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MECHANICAL PROPERTIES, PHYSICS OF STRENGTH, AND PLASTICITY

Influence of High Hydrostatic Pressure on the Vibrational Spectrum of an Edge Dislocation and Its Dynamic Interaction with Point Defects

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Abstract—The slip of a single edge dislocation in an elastic field of point defects chaotically distributed over a crystal with allowance for a high hydrostatic pressure has been studied theoretically. The numerical estimations have demonstrated that hydrostatic compression of some metals and alloys increases the dislocation drag force by point defects in them by several tens of percent.

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One of the methods of designing new functional materials that combine a high strength with a high plasticity is the processing under a high hydrostatic pressure [1–4]. As is known, the mechanical properties of a crystal are determined to significant degree by the existence and motion of dislocations [5]. A dislocation itself undergoes during its motion a strong influence of potential barriers induced by structural defects; a moving dislocation can surmount the barriers by two methods, namely, due to thermal fluctuations when the dislocation kinetic energy is lower than the barrier height and dynamically (overbarrier slip) in the opposite case; the latter is commonly realized at rates of dislocation motion of $10^{-2}c$ and higher (c is the velocity of propagation of transverse acoustic waves in a crystal) [6]. During the dynamic dislocation motion in the field of other structural defects, its kinetic energy is irreversibly transformed into the energy of dislocation vibrations in the slip plane. The dynamic drag force appeared during the process is dependent on both the interaction of a dislocation with defects and it vibrational spectrum [7–10]. In [11], the influence of the hydrostatic compression on the dynamic drag of moving dislocation pairs by pinned individual dislocations and also on the drag of individual dislocations by dislocation dipoles was studied. In [12], the dynamic drag of moving dislocation pairs by point defects in a crystal subjected to hydrostatic compression was analyzed. In that work, the effect of pressure on the interaction between dislocations forming pairs was taken into account, which, as a result, led to renormalization of the spectrum of dislocation vibrations in the case when the interaction between dislocations themselves influences predominantly the shape of this spectrum. The effect of hydrostatic compression on the interaction of point defects with dislocations was not taken into account in [12]; however, as is shown in what follows, it can be very substantial in a number of practically important cases.

The aim of this work is to theoretically study the specific features of the dynamic dislocation drag by point defects and the transformation of the dislocation vibrational spectrum as a result of an increase in the interaction of defects with a dislocation under hydrostatic compression.

Let an infinite edge dislocation to move under action of the external stress σ_0 at a constant rate v in the field of point defects that are randomly distributed over the volume of a hydrostatically compressed crystal. The dislocation line is parallel to the OZ axis, and the Burgers vector of the dislocation is parallel to the OX axis, so that the dislocation slips in the positive direction of this axis. The dislocation position is determined by function $X(z, t) = vt + w(z, t)$, where $w(z, t)$ is a random variable whose average value over the ensemble of defects and arrangement of dislocation elements is zero.

The dislocation motion is described by the equation

$$\tilde{m}\left\{\frac{\partial X^2(z, t)}{\partial t^2} + \tilde{\delta}\frac{\partial X(z, t)}{\partial t} - \tilde{c}^2\frac{\partial^2 X(z, t)}{\partial z^2}\right\} = \tilde{b}\sigma_0 + \tilde{b}\tilde{\sigma}_{xy}(vt + w; z). \tag{1}$$

Here, $\tilde{\sigma}_{xy}$ is the stress tensor component induced by point defects in the dislocation line in a hydrostatically compressed crystal; $\tilde{m}$ is the mass of the unit dislocation length; $\tilde{c}$ is the velocity of propagation of transverse acoustic waves in the crystal (the tilde indicates that the corresponding values are taken for the hydrostatically compressed crystal); $\tilde{\delta}$ is the damping coefficient; $\tilde{\delta} = B/\tilde{m}$; and B is the damping constant determined primarily by the phonon dissipation mechanism. As is shown in [13], the influence of these dissipation mechanisms on the drag force induced by the field of randomly distributed defects is insignificant because of the smallness of the dimensionless parameter $\gamma = \tilde{\delta} r_0 v/c^2$, where r_0 is the cutoff parameter ($r_0 \approx b$). Since, in order of magnitude, $B \leq 10^{-4}$ Pa s, and the linear density of the dislocation mass $m \approx 10^{-16}$ kg/m, we obtain $\tilde{\delta} \leq 10^{12}$ s^{-1}. With typical values $r_0 \approx b \approx 3 \times 10^{-10}$ m, $c \approx 3 \times 10^3$ m/s, and $v \leq 10^{-1}c$, we find that $\gamma \ll 1$. This estimation performed for crystals not subjected to hydrostatic compression also is valid for our case, since the hydrostatic pressure does not change the orders of the values used here. Because of this, when calculating the dislocation drag force by defects, we, as in [7–13], neglect the influence of phonon and other dissipation mechanisms contributing to the damping constant B and consider the damping coefficient $\tilde{\delta}$ as an infinite small quantity that provides the convergence of the integrals obtained.

In [14–16], it was shown that the elastic field of defects, among them point defects, in a hydrostatically compressed crystal can be described by the same expressions that are used for a crystal not subjected to compression; however, in this case, the elastic moduli must be replaced by the renormalized expressions obtained in [14–16] and containing in an explicit form the dependence on the hydrostatic pressure p. In particular, in the case $\Omega = \dfrac{p}{3\lambda + 2\mu} \ll 1$ (where λ and μ are the Lamé coefficients), according to [16], the stress tensor of point defects in the hydrostatically compressed crystal can be represented as

$$\tilde{\sigma}_{xy} = \sigma_{xy}(1 + \alpha p), \quad \alpha = \frac{0.5n - 3\lambda - \mu - 3m}{\mu(3\lambda + 2\mu)}, \quad (2)$$

where σ_{xy} is the stress tensor in the crystal not subjected to hydrostatic compression; and m and n are the Murnaghan coefficients.

As was done in [7, 17, 18], the point defects are considered as dilatation centers with a smoothly cut stress fields at the distances of an order of the defect radius R; because of this

$$\sigma_{xy}(\mathbf{r}) = \mu R^3 \varepsilon \frac{\partial^2}{\partial x \partial y} \frac{1 - \exp(-r/R)}{r}. \quad (3)$$

Using the method developed in [7–10, 17, 18], we calculate the dynamic dislocation drag by point defects by formula

$$F = \frac{\tilde{n}\tilde{b}^2}{8\pi^2 \tilde{m}} \int d^3q |q_x| |\sigma_{xy}(\mathbf{q})|^2 \delta[q_x^2 v^2 - \omega^2(q_z)], \quad (4)$$

where $\omega(q_z)$ is the dispersion law of dislocation vibrations; and $\tilde{n}$ is the point defect concentration.

Using the standard procedure of the Fourier transform and going to the system of the dislocation center of masses, we obtain the dispersion law in an explicit form

$$\omega(q_z) = \sqrt{\Delta^2(p) + c^2 q_z^2}, \quad (5)$$

where

$$\Delta(p) = \Delta_0 (1 + \alpha p)^{2/3}, \quad \Delta_0 = \frac{\tilde{c}}{\tilde{b}} (\tilde{n}_0 \tilde{\varepsilon}^2)^{1/3}. \quad (6)$$

Here, $\tilde{n}_0$ is the dimensional concentration of point defects, $\tilde{n}_0 = \tilde{n} R^3$.

As is known, the dynamic interaction of defects with a dislocation in the dependence on the dislocation slip rate can have both the collective character and the character of independent collisions [7, 17, 18]. To remember the sense of these concepts, denote the time of the interaction of a dislocation with a point defect as $t_{\text{def}} = R/v$, the propagation time of a perturbation along the dislocation at the distance on an order of the average distance between defects as $t_{\text{dis}} = l/c$, where l is the average distance between defects. In the region of the independent collisions $v > v_d = R\Delta$, the inequality $t_{\text{def}} < t_{\text{dis}}$ is obeyed, i.e., a dislocation element does not undergo the influence of other defects. In the region of the collective interaction ($v < v_d$), conversely, $t_{\text{def}} > t_{\text{dis}}$; i.e., for the time of interaction of a dislocation with a defect, the dislocation element has time to feel the influence of other defects that cause the perturbation of the dislocation form. At high ($v > v_d$) and low ($v < v_d$) rates, the character of the dislocation drag are substantially different.

It follows from Eq. (6) that, in a hydrostatically deformed crystal, the critical rate determining the boundary between these regions, also will be dependent on the hydrostatic pressure

$$v_d(p) = \tilde{b}\Delta_0 (1 + \alpha p)^{2/3}. \quad (7)$$

Performing the calculations, we obtained that, in the region of independent collisions ($v > v_d$), the dislocation drag force due to point defects is determined by the expression

$$F = \frac{\pi \tilde{n}_0 \tilde{b}^2 \tilde{\mu}^2 \tilde{\varepsilon}^2 R}{3 \tilde{m} \tilde{c} v} (1 + \alpha p)^2. \quad (8)$$

In the region of collective interaction, the dependence of this force on the hydrostatic pressure is significantly weaker:

$$F = \frac{\pi\tilde{n}_0\tilde{b}^2\tilde{\mu}^2\tilde{\varepsilon}^2 v(1+\alpha p)^{2/3}}{3\tilde{m}\tilde{c}R\Delta_0^2}. \qquad (9)$$

We perform numerical estimations of the effect under study for a pressure of 10^9 Pa. According to [14–16], the constants entering into the formulas obtained at such a pressure are insignificantly changed; thus, the main dependence on the hydrostatic pressure is determined by the factor $(1 + \alpha p)$. To estimate the degree of the influence of hydrostatic pressure on the quantities under study, we used the data from [19, 20]. Thus, in the aluminum-based D54S alloy, the increases in the dynamic drag force in the region of independent collisions and in the region of collective interaction are 32 and 10%, respectively; these values are, respectively, 28 and 8% for commercial magnesium, 8 and 3% for copper, 3 and 1% for molybdenum, and 2 and 1% for tungsten.

Thus, in the number of materials, the hydrostatic compression of a crystal can lead to a significant increase in the dynamic dislocation drag force by point defects.

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