Dragging and deceleration of mobile defects in metals by conduction electrons. Role of electron dispersion law

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It is shown that dragging and deceleration of defects (ions, atoms, dislocations) by conduction electrons in metals depends substantially on the electron dispersion law. Electrons and holes drag defects in opposite directions, whereas the contributions of decelerated defects are additive.

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The interaction of conduction electrons with defects in metals makes a substantial and frequently decisive contribution to the acceleration and deceleration of mobile defects. Ion motion due to the action of "electron wind"[1,2] and acceleration and deceleration of dislocations[3,4] depend significantly on the interaction of the defects with the conduction electrons. An important role is played here by the character of the electron spectrum–the electron dispersion law. The role of the dispersion law was investigated in detail in mass transport phenomena due to the electron wind, but the theory of the dragging and deceleration of dislocations by conduction electrons[3,4] is restricted to the free-electron approximation and gives therefore no idea of how these phenomena can be changed in metals with complicated electron dispersion.

We shall consider the dragging and deceleration of defects by electrons within the framework of the electron-wind model.[2] Let a certain defect move in the metal with velocity $\mathbf{V}_d$, and let an electric field E be maintained and a current of density j flow in the metal. The general expression for the electron-wind force is of the form[2]

$$\mathbf{F}=\frac{2}{(2\pi)^3 N_d}\iint_{\mathbf{k}\mathbf{k}'}\sum_{\mathbf{b}_g}(\hbar\mathbf{k}-\hbar\mathbf{k}'-2\pi\mathbf{b}_g)W_{\mathbf{k}\mathbf{k}'}^{\mathbf{b}_g}f(\mathbf{k})[1-f(\mathbf{k}')]d^3\mathbf{k}d^3\mathbf{k}', \quad (1)$$

where $\mathbf{b}_g$ is the reciprocal-lattice vector, N_d is the defect density, $f(\mathbf{k})$ is the nonequilibrium distribution function of the electrons, and $W_{\mathbf{k}\mathbf{k}'}^{\mathbf{b}_g}$ the probability of the transition of the electrons from the state $|\mathbf{k}\rangle$ to the state $|\mathbf{k}'\rangle$ when scattered by a defect. We neglect hereafter umklapp processes, assuming that $W_{\mathbf{k}\mathbf{k}'}^{\mathbf{b}_g}=0$ at $\mathbf{b}_g\neq 0$.

Expression (1) can be written in the form

$$\mathbf{F}=\frac{2}{(2\pi)^3 N_d}\int\frac{\hbar\mathbf{k}}{\tau_d}f_1(\mathbf{k})d^3\mathbf{k}, \quad (2)$$

where τ_d is the time of electron relaxation when scattered by defects.

Neglect of umklapp processes and the use of the τ approximation make it possible to obtain final expressions that are physically lucid, but the entire approach is then not quite rigorous. The experience of the entire electron theory of metals shows that a similar simplification is needed to clarify those features of the phenomenon which are lacking in the free-electron approximation and are not directly connected with the actual scattering mechanism. Principal attention will therefore be paid here just to the electron dispersion law, or more accurately speaking, to the geometry of the Fermi surface.

Of course, it must be borne in mind that the relaxation time τ_d depends on the electron dispersion law. This would have to be taken into account in quantitative calculations of the dragging and deceleration effects. We, however, are interested here in the qualitative aspect of the process. Neglect of the umklapp transforms the quasimomentum into the true momentum[5] and makes it possible by the same token to use the Galileo transformation.

To be able to take into account the motion of the defect, we change to a coordinate frame that moves together with the defect with velocity $\mathbf{V}_d$. In this coordinate frame, the electron distribution function is of the form

$$f'(\varepsilon)=f(\varepsilon-\hbar\mathbf{k}\mathbf{V}_d). \quad (3)$$

Since $\hbar\mathbf{k}\cdot\mathbf{V}_d\ll\varepsilon(\mathbf{k})$, we have in the linear approximation

$$f'(\varepsilon)=f(\varepsilon)-\frac{\partial f_0}{\partial\varepsilon}\hbar\mathbf{k}\mathbf{V}_d. \quad (4)$$

Since current flows in the metal, we have in the approximation of the electron relaxation time in the lattice

$$f(\varepsilon)=f_0(\varepsilon)-\frac{\partial f_0}{\partial\varepsilon}e\mathbf{v}\mathbf{E}\tau_L, \quad (5)$$

where E is the electric field intensity, e is the electron charge, and τ_L is the mean free path of the electron in the lattice and determines the electric resistivity of the metal.

Thus, the nonequilibrium increment to the distribution function $f_1(\mathbf{k})$ in the laboratory frame is equal to

$$f_1(\mathbf{k})=-\frac{\partial f_0}{\partial\varepsilon}e\mathbf{v}\mathbf{E}\tau_L+\frac{\partial f_0}{\partial\varepsilon}\hbar\mathbf{k}\mathbf{V}_d. \quad (6)$$

Substituting (6) in (2) we obtain the following expression for the force exerted on the defect by the electrons:

$$\mathbf{F}=-\frac{2}{(2\pi)^3 N_d}\int\frac{\hbar\mathbf{k}}{\tau_d}\frac{\partial f_0}{\partial\varepsilon}\{e(\mathbf{v}\mathbf{E})\tau_L-\hbar(\mathbf{k}\mathbf{V}_d)\}d^3k. \quad (7)$$

We see that this force consists of two components:

$$\mathbf{F}=\mathbf{F}^{(dr)}+\mathbf{F}^{(dec)}. \quad (8)$$

$\mathbf{F}^{(dr)}$ is the electric-wind force acting on the defect 2:

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$$F_i^{(dr)}=-\frac{2e}{(2\pi)^3N_d}\int\frac{\hbar k_i}{\tau_d}\frac{\partial f_0}{\partial\varepsilon}\mathbf{v}\mathbf{E}\tau_L d^3k=Z_{is}E_s, \tag{9}$$

where Z_{is} is the tensor of the effective charge of the defect dragging by the electrons:

$$Z_{is}=-\frac{2e}{(2\pi)^3N_d}\int\hbar k_i v_s\frac{\partial f_0}{\partial\varepsilon}\frac{\tau_L}{\tau_d}d^3k. \tag{10}$$

Recognizing that

$$-\partial f_0/\partial\varepsilon=\delta(\varepsilon-\varepsilon_F),$$

we have

$$Z_{is}=\frac{2e}{(2\pi)^3N_d}\oint_{s_F}\frac{\hbar k_i v_s}{v}\frac{\tau_L}{\tau_d}ds_F, \tag{11}$$

where ds_F is the element of area on the Fermi surface.

The second term $F^{(dec)}$ is the force of deceleration of the defect by the electrons:

$$F_i^{(dec)}=-B_{is}V_{ds}=\frac{2}{(2\pi)^3N_d}\int\frac{\hbar k_i}{\tau_d}\frac{\partial f_0}{\partial\varepsilon}(\hbar\mathbf{k}\mathbf{V}_d)d^3k, \tag{12}$$

where B_{is} is the tensor of the coefficients of the defect deceleration by the electrons

$$B_{is}=-\frac{2}{(2\pi)^3N_d}\int\frac{\hbar k_i\hbar k_s}{\tau_d}\frac{\partial f_0}{\partial\varepsilon}d^3k=\frac{2}{(2\pi)^3N_d}\oint_{s_F}\frac{\hbar k_i\hbar k_s}{\tau_d}ds_F. \tag{13}$$

Recognizing that in the free-electron approximation $\mathbf{j}=en\langle\mathbf{v}\rangle$, where $\langle\mathbf{v}\rangle$ is the drift velocity of the conduction electrons and n is their density, we obtain from (7), (9), and (12) the following expression for the total force (cf. Ref. 4):

$$\mathbf{F}=(\langle\mathbf{v}\rangle-\mathbf{V}_d)nmv_F\sigma_d=\frac{j}{e}\left(1-\frac{V_d}{\langle v\rangle}\right)mv_F\sigma_d, \tag{14}$$

where m is the electron mass, v_F is the electron velocity on the Fermi surface, and σ_d is the cross section for the electron scattering by the defect.

Different defects, such as ions, atoms, dislocations, or crowdions, have different scattering cross sections. If the moving defect is of atomic size ("pointlike"), then

$$\sigma_d\sim(10^{-15}-10^{-16})\ \text{cm}^2.$$

If the moving defect is a dislocation ("linear" defect), then $\sigma\sim b$ per unit length of the dislocation, where b is the Burgers vector. Thus, the force on a dislocation, normalized to unit dislocation length, is equal to

$$\mathbf{F}\approx n(\langle\mathbf{v}\rangle-\mathbf{V}_d)mv_Fb. \tag{15}$$

In the case of complicated dispersion law, however, the expressions for Z_{is} and B_{is} can change significantly. To illustrate this, we consider the band model of a metal (electron and hole bands) with a quadratic dispersion law. For such a metal we obtain, summing the contributions of both bands:

$$Z=enl\sigma_d-enl^{(h)}\sigma_d^{(h)}, \tag{16}$$

$$B=nmv_F\sigma_d+nm^{(h)}v_F^{(h)}\sigma_d^{(h)}, \tag{17}$$

l is the electron mean free path, the superscript h refers to holes ($m^h>0$), and the electrons and holes produce forces that drag the defect in opposite directions. In the decelerating force, the contributions of the electrons and the holes are summed. Thus, in metals in which the hole wind predominates ($Z>0$), the dislocations will be dragged by the current towards the cathode, whereas in electronic metals ($Z<0$) the dragging is towards the anode. This may turn out to be important when it comes to explaining the mechanism of the electroplastic effect.[6] By observing the motion of single dislocation under the influence of the current, in n- and p-type metals, it becomes possible to explain fully this phenomenon. Metals with predominant "hole wind" can be chosen by using experiments on electron transport. These include β-Zr, W, Mo, γ-Fe and Co, in which $Z>0$.[7]

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