Electrical conductivity and strength of ultrafine-grained copper containing deformation vacancies, alloying atoms and dislocations

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Abstract. The processes of electron scattering by crystal lattice defects such as vacancies, impurity atoms and dislocations are considered. The refined values of the sizes of the regions of interaction of electrons with the defects are obtained. The contribution of these defects to the resistivity and strength of the nanostructured Cu-0.5wt.% Cr alloy is estimated.

1. Introduction
In order to increase the strength properties of metallic materials, they are subjected to severe plastic deformation (SPD), which allows introducing various crystal lattice defects into the material. The influence of defects on the mechanical strength of ultrafine-grained materials obtained by SPD has been thoroughly studied. To analyze the effect of structural defects on physical properties and to predict their changes depending on the factors to which they are sensitive, the appropriate analytical dependencies between the quantities characterizing them are necessary. In particular, materials with high strength and sufficient electrical conductivity are in demand [1]. The introduction of a large number of dislocations into the material strengthens the material. The calculation of their contribution to the resistivity, performed in [2], establishes its dependence on the density of dislocations and the size of the region of interaction of an electron with a dislocation (size of the dislocation core). The estimates, based on the obtained analytical dependence [2] showed the correspondence with the known experimental data in order of magnitude. The purpose of this paper was to calculate the average scattering probability per unit time of an electron on vacancies and impurity atoms, which makes it possible to determine the contribution to the resistivity of the specified point defects. Comparison of the results with known experimental data will allow us to obtain refined data on the dimensions of the regions of interaction of an electron with the lattice imperfections under consideration.

2. Specific resistance and strength of metals containing vacancies
The contribution to the resistivity of metals of defects in the crystal lattice depends on the probability \( P \) of the scattering of electrons by them per unit time, which is determined by the dimensions of the scattering region. To calculate the value of \( P \), it is necessary to specify the form of the scattering potential \( U \).

Consider a system of \( N_e \) electrons-non-interacting fermions with spin \( \frac{1}{2} \), enclosed in a volume \( V \) at a temperature \( T=0 \). The solutions of the Schrödinger equation for a free particle have the form of plane waves: \( \psi_k = \exp(\mathbf{i} \mathbf{k} \cdot \mathbf{r}) \), where \( \mathbf{r} \) is the radius vector, \( \mathbf{k} \) is the wave vector. The density of electronic...
states in a metal (the density of allowed electron states in a single energy interval) is equal to

\[ g(E) = \frac{d(N_e / V)}{dE} = \frac{dn_e}{dE} = \frac{3n_e}{2E^2} \sqrt{\frac{E}{E^2}}. \]  

At the Fermi level \( g(E_r) = 3n_e / 2E_r \), where \( n_e \) is the bulk density of electrons, \( E_r \) is the Fermi energy. The potential of the vacant region is defined as \( U = n_e / g(E_r) = (2/3)E_r \) [2]. If the probability \( P \) of the fact that an electron per unit of time experiences a collision with a vacancy is known, then the relaxation time is \( \tau = 1/P \). Only the electrons in the vicinity of the Fermi energy are scattered. We represent the density of quantum states in the form \( \rho = \frac{dN_e}{dE} = km^* \sqrt{2\pi / h} \), where \( m^* \) is the effective mass. Then the scattering probability (2) takes the form

\[ P = A \frac{\sin^2(kl\sin(\Theta / 2))}{k^2l^2\sin^2(\Theta / 2) / 4\pi^3h^2u^*} \int dw. \]  

Then the contribution to the resistivity of vacancies is determined by the expression:

\[ \rho_v = \frac{m^*}{n_e^{\*2}} \frac{1}{\tau} \frac{k^3h^2l^4C_{uv}}{9m^{*2}n_e^{\*2}} \left[ 1 - \frac{2k^{2}l}{2k^{2}l} \right]. \]  

According to well-known theoretical estimates [3 - 5], the contribution to the resistivity of noble metals per one percent of vacancies is equal to \( \rho_v = 1.5 \mu\Omega\cdot\text{cm/at}\% \), which coincides with the experimental values. Also known are the values obtained by a number of authors for copper, equal to 1.64 [6], 1.70 [7] and 1.73 \mu\Omega\cdot\text{cm/at}\% [8]. The contribution of vacancies to the resistivity of copper, according to formula (7), is equal to \( \rho_v \approx 1.0C_{uv} \mu\Omega\cdot\text{m}, or 1.0 \mu\Omega\cdot\text{cm/at}\% \), if we assume that the
volume of the interaction region is equal to \( l^3 = a^3 / 4 \), where \( a \) is the lattice parameter. The obtained estimate is lower than the known theoretical estimates. The result obtained in this paper using the potential \( U \) [2] depends on the size of the interaction region \( l \) and corresponds to the known data in order of magnitude. At \( l = 1.06b \), the increase in the resistivity of copper is \( \rho_v \approx 1.73 \ \mu\Omega\cdot\text{cm/at.\%} \). In the SPD process, many deformation vacancies are formed. Their concentration can reach values of \( C_v = 10^5 \), the value \( \rho_v \) is respectively \( 1.73 \times 10^3 \ \mu\Omega\cdot\text{cm} \). At the same time, the resistivity of pure copper at room temperature is equal to \( \rho_v \approx 1.724 \ \mu\Omega\cdot\text{cm} [1] \). Thus, the contribution of vacancies to the electrical conductivity is very small.

The effect of vacancies on the strength and ductility of the metal is small and can be neglected.

3. Specific resistance and strength of metals containing impurity atoms

The introduction of an impurity atom into the crystal lattice leads to a change in its potential, which can be represented as the appearance of a Coulomb field of a point charge having the order of the elementary charge \( e \). Scattering on a dissolved atom occurs as a result of the interaction of a free electron with this potential. The dependence on the distance \( r \) of the potential \( \varphi \) of the point charge \( q \) surrounded by an electron Fermi gas has the form \( \varphi = qe^{-br} / r \) [9]. The Coulomb potential of a point charge is screened at distances \( r > 1/\delta \), where \( 1/\delta \approx 0.554 \times 10^{-10} \) m for copper. The contribution to the resistivity of impurity atoms the volume concentration of which is \( C_{\text{at}} \), is calculated by the formula

\[
\rho_{\text{at}} = m_{\text{at}} C_{\text{at}} S_a / n_e e^2.
\]

The scattering cross section is \( S_a = \pi r^2 \). If the screening length is assumed to be \( r = 3/\delta \), then at an atomic concentration of \( C_{\text{at}} = C_{\text{at}} / n_e = 6.1 \times 10^{-3} \) (0.5 wt\%), the increase in the resistivity of copper is \( \rho_{\text{at}} = 2.96 \ \mu\Omega\cdot\text{cm} (\rho_{\text{at}} = 4.85 \ \mu\Omega\cdot\text{cm/at.\%}) \).

The resistivity due to scattering of electrons by alloying atoms can also be calculated from formula (7) using the atomic concentration \( C_{\text{at}} \) of atoms. The results of the calculations lead to the value of \( \rho_{\text{at}} \approx 3.14 \ \mu\Omega\cdot\text{cm} \) for \( l = 1.35b \) and \( C_{\text{at}} = 6.1 \times 10^{-3} \) (\( \rho_{\text{at}} = 5.15 \ \mu\Omega\cdot\text{cm/at.\%}) \).

The solid-solution hardening is proportional to the value of \( C_{\text{at}}^{1/2} \). Practically, the dependence of hardening on concentration does not differ from linear [10]. In the case of the Cu-0.5 wt.% Cr alloy, its contribution can be neglected.

4. Specific resistance and strength of metals containing dislocations

To calculate the resistivity due to the presence of dislocations in the material, we can use the method described above to calculate the same for vacancies. It is assumed that electron scattering takes place at the dislocation core. The scattering potential is equal to \( U \). The interaction region is represented in the form of a rectangular parallelepiped whose volume is equal to \( Ll^2 \). The averaged probability of scattering per unit time for an electron with a wave number \( k \) on \( N_{\text{disl}} = \rho_{\text{disl}} L^2 \) dislocations is determined by the formula

\[
\langle P_\chi \rangle = \frac{1}{\tau_k} = \frac{k^2 \hbar^2 L}{9m^*V}\rho_{\text{disl}} L^2 \left[ 1 - \sin 2kl \right] / 2kl.
\]

This formula leads to the value of the resistivity per unit dislocation density in copper \( \rho_{\text{disl}} = 5.24 \times 10^{-26} \ \Omega\cdot\text{m}^3 \) for the size of the interaction region \( l = a / \sqrt{\lambda} \) [2]. The values of \( 0.78 \times 10^{-25} \) and \( 1.9 \times 10^{-25} \ \Omega\cdot\text{m}^3 \) were obtained in [11, 12], respectively. At the same time, experimental data are known that are equal to \( 1.6 \pm 0.2 \times 10^{-25} \) [13], \( 1.7 \times 10^{-25} \) [14], \( 1.8-2.3 \times 10^{-25} \ \Omega\cdot\text{m}^3 \) [15, 16]. The result, consistent with the experimental data \( \rho_{\text{disl}} = 1.7 \times 10^{-25} \ \Omega\cdot\text{m}^3 \), can be obtained using formula (8) for the scattering area sizes equal to \( l = 1.55b \).

The electrical conductivity of the Cu-0.5 wt.% Cr alloy subjected to 4 passes of equal-channel angular pressing is 35% IACS (\( \rho = 4.93 \times 10^{-8} \ \Omega\cdot\text{m} \)) [17]. The characteristic value of the dislocation density is \( \rho_{\text{disl}} = 8.33 \times 10^{14} \) m\(^2\), whose contribution to the resistivity of the alloy is \( \rho_{\text{disl}} = 1.42 \times 10^{-10} \ \Omega\cdot\text{m} \).

Taking into account the contribution of vacancies \( (C_v = 10^4, \rho_v = 1.73 \times 10^{-3} \ \mu\Omega\cdot\text{cm}) \) and the resistivity of pure copper, it is possible to determine the resistivity due to the alloying chromium atoms: \( \rho_c = \rho - \rho_v - \rho_{\text{disl}} \).
\( \rho_{\text{disl.}} = 3.19 \cdot 10^{-8} \, \Omega \cdot \text{m} \), which corresponds to the dimensions of the interaction region of atoms with electrons, equal to \( l \approx 1.354b \).

The dislocation hardening is described by the dependence 
\[ \sigma_{\text{disl. tot}} = M \alpha G b \rho \]  
[18], where \( \alpha \) is the coefficient [17], \( \alpha = 0.37 \). \( M \) is the Taylor factor, \( M = 3.06 \). The shear modulus is \( G = 42.1 \, \text{GPa} \). In the specified state of the alloy, Cu-0.5wt.% Cr \( \sigma_{\text{disl}} \approx 352 \, \text{MPa} \).

5. Summary and conclusions

The results obtained by the formulas presented in the paper agree with the experimental data in order of magnitude. From the known experimental data, the dimensions of the region of interaction of electrons with crystal lattice defects can be refined, which makes it possible to improve the accuracy of estimates. Vacancies have the smallest area of scattering (\( l \approx 1.06b \)), dislocations - the largest (\( l \approx 1.55b \)). The region of interaction of atoms is \( l \approx 1.35b \). As follows from the calculations, the resistivity of the Cu-0.5wt.% Cr alloy is substantially increased by chromium atoms dissolved in the matrix, which do not exert a noticeable effect on its strength. The presence of vacancies and dislocations does not have any noticeable effect on the electrical conductivity of the material. At the same time, dislocations strengthen the material.

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