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Self-Consistent Description of the Effect of Point Defects on Spectrum and Dynamic Deceleration of Dislocations

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A self-consistent equation of dislocation motion in elastic fields created by defects is obtained. The deceleration force value is calculated due to defect collisions and it is shown to have a quasi-viscous character under low velocities.

Получено самосогласованное уравнение движения дислокации в упругих полях, созданных дефектами. Вычислена величина силы торможения за счет столкновения с дефектами и показано, что при низких скоростях она имеет квазивязкий характер.

1. Introduction

To study dynamic deceleration of dislocations in a medium containing point defects the Granato-Lücke model is commonly used, i.e. a dislocation is treated as a string whose vibrational spectrum is described by a linear dispersion law [1 to 4]. The effect of point defects on the dislocation vibrational spectrum is usually not taken into account. In this case the deceleration force of the dislocation varies inversely as dislocation velocity and depends linearly on the concentration of defects and is quadratic over the misfit parameter. The available experiment does not, however, conform these dependences. Thus, the force of dislocation deceleration by defects in copper found in [5] depends linearly on the velocity and the misfit parameter and is proportional to the square root of the defect concentration.

In the dynamic region of velocities the dislocation executes an overbarrier slip, i.e. its kinetic energy is greater than the energy of the interaction with the defects. But still in this region the character of overcoming the local fields of the defect may be different for different velocity intervals. Let the dislocation move with mean velocity v. We denote the radius of the defect by a, the velocity of transverse sound by c_t, the mean distance between defects by $l \sim n^{-1/3}$, where n denotes the concentration. If the dislocation moves with a velocity at which the dislocation–defects interaction time is less than the time of perturbation propagation along the dislocation at distance l, i.e. $(a/v) \ll l/c_t$, then defects interact with the dislocation independently and the dislocation overcomes them in turn. Otherwise $(a/v \gg l/c_t)$ the dislocation interacts with many defects simultaneously. It is clear that the case of collective interaction between the defects and the dislocation should differ from that of independent single collisions. In particular, the velocity dependence of the deceleration force should be different in these cases (see [2]). The velocity region $v \gg c_t a/l$ was studied in [2 to 4]. As was stated above, in this region the deceleration force is proportional to v^{-1}.

In this paper an attempt has been done to study the velocity regions where the interaction of defects with the dislocation is of collective character.

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2. Dislocation Vibrational Spectrum

Let us consider an infinite edge dislocation moving in a field of randomly distributed defects under uniform constant external stress σ_0. In the stationary case when the external force $F \sim b\sigma_0$ is balanced by the defect deceleration force, the dislocation, as a unit, is moving with a constant velocity, but separate dislocation segments vibrate around the dislocation "centre-of-mass" position when it overcomes the inhomogeneous field created by the defects. Let the $0Z$-axis go along the dislocation line and the $0X$-axis be parallel with the Burgers vector $\boldsymbol{b}$. Also, let the dislocation move in positive direction of the $0X$-axis and vibrate in the slip plane $Z0X$. Vibrations in the plane perpendicular to the slip plane are not taken into account in this problem. The position of dislocations in the slip plane is described by the function $x(z, t) = vt + w(z, t)$, where $w(z, t)$ is a random quantity, its mean value over the ensemble of defects and the position of dislocation elements is zero,

$$\langle x(z, t)\rangle = vt\,, \qquad \langle w(z, t)\rangle = 0\,.$$

In this notation the equation of dislocation motion in the field of randomly distributed defects is of the form

$$m\left(\frac{\partial^2 x}{\partial t^2} + \delta\,\frac{\partial x}{\partial t} - c_t^2\,\frac{\partial^2 x}{\partial z^2}\right) = b\sigma_0 + b\sigma_{xy}^{(d)}(vt + w, 0, z)\,. \tag{1}$$

Here $\sigma_{xy}^{(d)}$ is the component of the tensor of stresses created by the defect on the dislocation line, $\sigma_{xy}^{(d)} = \sum_i \sigma_i$, m is the mass of the dislocation length unit, N the number of defects in the crystal. Infinitely small damping δ is formally introduced to provide convergence of the appearing integrals. Change over to the coordinate system relating to a moving dislocation. Then

$$\frac{\partial^2 w}{\partial t^2} + \delta\,\frac{\partial w}{\partial t} - c_t^2\,\frac{\partial^2 w}{\partial z^2} = \frac{b}{m}\,\sigma_{xy}^{(d)}(vt + w, 0, z)\,. \tag{2}$$

Considering dislocation vibrations to be small, we expand the function $\sigma_{xy}^{(d)}$ (later on referred to as σ) in terms of $w(z, t)$ up to the second order. We approximately replace $\frac{1}{2}\sigma'' w_1(z, t)\, w_2(z, t)$ (indices 1, 2 are introduced to distinguish $w(z, t)$) for

$$\tfrac{1}{2}\,\{\langle\sigma'' w_1\rangle\, w_2 + \langle\sigma'' w_2\rangle\, w_1\} = \langle\sigma'' w\rangle\, w\,,$$

where $\langle\ldots\rangle$ denotes averaging over dislocation length and ensemble of defects by the Poisson distribution

$$\langle\ldots\rangle = \lim_{\mathcal{L}\to\infty} \int\limits_{-\mathcal{L}/2}^{\mathcal{L}/2} \frac{dz}{\mathcal{L}} \int\limits_V \prod_{i=1}^N \frac{d\boldsymbol{r}_i}{V^N}\,. \tag{3}$$

In this expression $\boldsymbol{r}_i$ is the radius-vector of the i-th defect, V the volume of the crystal, $\mathcal{L}$ the dislocation length. Such a procedure means that the nonlinear interaction of the dislocation with defects is replaced by the dislocation interaction with the self-consistent field $\langle\sigma'' w\rangle$ which in some sense is analogous to a self-consistent field in the Vlasov kinetic equation for a plasma or to the Hartree self-consistent procedure for the calculation of wave functions of many-particle problems in quantum mechanics.

Note that the summand $\langle\sigma' w\rangle$ does not contribute to the renormalization of the dislocation vibrational spectrum and will be treated later on only in connection with the calculation of the dislocation force acting on the dislocation.

If the dislocation centre moves with a constant velocity and the impurities are distributed by the Poisson law, then it is easy to show that the quantity $\langle \sigma'' w \rangle$ does not depend neither on time nor on the coordinate. For this reason we transpose the summand $\frac{b}{m} \langle \sigma'' w \rangle \, w$ in (2) to the left-hand side. We obtain a linear equation the right-hand side of which is, after the Fourier transformation, of the form

$$(-\omega^2 - i\delta\omega + c_t^2 q^2 + \Delta^2) \, w(q, \omega) = \frac{b}{m} \, \sigma_{q\omega}(0) \, . \tag{4}$$

Here we denote

$$\Delta^2 = \frac{b}{m} \langle \sigma'' w \rangle \, , \qquad q \equiv p_z \, , \tag{5}$$

$\sigma_{q\omega}(0)$ is the Fourier component of stresses from defects on the line of the uniformly moving dislocation. From (4) it is seen that the account of the self-consistent field due to collisions with defects results in the appearance of activation in the vibrational spectrum at $q = 0$, $\omega = \Delta$. Solving (4) we have

$$w(q, \omega) = G(q, \omega) \, \frac{b}{m} \, \sigma_{q\omega}(0) \, , \tag{6}$$

where

$$G(q, \omega) = (-\omega^2 - i\delta\omega + c_t^2 q^2 + \Delta^2)^{-1} \tag{7}$$

is the Fourier component of the Green function of (4). Now substituting (6) and (7) into (5) and averaging according to (3) we obtain a self-consistent equation to determine the energy gap in the dislocation vibrational spectrum,

$$\Delta^2 = \frac{n b^2}{(2\pi)^3 \, m^2} \int \mathrm{d}^3 p \, \frac{p_x^2 \, |\sigma_{\boldsymbol{p}}|^2}{c_t^2 q^2 + \Delta^2 - p_x^2 v^2} \, ; \tag{8}$$

in this formula $\sigma_{\boldsymbol{p}}$ is the Fourier component of the stresses $\sigma_{xy}(\boldsymbol{r})$ created by a single defect. From (8) it is seen that Δ^2 does not depend on time and coordinate. This is a consequence of the homogeneity of motion and the isotropy of space due to averaging.

3. Dynamic Deceleration of Dislocation

Now we study the question on the influence of the gap in the dislocation vibrational spectrum on the form of the dependence of deceleration force F created by defects on the velocity. Using the Peach-Koehler formula we present the deceleration force in the form

$$F = \frac{b}{(2\pi)^4} \int \mathrm{d}^3 p \, \mathrm{d}\omega \, \sigma_{\boldsymbol{p}} \, \langle \mathrm{e}^{i p_x w(z,t)} \, f_{\boldsymbol{p}} \rangle \, \mathrm{e}^{i p_x v t + i p_z z - i\omega t} \, , \tag{9}$$

where $f_{\boldsymbol{p}} = \sum\limits_k \exp\,(i \boldsymbol{p} \boldsymbol{r}_k)$, summation is performed over the positions of the defects. Expanding the expression for the deceleration force in terms of small vibrations and taking account of the fact that terms linearly containing a random quantity vanish after averaging, we obtain

$$F = -b \, \langle \sigma'(vt) \, w \rangle = \frac{ib}{(2\pi)^4} \int \mathrm{d}^3 p \, \mathrm{d}\omega \, \sigma_{\boldsymbol{p}} p_x \, \mathrm{e}^{i p_x v t + i p_z z - i\omega t} \, \langle w f_{\boldsymbol{p}} \rangle \, . \tag{10}$$

Using (6) and (7) we can calculate $\langle w f_{\boldsymbol{p}} \rangle$, then (10) is rewritten in the following way:

$$F = -\frac{nb^2}{8\pi^2 m} \int \mathrm{d}^3p \, |p_x| \, |\sigma_{\boldsymbol{p}}|^2 \, \delta\{p_x^2 v^2 - \mathcal{E}^2(p_z)\} \,, \tag{11}$$

where $\mathcal{E}(p_z) = \sqrt{\Delta^2 + c_t^2 p_z^2}$. It is evident that the deceleration force tends to zero if the dislocation velocity does.

Next we study the stress tensors with components

$$\sigma_{xy}(\boldsymbol{p}) \equiv \sigma_{\boldsymbol{p}} = p_x p_y f(p^2) \,.$$

Integrating in (11) and taking into account that p_z enters $|\sigma_{\boldsymbol{p}}|^2$ only as the combination $p_x^2 + p_y^2 + p_z^2$, and $p_x^2 \geqq \Delta^2 v^{-2} \gg \Delta^2 c_t^{-2}$, we may suppose in the integrand (11) that

$$|\sigma(p_x, p_y, p_z)|^2 \approx |\sigma(p_x, p_y, 0)|^2 \,.$$

As a result, the deceleration force will be of the form

$$F = -\frac{nb^2}{4\pi^2 m c_t v} \int\limits_{-\infty}^{\infty} \mathrm{d}p_y \int\limits_{\Delta/v}^{\infty} \mathrm{d}p_x \, \frac{p_x \, |\sigma(p_x, p_y, 0)|^2}{\sqrt{p_x^2 - \Delta^2/v^2}} \,. \tag{12}$$

Let $\varkappa$ denote the characteristic wave vector of the stress-tensor Fourier transform. First consider the case $v \gg \Delta/x$. Here the wave vectors of the order of $\varkappa$ are the main contributors to (12). Then we can approximately write

$$F \approx -\frac{nb^2}{4\pi^2 m c_t v} \int\limits_{-\infty}^{\infty} \mathrm{d}p_y \int\limits_{0}^{\infty} \mathrm{d}p_x \, p_x \, |\sigma(p_x, p_y, 0)|^2 \,. \tag{13}$$

An analogous expression is obtained for the Fourier transforms divergent at infinity if $\varkappa$ is taken as the cut-off parameter of the integration over the wave vectors. Formula (13) is in agreement with the results of [2 to 4] obtained for dislocations moving with high velocities. Thus, in the region of high dislocation velocities ($v \gg \Delta/\varkappa$) the presence of a gap in the vibrational spectrum does not influence the dependence of the deceleration force on velocity. To study the velocity region $v \ll \Delta/\varkappa$ we replace the variables in the integral (12),

$$F = -\frac{nb^2 \Delta^6}{4\pi^2 m c_t v^7} \int\limits_{-\infty}^{\infty} \mathrm{d}y \int\limits_{1}^{\infty} \mathrm{d}x \, \frac{x^3 y^2}{\sqrt{x^2 - 1}} \, f^2\left(\frac{\Delta^2}{v^2}(x^2 + y^2)\right). \tag{14}$$

From (14) it follows that in this region the influence of the gap turns out to be essential, the form of the force-velocity dependence being determined by the form of the Fourier transform of the tensor of stresses created by the defect, and because it is impossible to find the $F(v)$ dependence in the general form we consider a number of simple model functions of $\sigma_{xy}(\boldsymbol{p})$.

(i) $\sigma_{xy}(\boldsymbol{p}) = \sigma_0 p_x p_y \theta(\varkappa^2 - p^2)$.

Here $\theta(x)$ is the Heaviside function. The deceleration force is equal to zero at $v < \Delta/\varkappa$, and at $v > \Delta/\varkappa$ it depends on v in the following way:

$$F \sim v^{-1} \sqrt{\varkappa^2 - \Delta^2/v^2} \,.$$

The force has a maximum at $v \approx 2\Delta/\varkappa$ and at $v \gg \Delta/\varkappa$ it behaves as v^{-1}.

(ii) The Fourier transform of Gaussian type

$$\sigma_{xy}(\boldsymbol{p}) = \sigma_0 p_x p_y \, \mathrm{e}^{-p^2\varkappa^{-2}} .$$

In this case

$$F = -\frac{nb^2\varkappa^2\sigma_0^2}{mc_t v} \, \mathrm{e}^{-\left(\frac{\Delta}{\varkappa v}\right)^2} .$$

At $v \to 0$ the deceleration force $F \to 0$, at $v = 2\Delta/\varkappa$ it has a maximum and at $v \gg \Delta/\varkappa$ decreases as v^{-1}.

(iii) Defects of the dilatation centre type. To eliminate the nonphysical divergence, let us introduce a cut-off for the defect field at the distance of the defect radius,

$$\sigma_{xy}(\boldsymbol{r}) = \mu b^3 \varepsilon \, \frac{\partial^2}{\partial x \, \partial y} \, \frac{1 - \mathrm{e}^{-\varkappa r}}{r} .$$

Here μ is the shear modulus, ε the misfit parameter, the dimensionless value characterizing the power of the defect (see [4]). The Fourier transform of the stress-tensor component needed is of the form

$$\sigma_{\boldsymbol{p}} = 4\pi\mu b^3 \varepsilon \varkappa^2 \, \frac{p_x p_y}{p^2(p^2 + \varkappa^2)} .$$

In this case the deceleration force is determined by the formula

$$F = -B_\mathrm{d} v \Phi\big(\Delta/(\varkappa v)\big) ,$$

where

$$B_\mathrm{d} = \frac{\pi n_0 b^5 \mu^2 \varepsilon^2 \varkappa^4}{3mc_t \Delta^2} , \tag{15}$$

$$\Phi(x) = x^2[1 + (6x^4 + 2x^2) \ln (1 + x^2) - 6x^2] . \tag{16}$$

Here n_0 is the dimensionless concentration of defects, $n_0 \approx nb^3$ (see [4]). At velocities $v \gg v_0 = \Delta/\varkappa$ the function $\Phi(x) \approx x^2$ and the deceleration force is proportional to v^{-1} which is in agreement with the results of [2 to 4]. At $v \ll v_0$ the function $\Phi(x) \approx 1$ and deceleration is of quasi-viscous character,

$$F = -B_\mathrm{d} v . \tag{17}$$

The obtained dependence of the deceleration force on dislocation velocity ($F \sim v$ at small velocities and $F \sim v^{-1}$ at high ones) agrees with the results of [6].

Basing on the above calculations we can conclude that at $p > \varkappa$ the behaviour of the Fourier transform of the tensor of the stresses created by the defect determines the dependence of the deceleration force on velocity at $v < v_0$. If at $p > x$ $\sigma_{xy}(\boldsymbol{p}) = 0$, then at $v < v_0$ $F = 0$. If at $p > \varkappa$ $\sigma_{xy}(\boldsymbol{p})$ exponentially decreases, then at $v < v_0$ F is exponentially small. Finally, if $\sigma_{xy}(\boldsymbol{p})$ decreases in a power-type manner, then the dependence of F on v will be of power type as well.

As was shown above, at the velocities $v > v_0$ the presence of the gap does not influence the deceleration force, but at small velocities its influence becomes essential. Thus, it is necessary to calculate the gap value in the region $v < \Delta/\varkappa$. First of all we pass to spherical coordinates in the integral (8)

$$p_x = p \sin \vartheta \cos \varphi ; \qquad p_y = p \sin \vartheta \sin \varphi ; \qquad p_z = \cos \vartheta ; \qquad x = \cos \vartheta .$$

Integrating over the angle φ we transform (8) to the form

$$1 = \frac{n_0}{4\pi^2 m^2 c_t^4 b} \left\{ \int_0^1 \mathrm{d}x\, x^2 \int_0^{\Delta/v\sqrt{1-x^2}} \mathrm{d}p\, p^4 f^2(p^2) \sqrt{\frac{\left\{1 + \left(\frac{c_t p}{\Delta}\right)^2 (1-x^2)\right\}^3}{1 - \left(\frac{pv}{\Delta}\right)^2 (1-x^2)}} - \right.$$

$$\left. - \frac{2}{3} \int_0^\infty \mathrm{d}p\, p^4 f^2(p^2) \left[1 + \frac{3}{5}\left(\frac{c_t p}{\Delta}\right)^2\right] \right\}. \tag{18}$$

In the case of a defect of centre-of-dilatation type,

$$f(p^2) = \frac{4\pi\mu b^3 \varepsilon \varkappa^2}{p^2(p^2+\varkappa^2)}.$$

We consider $\Delta \ll \varkappa c_t$. This means that the gap is less than the Debye frequency, as regards its order of magnitude, because $\omega_D \sim c_t b^{-1} \sim c_t \varkappa$. So, $\varkappa v \ll \Delta \ll \varkappa c_t$. In this case (18) becomes simpler,

$$1 = n_0 \varepsilon^2 \left(\frac{c_t \varkappa}{\Delta}\right)^3 \ln (\Delta/\varkappa v). \tag{19}$$

Here we have also used the approximate evaluation of the mass of the dislocation unit length $m \approx \varrho b^2$. A solution of this equation exists only for $v < v_1$, where

$$v_1 = c_t (n_0 \varepsilon^2)^{1/3} \tag{20}$$

and in rough approximation it has the form

$$\Delta \approx \varkappa v_1 \ln (v_1/v). \tag{21}$$

Because the mean distance between defects $l \sim b n_0^{-1/3}$, then $v_0 \sim c_t b/l$ which is in agreement with the conclusions of the authors [2]. The condition $v > v_1$ will be rewritten in the form $(l/c_t) > (a/v)$. As was mentioned above, this means predominance of single interactions of defects with the dislocation. The condition $v < v_1$ suggests predominance of collective interaction, resulting in the appearance of the gap essentially changing the character of dislocation deceleration. The above model is valid in the dynamic region of velocities, i.e. when the dislocation kinetic energy is greater than the energy of dislocation interaction with the impurities $\mathcal{L} U_0 b^{-1} n_0$, where U_0 is the energy of dislocation bonding to the impurity atom. According to [4], for the centre of dilatation $U_0 \sim \mu b^3 \varepsilon$. Making use of this expression $m \approx \varrho b^2 = \mu b^2 c_t^{-2}$ for the evaluation of the dislocation mass we obtain the applicability condition for our model in the form $v > c_t (n_0 \varepsilon)^{1/2}$. Thus, the force of dislocation deceleration at defects is of quasi-viscous character in the velocity region

$$c_t (n_0 \varepsilon)^{1/2} < v < c_t (n_0 \varepsilon^2)^{1/3}$$

and is proportional to v^{-1} in the region $c_t (n_0 \varepsilon^2)^{1/3} < v \ll c_t$. The concentration of defects is usually within the limits 10^{-6} to 10^{-3} and $\varepsilon \approx 10^{-1}$. For $n_0 \approx 10^{-4}$ the gap value is $\Delta \approx 10^{11}\ \mathrm{s}^{-1}$. In this case the damping constant $B_d \approx 10^{-5}$ kg/m s which is in order-of-magnitude agreement with data of [5]. From (21), (20), and (15) it follows that the constant B_d is proportional to $n_0^{1/3} \varepsilon^{2/3}$. The gap value $\Delta \sim (c_t/l) \sim \omega_D b/l$, i.e. $\omega_D \gg \Delta$.

4. Conclusion

It has been shown that the collective interaction of defects with a dislocation results in the appearance of a gap in the dislocation vibrational spectrum and the presence of the gap essentially changes the velocity dependence of the deceleration force, in particular, it results in the initiation of the experimentally observed quasi-viscous deceleration by defects.

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