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DYNAMIC DRAG OF DISLOCATION BY POINT DEFECTS IN NEAR-SURFACE CRYSTAL LAYER

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The effect of the surface on edge dislocation glide in the crystal with point defects both on the surface and in the bulk is studied theoretically. It is shown that the drag force of dislocation can be reduced by the image forces to several orders of magnitude in nanoscale region.

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1. Introduction

Crystal surface can essentially affect different properties of the crystal, including plastic ones.[1] In nanocrystals, the role of the surface is highly important. As it is known, the plastic properties of crystals are to a considerable extent formed by dislocation motion. The moving dislocations interact with different point defects distributed both on the surface and in the bulk of crystal. The image force action on moving dislocations is numerically studied in Refs. 2–6, however, influence of these forces on the dislocation drag by point defects has not been investigated yet.

The velocity range of dislocation motion in the crystal can be subdivided into two: a region of thermally activated motion, where local barriers created are overcome due to thermal fluctuations, and a dynamic one, where the kinetic energy of dislocation motion is greater than the energy of interaction with local bariers, which is why the dislocation motion can be described by dynamic equations. Though the dynamic range includes the velocities of motion $10^{-2}c \leq v \ll c$, where c is velocity of propagation of transverse sound waves, however the dynamic mechanisms of dissipation may be important for fluctuations overcoming the barriers by the moving dislocation. Moreover, for soft metals (copper, zinc, aluminum, lead, etc.) the region of high velocities starts at relatively low external stresses.

The dynamic drag of dislocations by point defects chaotically distributed in crystal bulk was studied in Refs. 7–9. Reference 10 investigates a motion of edge dislocation in parallel to the free crystal surface containing point defects. It was shown that the velocity dependence of the force of dislocation drag by surface point defects is nonmonotonic. The influence of image forces was not considered there.

This paper deals with the investigation of image forces effect on the dynamic drag of dislocations by point defects chaotically distributed both on the crystal surface and in the bulk. We show that the image forces greatly reduce the resistance of point defects to edge dislocation motion in the near-surface layer.

2. Model and Calculation

Let an infinite edge dislocation be moving under the influence of a continuous external stress σ_0 in the positive direction of axis OX at a constant velocity v and in parallel to crystal surface XOY. The dislocation line is parallel to axis OY, the Burgers vector being parallel to axis OX. For crystal points $z \leq 0$. The dislocation glide plain coincides with plane $z = -L$. The dislocation position is defined by the function

$$X(z = -L, y, t) = vt + w(z = -L, y, t)\,, \tag{1}$$

where function $w(z = -L, y, t)$ describes random fluctuations of the dislocation elements in the glide plane relative to the undisturbed dislocation line.

The equation of dislocation motion may be written in the following form:

$$m\left\{\frac{\partial X^2}{\partial t^2} - c^2\frac{\partial^2 X}{\partial y^2}\right\} = b[\sigma_0 + \sigma_{xz}^i + \sigma_{xz}^S + \sigma_{xz}^V] - B\frac{\partial X}{\partial t}\,. \tag{2}$$

Here σ_{xz}^S and σ_{xz}^V are tensor components of the stresses created on the dislocation line by point defects chaotically distributed on the surface and in the bulk of the crystal, respectively; σ_{xz}^i are image forces acting on the dislocation due to available free surface, b is the modulus of dislocation Burgers vector, m is the mass of dislocation unit length, B is the damping constant dependent on phonon, magnon, electron or another dissipation mechanism characterized by a linear dependence of dislocation drag force on the velocity of its slip, c is the propagation velocity of transverse sound waves in the crystal. As was shown in Ref. 7, the drag force induced by a field of randomly distributed defects depends only slightly on the phonon mechanisms of dissipation because of the smallness of the dimensionless parameter $\alpha = Bbv/(mc^2)$, which is small in most cases.

Let us study how the image forces affect the type of dislocation oscillation spectrum. To calculate the image force acting on the dislocation we use the standard method of images.[11] According to this method, the dislocation image is constructed such that the sum of the stresses of dislocation σ_{ik}^d and its image σ_{ik}^i on the free surface are equal to zero. If $\sigma_{ik}^d + \sigma_{ik}^i \neq 0$, we add a term calculated using stress function ψ to satisfy the boundary conditions.

Let us construct a simple image of the edge dislocation (Fig. 1). Under superposition of stresses created by the dislocation and its image all stress components

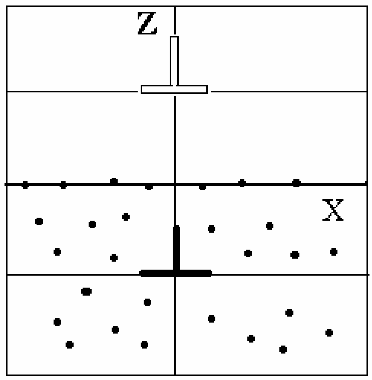

Fig. 1. Semi-infinite crystal with point defects on the surface and in the bulk. Edge dislocation and its image.

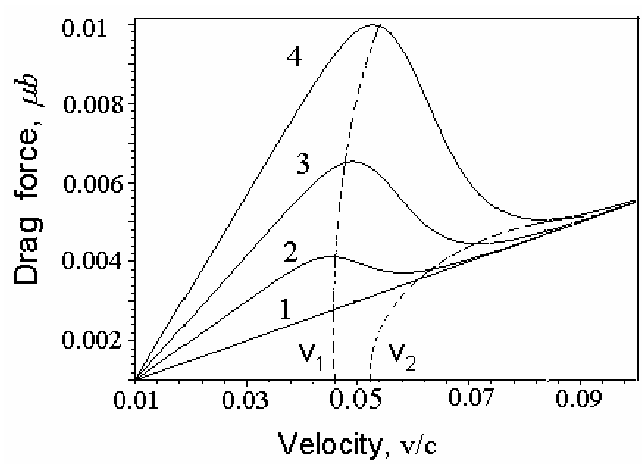

Fig. 2. The velocity-dependence of the drag force for different values of defect concentration. ($n_4 > n_3 > n_2 > n_1 = 0$). Point defects are distributed in infinite crystal bulk.

on the three surface, apart from σ_{xz}, turn to zero. After simple algebra we get additional stresses occuring on the dislocation line due to the free surfaces as follows:

$$\sigma_{xz}^{i} = M\frac{x(12zLz_-^2 - 4zLx^2 + z_-^4 - x^4)}{r^6}\,, \tag{3}$$

$$M = \frac{\mu b}{2\pi(1-\gamma)}, \qquad r = \sqrt{x^2 + z_-^2}, \qquad z_- = z - L\,. \tag{4}$$

On the undisturbed dislocation line the stresses are equal to zero: $\sigma_{xz}^{i} = 0$ for $x = 0$, and the surface does not affect the linear edge dislocation in the glide plane parallel to that surface. However, the surface changes the dislocation oscillation spectrum. Expanding $\sigma_{xz}^{i}(vt + w; y)$ with respect to small parameter w/L and

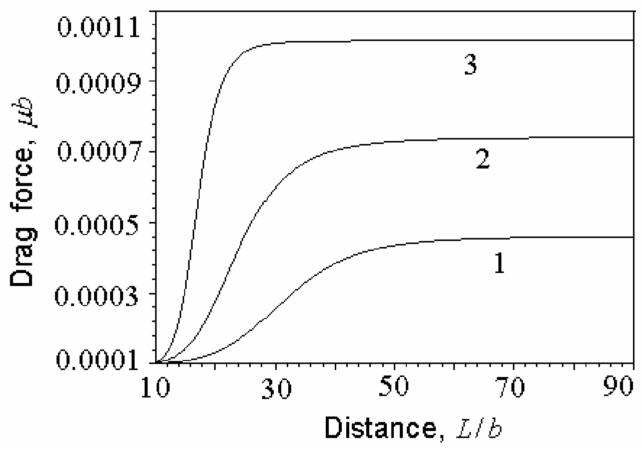

Fig. 3. Distance-dependence of the drag force for different values of defect concentration ($n_3 > n_2 > n_1$). Point defects are distributed in semi-infinite crystal bulk.

changing variables to the system of dislocation mass center we obtain the oscillation spectrum

$$\omega^2 = c^2 p_z^2 + \Delta^2, \qquad \Delta = \Delta_S = \frac{1}{L}\sqrt{\frac{bM}{2m}} \approx \frac{c}{L}\,. \tag{5}$$

Index s means that in this case the gap value is defined by the image forces caused by the free surface. Below it will be shown that other interactions can contribute to the spectral gap, in particular, the collective effects of point defects distributed in crystal bulk. Thus, the edge dislocation glide is, in a sense, equivalent to the motion of a pair of dislocations.[9] In this case, a pair is formed by the dislocation and its image.

Using the results of Ref. 10 we can write the dislocation drag force by point surface defects

$$F = \frac{n_S b^2}{4\pi m}\int dq_x dq_y |q_x| \cdot |\sigma_{xz}(q_x, q_y, z)|^2 \delta(q_x^2 v^2 - \omega^2(q_y))\,, \tag{6}$$

where n_S is the surface concentration of point defects, $\delta(q_x^2 v^2 - \omega^2(q_y))$ is the Dirac delta function, $\omega(q_y)$ is the dislocation oscillation spectrum. In our case, condition $L\Delta_S \ll v$ cannot be satisfied, as $L\Delta_S \approx c \gg v$, i.e. only condition $L\Delta_S \gg v$ is satisfied. Then the drag force may be written in the following form:

$$F_d = n_{0S}\varepsilon_S^2 \mu b \left(\frac{R}{L}\right)^3 \left(\frac{c}{v}\right)^{\frac{11}{2}} \exp\left(-\frac{2c}{v}\right)\,. \tag{7}$$

Here $n_0 = n_S R^2$ is the dimensionless surface concentration of point defects, μ is the shear modulus, ε_S is the dimensionless misfit parameter of surface defect, characterizing its power, R is a value of the order of defect radius, $R \approx b$. To simplify the formula we approximate dislocation mass by $m \approx \rho b^2$, where ρ is the crystal density, as well as the relation $c^2 = \mu/\rho$. The analysis shows that in the dynamic region the drag force is exponentially small. One can say that the dislocation drag, related to the dislocation excitations by surface impurities, is locked. Thus, the free surface does not generate force acting on the dislocation in the glide plane, but it suppresses the origination of dislocation oscillations in this plane and, as a result, locks the dynamic drag of the dislocation by surface defects.

The gap in the spectrum of dislocation oscillations, that occurred due to the free surface, affects dislocation drag by not only surface point defects but also the defects distributed in crystal bulk. But the interaction of those defects with dislocation initiates a spectral gap too. The dynamic interaction of defects with the dislocation can be of collective character and in the form of independent collisions and it is determined by the dislocation velocity.[8]

Let us denote the time of dislocation interaction with impurity atom as $\tau_{\rm def} \approx R/v$. The time of perturbation propagation along the dislocation for a distance of the order of the average distance between defects l_d is denoted by $\tau_{\rm dis} \approx l_d/c$. In the region of independent collisions $v > v_1 = R\Delta_d$ the inequality $\tau_{\rm def} < \tau_{\rm dis}$ is satisfied, i.e. the dislocation element for the time of interaction with the point defect is not affected by other defects. In this region point defects do not create a gap in the dislocation spectrum. In the region of collective interaction ($v < v_1$) we have $\tau_{\rm def} > \tau_{\rm dis}$, i.e. during the time of dislocation interaction with point defect this dislocation element has time to receive a signal from other defects. The collective interaction of defects creates the spectrum gap

$$\Delta_d = \frac{c}{b}(n_{0V}\varepsilon^2)^{1/3} = \frac{c}{l}, \qquad (n_{0V}\varepsilon^2)^{-1/3} = l \approx l_d\,. \tag{8}$$

Here n_0 is the dimensionless concentration of point defects, $n_{0V} = n_V R^3$. Dependence of the drag force by point defects on dislocation velocity in an infinite crystal is schematically shown in Fig. 2. The values of $v > v_2 = v_1\sqrt{B_{\rm def}/B} = 2\pi\varepsilon\sqrt{(1-\gamma)n_{0V}\mu bc/3B}$ correspond to the region where the phonon drag exceeds drag by defects. In the region $v < v_2$ the drag by defects dominates, and values $v_1 < v < v_2$ correspond to the region of independent collisions, while for $v < v_1$ we have the collective interaction region.

When the edge dislocation is moving in near-surface layers of the crystal with point defects chaotically distributed in crystal bulk, the gap in the dislocation spectrum is defined as

$$\Delta^2 = \Delta_S^2 + \Delta_d^2\,, \tag{9}$$

where Δ_S is described by Eq. (5). To analyze the dislocation drag we consider three limiting cases:

Case 1. $\boldsymbol{\Delta_d \gg \Delta_S;\ b\Delta_d \gg v}$

This is the collective interaction region in which the defect contribution to spectral gap value strongly exceeds the image force contribution, $\Delta \approx \Delta_d$. By using Eqs. (5)

and (8), we obtain that region boundaries are approximately present inequalities $(bc/v) \gg l$ and$L \gg l$. In this case, the drag force is defined by the expression

$$F_d = \mu b(n_{0V}\varepsilon^2)^{\frac{1}{3}}\frac{v}{c}\,. \tag{10}$$

Case 2. $\boldsymbol{\Delta_S \gg \Delta_d; b\Delta_S \gg v}$

In this case, the image forces are the main contributors to gap formation. Boundaries of the region are defined by the inequalities $(bc/v) \gg L$ and $l \gg L$. In the region the drag force depends on distance to the surface

$$F_d = \mu b n_{0V}\varepsilon^2\frac{v}{c}\left(\frac{L}{b}\right)^2\,. \tag{11}$$

Case 3. $\boldsymbol{b\Delta_d \ll v; b\Delta_S \ll v}$

This is the independent collision region. Its boundaries are defined by the inequalities $(bc/v) \ll l \ll L$, if $l \ll L$, and $(bc/v) \ll L \ll l$, if $L \ll l$. In this range the drag force is not sensitive to the presence of spectrum gap, and, for the same in Ref. 7, it is inversely proportional to the dislocation velocity

$$F_d = \mu b n_{0V}\varepsilon^2\frac{c}{v}\,. \tag{12}$$

3. Conclusion

As follows from the analysis, the existence of surface essentially influences the edge dislocation drag only in Case 2. To estimate the role of surface effect we take the ratio of drag forces in Case 2 and in Case 1:

$$\frac{F_{d2}}{F_{d1}} = \left(\frac{L}{l}\right)^2\,. \tag{13}$$

For $n_{0V} \approx 10^{-4}$, $\varepsilon \approx 10^{-1}$, $L \approx 10b$ we obtain $(F_{d2}/F_{d1}) \approx 10^{-2}$, i.e. surface effect reduces the drag force by two orders of magnitude. So, the existence of surface makes the drag force of the dislocation by point defects much weaker. Figure 3 schematically presents the $F_d(L)$-dependence.

In our case, the thickness of the near-surface layer (with dominating surface effect) typically varies from several nanometers to tens of nanometers, so the present results can be useful for the analysis of the nanocrystal properties.

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