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Influence of point defect misfit parameter on the dynamic yield strength of metals and alloys

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The motion of an ensemble of edge dislocations in case of high strain rate deformation of metals and alloys with a high concentration of point defects was theoretically analyzed. An analytical expression of the dependence of the dynamic yield strength on the point defect misfit parameter for various cases of high strain rate deformation is obtained. A qualitative analysis of the obtained results has been performed within the framework of the theory of dynamic interaction of defects (DID). Numerical estimates of the field of applicability of the obtained results have been made.

Keywords: dislocations, point defects, high strain rate deformation.

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1. Introduction

High strain rate deformation of metals and alloys occurs under conditions of high-energy external influences both at the stage of processing functional materials and during their operation [1–9]. It significantly differs from quasi-static deformation. Te kinetic energy of the dislocation exceeds the energy of its interaction with the structural defects of the crystal due to strong external influences. The dislocation performs an over-barrier sliding, overcoming crystal defects without the help of thermal fluctuations. The mechanism of energy dissipation is radically changing and the role of collective dynamic effects is significantly increasing. As a result, the dependence of the dynamic drag force of dislocations on the characteristics of structural defects becomes significantly more complicated. This leads to a more complicated dependence of the mechanical properties of materials on these characteristics. The dynamic interaction of dislocations with other defects in the crystal structure, in particular, with the Guinier-Preston zones formed at the first stage of aging of alloys, has a significant effect on the mechanical properties of crystals [10]. The dependence of the dynamic yield strength on the concentration of point defects and dislocation density under high strain rate deformation conditions was theoretically analyzed in Ref. [11,12]. It has been shown that this dependence has a non-monotonic character. The purpose of this work is to obtain an analytical dependence of the dynamic yield strength on the point defect misfit parameter.

2. Formulation of the problem, solution, analysis of results

The studied region of dislocation velocities is determined by the inequality $10^{-2}c \leq v \ll c$, where c is the velocity of propagation of transverse sound waves in a crystal. These are the rates 10^{-2}–$10^{-1}c$. The problem is solved within the framework of the theory of dynamic interaction of defects (DID), which has been successfully applied to solve a number of problems of dislocation dynamics [13–16]. Dislocation is considered as an elastic string with effective tension and effective mass. The dissipation mechanism in the dynamic domain consists in the irreversible transformation of the energy of external influences into the energy of dislocation vibrations in the plane of sliding. These fluctuations are considered small, which makes it possible, in the second order of perturbation theory, to calculate the force of dynamic drag of dislocation by structural defects using the following formula

$$F_{def} = \frac{nb^2}{8\pi^2 m} \int d^3q |q_x| \cdot |\sigma_{xy}(\mathbf{q})|^2 \delta\left(q_x^2 v^2 - \omega^2(q_z)\right). \quad (1)$$

Here n — the volume concentration of the corresponding defects, m — the mass of the dislocation unit, $\sigma_{xy}(\mathbf{q})$ — the Fourier transform of the stress tensor components created by the corresponding defect, $\omega(q_z)$ — the spectrum of dislocation vibrations. We can find the contribution of the corresponding structural defects to the dynamic yield strength of the crystal by calculating the dynamic drag force of the dislocation.

Consider an ensemble of infinite edge dislocations moving under the action of constant external stress σ_{xy}^0 along the axis OX with constant velocity v in planes of sliding parallel to XOZ. Point defects are randomly distributed throughout the crystal. The dislocation lines are parallel to the axis OZ, their Burgers vectors are parallel to the axis OX. The position of the kth dislocation is determined by the function

$$X_k(y = 0, z, t) = vt + w_k(y = 0, z, t). \qquad (2)$$

Here $w_k(y = 0, z, t)$ is a random variable describing transverse dislocation vibrations in the sliding plane as a result of interaction with structural defects.

The equation of motion of the kth dislocation can be represented as

$$m\left\{\frac{\partial^2 X}{\partial t^2} - c^2\frac{\partial^2 X}{\partial z^2}\right\} = b\left[\sigma_0 + \sigma_{xy}^d + \sigma_{xy}^{dis}\right] - B\frac{\partial X}{\partial t}. \qquad (3)$$

Here σ_{xy}^d — component of the stress tensor created by point defects on the dislocation line, σ_{xy}^{dis} — component of the stress tensor created on this line by other dislocations of the ensemble, B — phonon damping constant.

It follows from the formula (1) that the magnitude of the dynamic drag force of dislocations, and, consequently, the dynamic yield strength, depends on the type of spectrum of dislocation vibrations. The collective interaction of point defects with dislocation and the collective interaction of other dislocations of the ensemble can generate a gap in the dislocation spectrum, which has a significant impact on the nature of dynamic drag. The spectrum of dislocation vibrations in this case has the following form

$$\omega(q_z) = \sqrt{c^2 q_z^2 + \Delta^2}. \qquad (4)$$

If the gap Δ is created by the collective interaction of point defects with dislocation, then according to [11], it has the form

$$\Delta = \Delta_d = \frac{c}{b}\left(n_d\chi^2\right)^{1/4}, \qquad (5)$$

where n_d — the dimensionless concentration of point defects, χ — the parameter of their dimensional discrepancy, which is determined by the expression [10]

$$\chi = \left|\frac{R_d - R_m}{R_m}\right|. \qquad (6)$$

Here R_d is the radius of the point defect atom, R_m is the radius of the matrix atom.

The contribution of the collective interaction of the ensemble dislocations to the formation of the spectral gap according to [12] is defined by the expression

$$\Delta_{dis} = \pi b\sqrt{\frac{\mu\rho}{6\pi m(1-\gamma)}} \approx c\sqrt{\rho}. \qquad (7)$$

Here ρ is the dislocation density, μ is the shear modulus, γ is the Poisson's ratio.

Let us first consider the case when point defects make the main contribution to the dynamic drag of dislocation, and the formation of the dislocation spectrum is dominated by the collective interaction of the dislocations of the ensemble. This happens at concentrations of

$$n_d < n_0 = \left(\frac{\rho b^2}{\chi}\right)^2. \qquad (8)$$

Let us make numerical estimations. We obtain $n_0 = 10^{-4}$ for the values $b = 3\cdot 10^{-10}$ m, $\chi = 10^{-1}$, $\rho = 4\cdot 10^{15}\,\mathrm{m}^{-2}$.

Using the results of the DID theory, we obtain the dependence of the dynamic yield strength of the metal on the defect misfit parameter. It is quadratic

$$\tau = K\chi^2; \quad K = \mu\frac{n_d}{(\rho b^2)^2}\frac{\dot{\varepsilon} b}{c}. \qquad (9)$$

Here $\dot{\varepsilon}$ — strain rate, μ — shear modulus.

Let us now analyze the case when the main contribution to both the dynamic drag of dislocation and the formation of a gap is made by the collective interaction of point defects. This situation is realized at point defect concentrations of $n_d > n_0$. Using the results of the theory of DID and performing the necessary transformations, we conclude that the dependence of the dynamic yield strength of the metal on the defect misfit parameter in this case is linear

$$\tau = D\chi; \quad D = \frac{\mu\dot{\varepsilon}\sqrt{n_d}}{\rho b c}. \qquad (10)$$

This formula is valid for dislocation velocities

$$v < v_0 = b\Delta_d = c(n_d\chi^2)^{1/4}. \qquad (11)$$

$v_0 = 3\cdot 10^2$ m/s is obtained for the values $c = 3\cdot 10^3$ m/s, $n_d = 10^{-4}$, $\chi = 10^{-1}$.

This type of dependence was observed by the authors of Ref. [17].

Next, let us consider the high strain rate deformation of an aged two-component alloy with a high concentration of Guinier-Preston zones. The most interesting case is when the Guinier-Preston zones make the main contribution to the dynamic drag of dislocations, and point defects dominate the formation of the spectral gap. This situation is realized with a volumetric concentration of Guinier-Preston zones of $n_G = 10^{23}-10^{24}\,\mathrm{m}^{-3}$ and a concentration of point defects of $n_d > n_0$. Dynamic drag of dislocations by Guinier-Preston zones has the character of dry friction (i.e., it does not depend on the sliding velocity) at velocities of $v < v_G = R\Delta$, where R is the average radius of the Guinier-Preston zone. For the values $R = 10b$ and $n_d = 10^{-2}$, we obtain that the critical velocity v_G is close to the velocity of transverse sound waves in metal, i.e. dry friction occurs in almost the entire considered velocity range. The dependence of the yield strength on the defect misfit parameter is determined in an aged alloy by the expression

$$\tau = \frac{G}{\sqrt{\chi}}; \quad G = \mu\frac{n_G b^2 R}{\sqrt[4]{n_d}}. \qquad (12)$$

It follows from the formula obtained that the yield strength decreases with the increase of the misfit parameter.

Let's analyze the results obtained within the framework of the DID theory. Dislocation drag occurs when irreversible energy losses occur as a result of defect overcoming. As noted above, the dissipation mechanism comprises the conversion of energy from external influences into the energy of dislocation oscillations. The greater the energy of these oscillations, the stronger the dislocation drag. The occurrence of a spectral gap reduces the efficiency of oscillation excitation, and therefore reduces the dislocation drag. Thus, there are two competing factors. On the one hand, the increase of the misfit parameter increases local elastic stresses, and, consequently, the drag force. On the other hand, the spectral gap increases according to formula (5) with the increase of the parameter χ which reduces the drag force. The competition of these factors explains the pattern of the obtained results. Point defects make the main contribution to the drag force in the first case, but they do not affect the spectral gap. This situation is characterized by the strongest (quadratic) increase of the yield strength with an increase of χ. These defects make the main contribution not only to drag, but also to the formation of a gap in the second case, as a result, the dependence $\tau(\chi)$ becomes weaker (linear). Point defects do not significantly contribute to drag in the third case, but they increase the spectral gap, as a result, an increase of the misfit parameter leads to a decrease of the yield strength.

3. Conclusions

It is shown within the framework of the theory of dynamic interaction of defects that collective effects in the field of high strain rate deformation have a significant effect on the specific type of dependence of the dynamic yield strength on the point defect misfit parameter. This dependence varies for different concentrations of point defects, since it is their concentration that determines the degree of influence of point defects on the formation of the total dynamic drag force and the magnitude of the spectral gap.

The obtained results may be useful for the analysis of high strain rate deformation of metal and alloys.

Conflict of interest

The author declares that he has no conflict of interest.

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