood, because in our approach the L-dependence of n_d has been considered correctly in the framework of the misorientation band model [15]. In [19] the increase of ρ with grain-size decreasing has been found experimentally for nanocrystalline Pd. These results are in qualitative agreement with our calculations.

Fig.2 demonstrates the n_d-dependence of ρ for uniaxial WDD with different strengths of defects ω. This dependence is nonlinear ($\rho(z = 2) \sim n_d^{1/2}$) as one can conclude from the previous reasonings. The nonlinear dependence of ρ has been found in [10] for isolated wedge disclinations as well. Similar result should be expected for edge dislocation walls as we have discussed in the beginning of this paper. Let us note that linear n_d-dependence of ρ had been observed only for isolated dislocations (See [3], and references therein). In addition, one can see from Fig.2 that ρ increases substantially with increasing ω reaching quite large values. For example, for the curve number one $\rho \approx 6 \times 10^{-7}$ Ω cm when $n_d \approx 3 \times 10^{13}$ cm^{-2} (that correspond to the dipole arm L equal to few nanometers).

In conclusion, we would like to mention, that the resistivity due to oriented in some direction disclination dipoles should be anisotropic (as in the case of dislocations [2]). For example, for edge dislocations with glide direction along the x-axis,

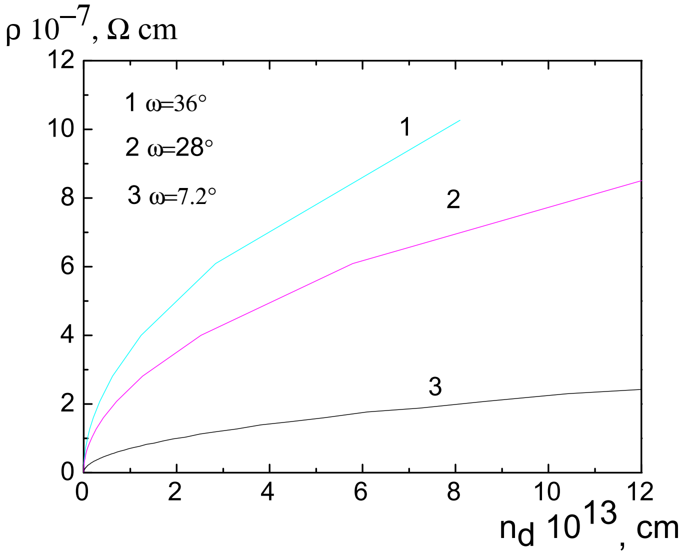

Figure 2: The residual resistivity as a function of the arial density of uniaxial dipoles n_d at different defect strengths ω.

the ratio ρ_x/ρ_y has been found to be equal to $\frac{1}{3}$ [20,21]. Calculations of ρ in different plane directions for disclination dipoles (dislocation walls) will be performed in the near future.

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Figure Captions

Fig.1.The residual resistivity as a function of the dipole arm of size L for symmetrical biaxial disclination dipole ($z = 0$); biaxial dipole with shifted axes of rotation ($z = 1/2$, $z = 1$); uniaxial dipole ($z = 2$). The curves have been plotted according to Eq.(4) and Eq.(6) with the set of the parameters: $B = 0.1$eV, $v_F \approx 1.2 \times 10^8$cm c^{-1}, $n = 5 \times 10^{22}$cm^{-3}, $m = 0.5 \times 10^6$eV .

Fig.2.The residual resistivity as a function of the arial density of uniaxial dipoles n_d at different defect strengths ω .