DEFECTS AND IMPURITY CENTERS, DISLOCATIONS, AND PHYSICS OF STRENGTH

Influence of Collective Effects on the Dynamic Behavior of a Single Edge Dislocation in a Crystal with Point Defects

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Abstract—The glide of a single edge dislocation in an elastic field of point defects randomly distributed over a crystal is investigated taking into account the influence of the phonon subsystem of the crystal. The force of retardation of the dislocation motion is calculated, and the velocities at which this force has a local maximum and a local minimum are determined. A comparative analysis of the glide of a single dislocation and the glide of a pair of edge dislocations is performed.

1. INTRODUCTION

The presence of point defects, which affect the dislocation motion in crystals, can have a substantial effect on the mechanical characteristics of a material. The influence of point defects on the glide of single dislocations in the dynamic regime has been investigated in a number of works [1–6].

Since the interaction of defects with dislocations executing motion gives rise to dislocation vibrations, the efficiency of energy dissipation turns out to be dependent on the spectrum of these vibrations [3–6]. In my previous paper [7], the motion of a pair of edge dislocations in parallel glide planes was investigated with due regard for the interaction of the dislocations with each other and with the phonon subsystem of the crystal containing randomly distributed point defects. It was demonstrated that, under certain conditions, the force of retardation of the dislocation motion as a function of the velocity of dislocation glide can exhibit two extrema (a minimum and a maximum) between which the dislocation motion is unstable. This paper reports on an analysis of the motion of a single edge dislocation. It will be shown that, under specific conditions, there can arise two extrema bounding the range of instability in the system under investigation; however, the position of the maximum in this case will be determined by other parameters of the crystal.

The purpose of this paper is to investigate the glide of a single edge dislocation in an elastic field of point defects randomly distributed over a crystal with due regard for the interaction of the dislocation with the phonon subsystem of the crystal. In order to take into account the effect of the phonon subsystem of the crystal on the glide of a single edge dislocation, the equation of motion of the dislocation, as was done earlier in [7], is supplemented with an additional quasi-viscous term. In essence, this means that any dissipation mechanism associated with the quasi-viscous retardation of dislocation motion, in particular, the mechanisms of interaction of a moving dislocation with electrons and magnons [8, 9], is included in the analysis.

2. THEORETICAL ANALYSIS

Let us consider a uniform glide of an infinitely long edge dislocation under a constant external stress σ_0 in a field of point defects randomly distributed in the bulk of a crystal. The line of this dislocation is parallel to the OZ axis, and the Burgers vector is aligned parallel to the OX axis. The dislocation moves in the positive direction of the OX axis at a constant velocity v. The plane of dislocation glide coincides with the XOZ plane. The location of the dislocation is determined by the function

$$X(y = 0, z, t) = vt + w(y = 0, z, t), \quad (1)$$

where the function $w(y = 0, z, t)$ is a random quantity that describes vibrations of elements of the edge dislocation in the glide plane with respect to the undisturbed dislocation line.

Since this study is concerned with the glide of a single edge dislocation, the right-hand side of the equation of motion, unlike the equation of motion in [7], does not include the term describing the interaction of dislocations with each other (recall that, for the motion of a pair of dislocations, this interaction determines both the spectrum of dislocation vibrations and the character of the retardation of the dislocation motion by point

defects). The motion of the dislocation can be described by the equation

$$m \left\{ \frac{\partial X^2}{\partial t^2} - c^2 \frac{\partial^2 X}{\partial z^2} \right\}$$

$$= b[\sigma_0 + \sigma_{xy}(vt + w; z)] - B \frac{\partial X}{\partial t}. \quad (2)$$

Here, m is the mass of the dislocation per unit length, which is determined by the relationship [10]

$$m = \frac{\rho b^2}{4\pi(1-\gamma)} \ln \frac{L}{r_0}; \quad (3)$$

ρ is the density of the crystal; L is a quantity of the order of the dislocation length; r_0 is a quantity of the order of the atomic distances ($r_0 \sim b$); γ is the Poisson ratio; B is the damping constant, which accounts for the phonon, magnon, electron, or other dissipation mechanisms characterized by a linear dependence of the force of retardation of the dislocation motion on the velocity of dislocation glide; c is the velocity of propagation of transverse acoustic waves in the crystal; σ_{xy} is the tensor component of the stresses generated by point defects along the dislocation line; and $\sigma_{xy} = \sum_{i=1}^{N} \sigma_{xy,i}$ (here, N is the number of point defects in the crystal). As in our earlier study [3], we use a smooth cutoff of the stress field of a point defect at distances of the order of the radius of this defect:

$$\sigma_{xy}(\mathbf{r}) = \mu R^3 \varepsilon \frac{\partial^2}{\partial x \partial y} \frac{1 - \exp(-r/R)}{r}, \quad (4)$$

where R is the radius of the point defect, ε is the mismatch parameter, and μ is the shear modulus.

As in [2, 7], the dimensionless parameter $\alpha = \beta \lambda v/c^2$ (where λ is the cutoff parameter, $\lambda \approx b$, and $\beta = B/m$) is assumed to be small. According to the estimates made in [2], this condition is satisfied in the vast majority of cases. Therefore, the force of retardation of the dislocation motion by point defects can be calculated by ignoring the phonon and other dissipation mechanisms that contribute to the damping constant B. However, when analyzing the total retarding force that acts on the dislocation, these mechanisms should be taken into account by adding the term Bv.

As follows from [3, 4], there is a range of dynamic glide of a single dislocation in which the dislocation vibrations are described by a nonlinear spectrum:

$$\omega^2 = c^2 p_z^2 + \Delta_d^2. \quad (5)$$

Here, the quantity Δ_d is the solution of the equation

$$\Delta_d^2 = \frac{nb^2}{8\pi^3 m^2} \iiint d^3 p \frac{p_x^2 |\sigma_{xy}(\mathbf{p})|^2}{\Delta_d^2 + c^2 p_z^2 - p_x^2 v^2}, \quad (6)$$

where n is the volume concentration of point defects.

It is known that the dynamic interaction of defects with a single dislocation can occur through the mechanisms of either collective interaction or independent collisions between the defects depending on the velocity of dislocation glide [3, 4]. Let $\tau_{def} \approx R/v$ be the time of interaction between the dislocation and the impurity atom, where R is the radius of this defect. The time of propagation of disturbance along the dislocation over a distance of the order of the mean distance between the defects is designated as $\tau_{def} \approx l/c$. In the range of independent collisions $v > v_0 = R\Delta_d$, these times satisfy the inequality $\tau_{def} < \tau_{dis}$; i.e., the element of the dislocation for the time of interaction with the point defect is not affected by other defects. In this range, there are no solutions to Eq. (6) and, hence, no gap arises in the spectrum of dislocation vibrations. By contrast, in the range of the collective interaction ($v < v_0$), we have $\tau_{def} > \tau_{dis}$; i.e., the element of the dislocation for the time of interaction of the dislocation with the point defect manages to be affected by other defects responsible for the distortion of the dislocation shape. In this range, the spectrum of dislocation vibrations involves the gap

$$\Delta_d = \frac{c}{b}(n_0 \varepsilon^2)^{1/3}, \quad (7)$$

where $n_0 = nR^3$ is the dimensionless concentration of point defects. Therefore, unlike the situation described in [7], where the spectral gap arises from the interaction between dislocations, exists over the entire range of velocities under investigation, and depends on the spacing of dislocations, the gap observed in the spectrum of dislocation vibrations in the given case originates from the collective interaction of defects with the dislocation, exists only at velocities lower than the critical velocity v_0, and depends on the concentration of defects.

According to [3, 4], the force of retardation of the dislocation motion by point defects can be represented in the following form:

$$F_d = \frac{nb^2}{4\pi^2 mcv} \int_{-\infty}^{\infty} dp_y \int_{\Delta/v}^{\infty} dp_x \frac{p_x |\sigma_{xy}(p_x, p_y, 0)|^2}{\sqrt{p_x^2 - (\Delta/v)^2}}. \quad (8)$$

At $v < v_0$, i.e., in the range of the collective interaction, the force of retardation of the dislocation motion by defects increases linearly with an increase in the dislocation velocity:

$$F_d = B_d v, \quad B_d = \frac{\pi n_0^{1/3} \mu^2 \varepsilon^{2/3} b^4}{3mc^3 R}. \quad (9)$$

It follows from expression (9) that the coefficient B_d depends on the defect concentration (in the case of two dislocations, this coefficient also depends on the distance between their glide planes).

By using the explicit formula (3) for the dislocation mass and taking into account that, under real conditions

[10], the quantity $\ln(L/r_0)/(4\pi(1-\gamma))$ is of the order of unity and $c^2 = \mu/\rho$, the qualitative evaluation can be performed using the simplified relationship

$$F_d = \mu b\left(\frac{b}{R}\right)^2 (n_0\varepsilon^2)^{1/3} \frac{v}{c}. \tag{10}$$

Relationships (9) and (10) were derived for defects of the type of dilatation centers with a smooth cutoff of the strain tensor at distances of the order of the defect radius, which is described by expression (4). As was shown earlier in [3, 4], the retardation of the dislocation motion by impurities at velocities in the range of the collective interaction is governed by the asymptotic behavior of the strain tensor in this range, i.e., at short distances. Furthermore, in our previous paper [11], we demonstrated that the near asymptotics identical to asymptotic expression (4) is characteristic of defects for which the strain vector components u_i at short distances are proportional to $(x_i/r) \sim \cos\varphi$; i.e., as the distance decreases, these strains do not tend toward an infinite increase and cease to increase after a limiting value is reached. Therefore, relationships (9) and (10) hold true within a constant numerical factor for all defects satisfying the above condition.

At $v > v_0$, the force of retardation of the dislocation motion by point defects is inversely proportional to the velocity of dislocation glide [3, 4]:

$$F_d = \frac{nb^2}{4\pi^2 mcv} \int_{-\infty}^{\infty} dp_y \int_0^{\infty} dp_x |\sigma_{xy}(p_x, p_y, 0)|^2. \tag{11}$$

The retarding force for defects such as dilatation centers has the form

$$F_d = \frac{\pi n_0 R b^2 \mu^2 \varepsilon^2}{3mcv}. \tag{12}$$

However, it should be noted that relationship (11) was derived without recourse to the explicit formula for the tensor of stresses generated by a point defect. This implies that relationship (11) is valid not only for defects such as dilatation centers but also for any point defects for which the stress tensor can be described by the expression

$$\sigma_{xy}(\mathbf{r}) = A\frac{\partial^2}{\partial x \partial y} f(r), \tag{13}$$

where A is a coefficient that characterizes the strength of the point defect and, hence, depends on the elastic moduli of the crystal and on the sizes of the defect; and $f(r)$ is an arbitrary function of the distance from the defect to the point under consideration. Thus, expression (12) is qualitatively valid for any defects satisfying formula (13) and the forces calculated for these defects can differ only by a numerical factor.

At $v = v_0$, the force of retardation of the dislocation motion reaches a local maximum,

$$F_{max} = \mu b\left(\frac{b}{R}\right)^{2/3} n_0^{2/3} \varepsilon^{4/3} \approx \mu b(n_0\varepsilon^2)^{2/3}. \tag{14}$$

It can be seen from this relationship that the local maximum of the retarding force depends on the concentration and strength of the defects and on the elastic moduli of the crystal. Now, we use the data taken from [2] to estimate the order of magnitude of the maximum force F_{max}. For $\varepsilon \approx 10^{-1}$, $n_0 \approx 10^{-3}$, $\mu \approx 5 \times 10^{10}$ Pa, $b \approx 3 \times 10^{-10}$ m, and $R \approx b$, we obtain $F_{max} \approx 10^{-2}$ N/m. For comparison, we estimate the maximum retarding force for the motion of two dislocations. For this purpose, we use the results obtained in [7] and derive the expression

$$F_{max} = \frac{2\pi^2(1-\gamma)}{3}\mu a(n_0\varepsilon^2) \approx \mu a(n_0\varepsilon^2). \tag{15}$$

After substituting the above parameters into this expression, we obtain the maximum force $F_{max} \approx 10^{-3}$ N/m at $a = 10b$ and $F_{max} \approx 10^{-2}$ N/m at $a = 100b$. For the glide of a single dislocation, the critical velocity v_0 is determined by the concentration of point defects and, according to the results obtained in [3, 4], corresponds to the transition from the collective interaction of point defects with the dislocation to independent collisions between the defects:

$$v_0 = c\frac{R}{b}(n_0\varepsilon^2)^{1/3} \approx c(n_0\varepsilon^2)^{1/3}. \tag{16}$$

Recall that, for a pair of dislocations, the critical velocity v_0 depends on the spacing of dislocations and is independent of the defect concentration. The velocity v_1 at which the total retarding force of the dislocation motion has a local minimum is determined by the same relationship both for a single dislocation and for two dislocations; that is,
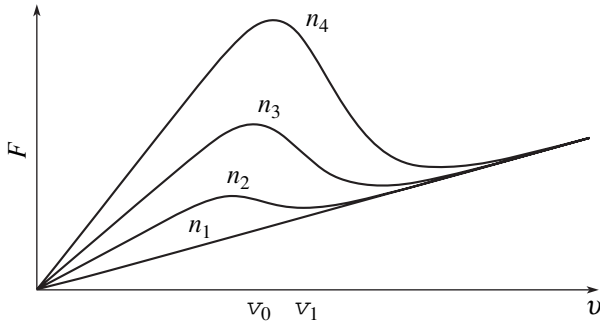
$$v_1 = v_0\sqrt{\frac{B_d}{B}} = 2\pi\varepsilon\sqrt{\frac{(1-\gamma)n_0\mu Rc}{3B}}. \tag{17}$$

The minimum retarding force can be estimated from the expression

$$F_{min} = 2\pi\mu b\sqrt{\frac{1-\gamma}{3}(n_0\varepsilon^2)\frac{Bc}{\mu b}\left(\frac{R}{b}\right)}$$
$$\approx \mu b\sqrt{(n_0\varepsilon^2)\frac{Bc}{\mu b}} \approx \sqrt{\mu b(n_0\varepsilon^2)Bc}. \tag{18}$$

The total retarding force can be approximately evaluated from the formula

$$F = F_d + Bv = \frac{B_d v}{1 + \frac{v^2}{v_0^2}} + Bv. \tag{19}$$

Fig. 1. Dependences of the retarding force of dislocation motion on the velocity of dislocation glide for different concentrations of point defects ($n_4 > n_3 > n_2 > n_1 = 0$).

Fig. 2. Dependences of the retarging force of dislocation motion on the concentration of point defects for different velocities of dislocation glide ($v_3 > v_2 > v_1$).

Therefore, the function $F(v)$ for the glide of a single dislocation has a form identical to that for the glide of two dislocations; however, the quantities B_d and v_0 are determined by other relationships and, in particular, have a different dependence on the defect concentration.
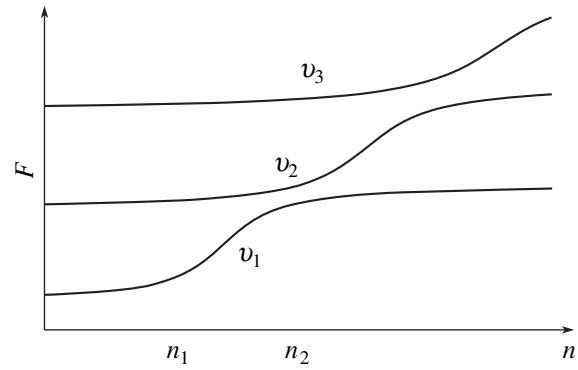
3. RESULTS AND DISCUSSION

The dependences of the total force of retardation of the dislocation motion on the velocity of dislocation glide for different concentrations of point defects are schematically depicted in Fig. 1. It follows from this figure and relationships (16) and (17) that, for the glide of a single dislocation, the positions not only of the minima (as is the case with two dislocations) but also of the maxima shift toward higher velocities with an increase in the defect concentration. The dependence $F(v)$ exhibits a minimum and a maximum under the following condition:

$$B < B_0 = \frac{B_d}{8} = \frac{\mu b (n_0 \varepsilon^2)^{1/3}}{8c}; \qquad (20)$$

i.e., the critical value of the phonon damping constant is determined by the defect concentration alone (for a pair of dislocations, this constant also depends on the distance between the dislocation glide planes).

Figure 2 schematically shows the dependences of the total force of retardation of the dislocation motion on the concentration of point defects. For a defect concentration $n < n_1 = \frac{1}{\varepsilon^2}\left(\frac{v}{c}\right)^3$, the retarding force is independent of the defect concentration because the phonon subsystem of the crystal makes a dominant contribution to the retardation of the dislocation motion. For a dislocation velocity $v \approx 10^{-2}\,c$, we obtain $n_1 \approx 10^{-4}$. In the case when the defect concentration lies in the range $n_1 < n < n_2$, where

$$n_2 = \frac{3}{4\pi^2 \varepsilon^2 (1-\gamma)} \frac{B v^2}{\mu R c} \approx \frac{1}{(\pi \varepsilon)^2}\left(\frac{B v}{\mu R}\right)\frac{v}{c}, \qquad (21)$$

the retarding force increases linearly with an increase in the defect concentration. It is worth noting that, as the velocity of dislocation glide increases, the slope of the dependence decreases in inverse proportion to the velocity in accordance with formula (12) (at $n_1 < n$, we have $F_d > Bv$; i.e., $F \approx F_d$). At concentrations $n > n_2$, the retarding force of the dislocation motion is described by expression (9); i.e., it is proportional to the cubic root of the defect concentration.

It should be noted that the dissipation mechanism under investigation is independent of temperature. By contrast, the damping constant depends substantially on the temperature and is governed by different mechanisms in different temperature ranges. Let us make a comparative analysis of the contributions from different mechanisms of retardation to the damping constant B with the use of the data taken from [1]. At a temperature $T < T_{el} = 25$ K, the dominant mechanism of energy dissipation for a moving dislocation is the interaction with conduction electrons: $B \approx B_{el} \approx 10^{-6}$ Pa s. In the temperature range $T_{el} < T < T_S \approx 100$ K, the magnon mechanism of retardation becomes dominant (the corresponding damping constant is estimated as $B \approx B_S \approx 10^{-5}$–$10^{-6}$ Pa s in the aforementioned temperature range). At a temperature $T_S < T < \Theta_C \sim 1000$ K (where Θ_C is the Curie temperature), the retardation of dislocations is determined primarily by the phonon mechanism of energy dissipation ($B \approx B_f \approx 10^{-4}$–$10^{-5}$ Pa s).

Now, we perform a numerical evaluation. For $\varepsilon \approx 10^{-1}$ and $n_0 \approx 10^{-4}$, we obtain the critical velocity $v_0 \approx 10^{-2}c \approx 30$ m/s and $v_1 \approx 80$ m/s. As is known, the plastic strain rate $\dot{\varepsilon}_d$, the density of mobile dislocations ρ_d, and the mean velocity of dislocation motion v are related by the expression $\dot{\varepsilon}_d = b\rho_d v$. For the density of mobile dis-

locations $\rho_d \approx 10^{11}$ m^{-2}, we find $\dot{\varepsilon}_d \geq 10^3$ S^{-1}. The coefficient of retardation by point defects is estimated as $B_d \approx 5 \times 10^{-5}$ Pa s. In this case, two extrema can exist when the damping constant B satisfies the condition $B \leq 6 \times 10^{-6}$ Pa s. These values of the damping constant for the majority of crystals are observed at temperatures $T \leq 25$ K. For the concentration of point defects $n_0 \approx 10^{-3}$, we obtain the following parameters: $v_0 \approx 60$ m/s, $v_1 \approx 160$ m/s, $B_d \approx 10^{-4}$ Pa s, and $B \leq 10^{-5}$ Pa s. This condition for the damping constant B is satisfied at temperatures $T \leq 100$ K. Theoretically, two extrema at very high concentrations of point defects $n_0 \geq 10^{-2}$ can exist at room temperature. However, at these concentrations of point defects, we have the critical velocities $v_0 \approx 10^{-1} c$, i.e., the velocities close to the maximum permissible velocities in the framework of the model under consideration. This circumstance decreases the reliability of the estimates obtained for room temperature.

Therefore, owing to the collective interaction of point defects with a dislocation, the dependence $F(v)$ can exhibit two extrema in the case of motion of a single dislocation. However, it should be noted that, for the glide of a pair of dislocations, the defects can also enter into a collective interaction with each dislocation. A question now arises regarding the conditions under which the dominant effect on the dislocation spectrum (and, hence, on the retardation) is exerted by the interaction of dislocations with each other or by the collective interaction of point defects with each dislocation. The answer can be found from a comparison of the gaps determined by each of the above interactions. Under the condition $\Delta_{\text{dis}} > \Delta_{\text{def}}$, i.e.,

$$\frac{c}{a}\sqrt{\frac{2}{\ln(D/L)}} > \frac{c}{b}(n_0\varepsilon^2)^{1/3}, \qquad (22)$$

where L is the dislocation length and D is a quantity of the order of the crystal size, the interaction of the dislocations with each other makes a dominant contribution. It is this case that was analyzed in my earlier work [7]. Inequality (22) can be approximately rewritten in the form

$$a < b(n_0\varepsilon^2)^{-1/3} \equiv a_1. \qquad (23)$$

For a defect concentration $n_0 \approx 10^{-4}$, we obtain $a_1 \approx 10^2 b$. Otherwise ($a > a_1$), the interaction between the dislocations appears to be insignificant. Consequently, the results obtained in this study hold not only for the glide of a single dislocation but also for the motion of two dislocations separated by a distance greater than a_1.

Since the force of retardation of the dislocation motion in the velocity range $v_0 < v < v_1$ is inversely proportional to the velocity of dislocation glide, the extrema bounding this range are actually the boundary values determining the range of dynamic instability for the dislocation motion. The specific features of the dislocation behavior in this range were investigated in [3, 4].

4. CONCLUSIONS

Thus, the numerical estimates obtained in this paper demonstrate that the studied mechanism of dissipation at high concentrations of point defects can have a profound effect on the dislocation dynamics, especially at low temperatures.

REFERENCES

1. V. I. Al'shits and V. L. Indenbom, Usp. Fiz. Nauk **115** (1), 3 (1975) [Sov. Phys. Usp. **18** (1), 1 (1975)].
2. V. D. Natsik and K. A. Chishko, Cryst. Res. Technol. **19**, 763 (1984).
3. V. V. Malashenko, V. L. Sobolev, and B. I. Khudik, Phys. Status Solidi B **143**, 425 (1987).
4. V. V. Malashenko, V. L. Sobolev, and B. I. Khudik, Fiz. Tverd. Tela (Leningrad) **29** (5), 1614 (1987) [Sov. Phys. Solid State **29** (5), 931 (1987)].
5. V. V. Malashenko, Fiz. Tverd. Tela (Leningrad) **32** (2), 645 (1990) [Sov. Phys. Solid State **32** (2), 380 (1990)].
6. V. V. Malashenko, Fiz. Tverd. Tela (St. Petersburg) **39** (3), 493 (1997) [Phys. Solid State **39** (3), 428 (1997)].
7. V. V. Malashenko, Fiz. Tverd. Tela (St. Petersburg) **48** (3), 433 (2006) [Phys. Solid State **48** (3), 460 (2006)].
8. M. I. Kaganov, V. Ya. Kravchenko, and V. D. Natsik, Usp. Fiz. Nauk **111** (6), 655 (1973) [Sov. Phys. Usp. **16** (6), 878 (1973)].
9. V. G. Bar'yakhtar and V. V. Tarasenko, Fiz. Tverd. Tela (Leningrad) **22** (2), 431 (1980) [Sov. Phys. Solid State **22** (2), 252 (1980)].
10. A. M. Kosevich, *Dislocations in the Theory of Elasticity* (Naukova Dumka, Kiev, 1978) [in Russian].
11. V. V. Malashenko and T. I. Malashenko, Fiz. Tekh. Vys. Davleniĭ (Donetsk, Ukr.) **9**, 30 (1999).

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