Conduction-electron-spin resonance linewidth due to edge dislocations*

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Recently, Beuneu and Monod measured both the electrical resistivity ρ and the conduction-electron spin resonance linewidth (CERSLW) $1/2\Delta H$ as a function of the density of dislocations C in cold-worked Cu, Ag, and Al metals. Here we calculate theoretically the spin-orbit induced CESRLW $1/2(\Delta H)_{ed}$ in the case of scattering by dislocations using a model structure factor for edge dislocations that reproduces the experimental ρ. It is shown that for Ag and Cu, $1/2(\Delta H)_{ed}$ coincides with the experimental values within the errors involved. However, in the case of Al, $1/2(\Delta H)_{ed}$ is three orders of magnitude smaller than the observed value. This gives indication that in this regard solid Al does not behave like a free-electron gas, which is probably related to large effects due to its anisotropic Fermi surface. Liquid Al, however, should have an isotropic Fermi surface and the theoretical value of $1/2(\Delta H)_{ed}$ for this case is calculated, which would be interesting to compare with experiment.

I. INTRODUCTION

The relaxation times corresponding to many electronic transport coefficients of metals have been written as integrals of the form[1,2]

$$\frac{1}{\tau_f} = \int_0^{2k_F} dq\, |V_q|^2 S_E(q) f(q) \tag{1}$$

with

$$S_E(q) = \frac{1}{4\pi} \int d\Omega_{\vec{q}} \int_{-\infty}^{\infty} d\omega\, S'(\vec{q}, \omega) \frac{\beta\omega}{e^{\beta\omega} - 1}, \tag{2}$$

where $S'(\vec{q}, \omega)$ is the inelastic part of the dynamical structure factor of Van Hove.[3] $|V_{\vec{q}}|^2$ is the electron-ion interaction pseudopotential and $f(q)$ is a function whose form depends on the coefficient considered. $\beta = \hbar/k_B T$ and k_F is the Fermi wave vector. $\hbar$ is Planck's constant, k_B is Boltzmann's constant, and T is the absolute temperature. The integrals involve an average over all directions of the vector $\vec{q}$. The usefulness of this approach in the calculation of electronic transport coefficients lies in the fact that an empirical dynamical structure factor can be used. Thus, the actual ionic structure of the metal, including its temperature dependence, as well as the umklapp processes are automatically taken into account. This is, for instance, the case in the calculation of the resistivity due to phonons.[4] However, to the best of our knowledge, neither x-rays nor slow-neutron scattering experiments have been performed on cold-worked metals which provide information about the structure factor corresponding to dislocations at large momentum transfers.[5] The purpose of this paper is to propose a model structure factor for edge dislocations which can be used in Eq. (1) to evaluate the contribution of dislocations to the transport coefficients. The structure factor proposed contains a single parameter which can be adjusted, for instance using resistivity data, and later on used to calculate any other transport coefficient. In particular we calculate the conduction-electron-spin resonance linewidth (CESRLW) produced by edge dislocations in cold-worked Cu, Ag, and Al and compare the results with data obtained by Beuneu and Monod.[6] For Cu and Ag the agreement is good. For Al there is a large discrepancy which may be associated with the highly anisotropic Fermi surface[6] of solid Al. In order to test if this is the case, we also calculate the CESRLW of liquid Al, whose Fermi surface should be isotropic. This result should be susceptible of direct comparison with experiment.

II. MODEL

The field of deformation due to an edge dislocation[7] in a metal has been studied in a continuum model[8] and also on an atomic level.[9,10] The contribution of this deformation field to the resistivity has been extensively discussed in the literature.[10-18] The continuum model underestimates the resistivity by factors of 10 to 50.[16,18] The disagreement has been attributed to the fact that the continuum model does not describe properly the core of the dislocation, which is the region that contributes overwhelmingly to the electron scattering. It has been shown that a model in which the dislocation is described by a hollow cylinder with a radius of the order of the interatomic distance leads to a resistivity which is much closer to the experimental data.[16,17]

Here, in order to calculate the structure factor corresponding to the deformation produced by edge

dislocations, we describe the deformation field by the continuum model at radial distances $r > r_0$ and by a hollow cylinder for $r < r_0$. Here r_0 is an adjustable parameter (of the order of the interatomic distance) that depends on the material.[19]

In the continuum model the dilatation field corresponding to an edge dislocation is given by[7,20]

$$\Delta(r,\theta) = \frac{-b}{2\pi}\,\frac{1-2\nu}{1-\nu}\,\frac{\sin\theta}{r}, \tag{3}$$

where b is the modulus of the Burger's vector and ν is the Poisson ratio. The axis of the dislocation defines the z-coordinate axis, r is a radial distance from the axis of the dislocation in the x-y plane, and θ is the angle between the radius vector $\vec{r}$ and the Burger's vector $\vec{b}$ which defines the x-direction. The density field is given by

$$D(r,\theta) = \frac{D_0}{1-\Delta} \simeq D_0(1+\Delta), \tag{4}$$

where D_0 is the number of atoms per unit volume in the unstrained crystal.

Thus, in our model, the density field is approximated by[21]

$$D(r,\theta) = \begin{cases} D_0(1+\Delta) & \text{for } r > r_0, \\ 0 & \text{for } r < r_0. \end{cases} \tag{5}$$

From this density field we substract the constant density D_0 which does not contribute to the electronic scattering. In a proper atomic treatment, D_0 would lead to Bragg scattering, which is usually taken into account through an effective electron mass. Therefore, the differential density field d is

$$d(r,\theta) = \begin{cases} D_0\Delta(r,\theta) & \text{for } r > r_0, \\ -D_0 & \text{for } r < r_0. \end{cases} \tag{6}$$

Its Fourier transform $d_{\vec{q}}$ is

$$d_{\vec{q}} = \frac{4\pi^2 D_0 r_0^2 \delta(q_z)}{q_\perp r_0}\left(-J_1(q_\perp r_0) - i\,\frac{b}{2\pi r_0}\,\frac{1-2\nu}{1-\nu} \times J_0(q_\perp r_0)\sin\phi\right). \tag{7}$$

Here, $\vec{q} = (q_\perp\cos\phi, q_\perp\sin\phi, q_z)$, where ϕ is the angle between the component of $\vec{q}$ in the x-y plane ($q_\perp$) and the x axis.

We assume that the density field is static, which should be an extremely good approximation since the times involved in dislocation displacements are extremely long compared to $k_B T$.[22] Then Eq. (2) reduces to

$$S_E(q) = \frac{1}{4\pi}\int d\Omega_{\vec{q}}\, S(\vec{q}), \tag{8}$$

where $S(\vec{q})$ is the static structure factor. By definition

$$S(\vec{q}) = |d_{\vec{q}}|^2 = \frac{(2\pi)^3 L D_0^2 r_0^4 \delta(q_z)}{(q_\perp r_0)^2} \times \left[J_1^2(q_\perp r_0) + \left(\frac{b(1-2\nu)}{2\pi(1-\nu)}\right)^2 \times \frac{1}{r_0^2} J_0^2(q_\perp r_0)\sin^2\phi\right], \tag{9}$$

where we have used the relation $\delta^2(q_z) = (L/2\pi)\delta(q_z)$. Here L is the length of the sample.[23] If there are n parallel dislocations, the structure factor to be used in the proper transport equations[18] is

$$nS(\vec{q}) = \frac{(2\pi)^3 NCD_0 r_0^4 \delta(q_z)}{(q_\perp r_0)^2} \times \left[J_1^2(q_\perp r_0) + \left(\frac{b(1-2\nu)}{2\pi(1-\nu)}\right)^2 \times \frac{1}{r_0^2} J_0^2(q_\perp r_0)\sin^2\phi\right], \tag{10}$$

where C is the number of dislocations per cm^2 and N the number of atoms in the sample. This form of the structure factor leads, of course, to anisotropic transport coefficients. The result (10) contains the assumption that the dislocations scatter incoherently.

If there are n dislocations randomly oriented we proceed to do the angular integrations indicated in Eq. (8)

$$nS(q) = \frac{n}{4\pi}\int d\Omega_{\vec{q}}\, S(\vec{q}) = \frac{4\pi^3 NCD_0 r_0^2}{q^3} \times \left[J_1^2(qr_0) + \frac{1}{2r_0^2}\left(\frac{b(1-2\nu)}{2\pi(1-\nu)}\right)^2 J_0^2(qr_0)\right]. \tag{11}$$

III. RESISTIVITY

The resistivity is given by

$$\rho = m/D_0 Z e^2 \tau_f, \tag{12}$$

where m is the electron mass, e is the electron charge, and Z is the number of conduction electrons per atom. The relaxation time τ_f is given by Eq. (1) with

$$f(q) = [2m/\hbar^3 N/3(2\pi)^2 D_0^2 Z]\, q^3. \tag{13}$$

We have calculated the resistivity for Cu, Ag, and Al, using the constants given in Table I and the pseudopotentials of Ref. 24 and 25 for Cu and Ag, and for Al, respectively. In the same table are shown the values of r_0 adjusted using experimental data, taken from Ref. 6.

TABLE I. Values of the various quantities used in the calculation of the resistivity induced by dislocations in Cu, Ag, and Al.

Metal	b[a] (Å)	ν[a]	k_F (cm^{-1})	D_0 (10^{23} atoms/cm^3)	Resistivity per dislocation[b] (10^{-10} nΩ cm^3)	r_0 (Å)
Cu	2.55	0.35	1.36	0.85	1.3	2.81
Ag	2.89	0.37	1.20	0.58	1.9	3.62
Al	2.86	0.34	1.75	0.60	1.8	5.52

[a]Reference 7. [b]Reference 6.

The resulting structure factors calculated with these parameters are shown in Fig. 1. In the following, we assume that such structure factors can be used to estimate other transport coefficients.

The values obtained for the resistivity per dislocation within the continuum theory (with $r_0 = 0$) are $\rho^c_{Ag} = 0.017 \times 10^{-10}$ nΩ cm^3, $\rho^c_{Cu} = 0.020 \times 10^{-10}$ nΩ cm^3, and $\rho^c_{Al} = 0.011 \times 10^{-10}$ nΩ cm^3. We see that the purely continuum model underestimates the resistivity by a factor ranging from 50 to 100.

IV. CESR LINEWIDTH

The conduction-electron-spin resonance (CESR) relaxation time T was calculated for Cu, Al, and Ag, using Eq. (14) of Ref. 2, which is valid only within the free electron model. The core-electron wave functions of the ions in the metal were approximated by the atomic wave functions tabulated by Herman and Skillman.[26] The structure factors $S(q)$ given by Eq. (10), with the corresponding values of r_0 (Table I) which reproduce the correct resistivity, were used. The results are presented in Table II together with the experimental values.

The same theory was used to calculate the CESRLW of liquid Al at 700 °C using the structure factor reported in Ref. 27. The result is also reported in Table II.

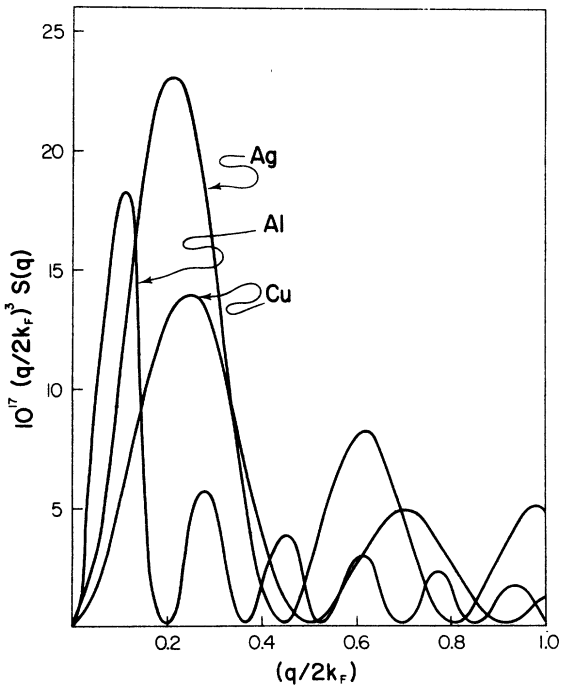

FIG. 1. Static structure factors of Al, Ag, and Cu per edge dislocation averaged over all directions.

V. DISCUSSION

This calculation involves several approximations: (a) The theory of Ref. 2 is appropriate for light simple metals whose Fermi surface lies completely within the first Brillouin zone and where anisotropy effects are not very important. These are the cases of Na, K, and their alloys.[28] Although with less accuracy, the theory may still be applied to Ag and Cu. In the case of Al, the Fermi surface extends up to the third Brillouin zone and anisotropy effects may become very important. For such cases the theory should be revised. It is not possible to give a simple estimate of the order of magnitude of the corrections to the present theory due to anisotropy. However, for liquid Al, with an isotropic Fermi surface, the above theory should again be a good approximation. (b) The use

TABLE II. Experimental and theoretical CESR linewidths for Ag, Cu, and Al.

Cold-worked metal	$\frac{1}{2}\Delta H$ experimental[a] (10^{-10} G cm^2)	$\frac{1}{2}\Delta H$ theoretical (10^{-10} G cm^2)
Ag	4.2	3.35
Cu	1.5	0.30
Al	4.7	0.002
Liquid Al	...	$\frac{1}{2}\Delta H = 501$ G

[a]Reference 6.

of a single orthogonalized plane wave to describe the conduction electrons leads to overestimates of the spin relaxation time. The corrections should be negligible for Al but they may be of up to a factor of 2 for heavier metals.[28] (c) It is assumed that the model structure factor fitted to the resistivity can be applied to estimate other transport coefficients. This is not necessarily correct because the structure factor is weighted by different functions in the calculation of the various transport coefficients. However, the hollow-cylinder model for the edge dislocations is not unreasonable and we do not think that the use of a more-refined model will change the results in order of magnitude. (d) The experimental data for ρ vs C used to obtain the parameter r_0 may involve an error of 50% in C due to the difficulty in counting the dislocations under the microscope (they constitute a complicated network).

In view of this, we consider that the theoretical results for the CESRLW of Cu and Ag are in agreement with the experimental values within the theoretical approximations and the experimental errors. However, there is a large discrepancy in the case of Al. We think that it is mainly due to the highly anisotropic Fermi surface of Al, whose effects are not described by this theory. A possible test of this conjecture is to compare the predictions of this theory for liquid Al with experimental data.

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