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Dynamic Blocking of the Influence of Surface Point Defects on the Glide of Edge Dislocations

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Abstract—The influence of image forces on an edge dislocation gliding parallel to the free crystal surface having point defects is studied theoretically. It is shown that image forces block the drag mechanism that involves the excitation of dislocation vibrations by surface defects.

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Properties of nanocrystals are largely dependent on intergrain boundaries [1] and the free crystal surface. The crystal surface itself can contain defects, e.g., impurities. Modern technology makes it possible to deposit them in a controlled manner. Interacting with dislocations, these impurities can have an effect on their motion and, therefore, on the plastic properties of crystals. Local barriers caused by defects are overcome by slowly gliding dislocations through thermal fluctuations. For rapidly gliding dislocations, thermal activation is not required, because their kinetic energy is greater than the height of potential barriers [2]. This dynamic regime of gliding corresponds to velocities $v \geq 10^{-2}c$, where c is the speed of transverse sound waves. In most metals, dislocations move at high velocities even under relatively weak external stresses. The dynamic drag exerted on edge dislocations by point defects randomly distributed over the crystal volume was studied in [3–7]. The drag of dislocations caused by surface point defects was studied in [8], where the dissipation mechanism was assumed to involve the irreversible transformation of the kinetic energy of a gliding dislocation into dislocation vibration energy. The influence of image forces was not taken into account in [8]. In this paper, we show that image forces cause the appearance of a gap in the dislocation vibration spectrum, which blocks the operation of this drag mechanism.

Let us consider an infinite edge dislocation gliding at a constant velocity v along the positive direction of the x axis parallel to the crystal surface (coinciding with the xy plane) under a constant external stress σ_0. The dislocation line is parallel to the y axis, and its Burgers vector is parallel to the x axis. The crystal occupies the region $z \leq 0$. The glide plane coincides with the $z = -L$ plane, and the position of the dislocation is described by the function

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

where $w(z = -L, y, t)$ is a random function describing vibrations of elements of the edge dislocation in the glide plane relative to the undistorted dislocation line.

The equation of motion of the dislocation is

$$m\left\{\frac{\partial X^2}{\partial t^2} - c^2\frac{\partial^2 X}{\partial y^2}\right\} = b[\sigma_0 + \sigma_{xz}(vt + w;\, y) + \sigma_{xz}^{\sigma}(vt + w;\, y)] - B\frac{\partial X}{\partial t}. \qquad (2)$$

Here, σ_{xz} is a component of the stress tensor produced by surface point defects at the dislocation line ($\sigma_{xz} = \sum_{i=1}^{N}\sigma_{xz,\,i}$, where N is the number of defects); σ_{xz}^{s} represents image forces acting on the dislocation due to the presence of the free surface; b is the magnitude of the dislocation Burgers vector; m is the dislocation mass per unit length; B is the damping constant due to phonons, magnons, electrons, and other dissipation mechanisms characterized by a linear dependence of the drag force exerted on the dislocation on its glide velocity; and c is the speed of transverse sound waves in the crystal. As in [3–8], we neglect the influence of the damping constant on the dislocation drag caused by point defects, because the dimensionless parameter $\alpha = Bbv/(mc^2)$ is small in most cases [3].

The required stress tensor component produced by a surface point defect is given by the expression [8]

$$\sigma_{xz}(\mathbf{r}) = -\frac{1}{2}\mu R^3 \varepsilon \frac{\partial^2}{\partial z \partial x}\frac{z^2}{r^3}. \quad (3)$$

where μ is the shear modulus, φ is the surface defect misfit parameter, and R is on the order of the defect radius. The Fourier transform of this component is

$$\sigma_{xz}(q_x, q_y, z) = \frac{2}{\pi} i\mu R^2 q_x \exp(-q|z|)(1-q|z|); \quad q = \sqrt{q_x^2 + q_y^2}. \quad (4)$$

As shown in [8], the dynamic drag force exerted on a dislocation by surface point defects can be written in the form

$$F = \frac{n_s b^2}{4\pi m}\int dq_x dq_y |q_x| |\sigma_{xz}(q_x, q_y, z)|^2 \times \delta(q_x^2 v^2 - \omega^2(q_y)), \quad (5)$$

where n_s is the surface density of point defects, $\delta(q_x^2 v^2 - \omega^2(q_y))$ is a Dirac δ function, and $\omega(q_y)$ is the spectrum of dislocation vibrations.

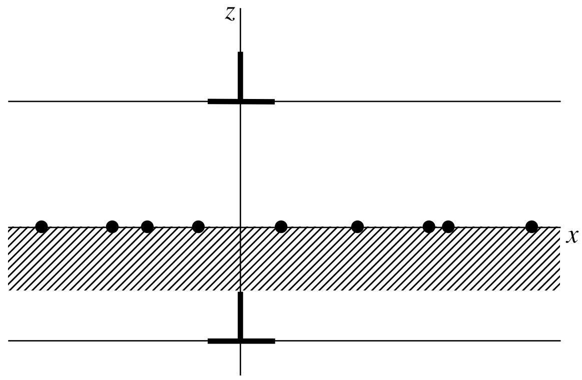
We calculate the image force exerted on the dislocation using the standard image method [9]. In this method, one should find the image of the dislocation for which the sum of the stresses produced by the dislocation (σ_{ik}^d) and its image (σ_{ik}^i) is zero at the free crystal surface. If certain components of this sum are nonzero at the surface, then to the solution should be added a term calculated using a stress function ψ in order to satisfy the boundary conditions. The stresses produced by a dislocation with coordinates ($x = 0$, $z = -L$) are given by

$$\sigma_{xx}^d = -D\frac{(z+L)(3x^2+(z+L)^2)}{(x^2+(z+L)^2)^2}, \quad \sigma_{zz}^d = D\frac{(z+L)(x^2-(z+L)^2)}{(x^2+(z+L)^2)^2}, \quad (6)$$

$$\sigma_{xz}^d = D\frac{x(x^2-(z+L)^2)}{(x^2+(z+L)^2)^2}, \quad D = \frac{\mu b}{2\pi(1-\gamma)}. \quad (7)$$

The mirror image of the edge dislocation (see figure) produces the stresses

$$\sigma_{xx}^i = -D\frac{(z-L)(3x^2+(z-L)^2)}{(x^2+(z-L)^2)^2}, \quad \sigma_{zz}^i = D\frac{(z-L)(x^2-(z-L)^2)}{(x^2+(z-L)^2)^2}, \quad (8)$$



Edge dislocation gliding in a plane parallel to the free crystal surface in the elastic field of surface point defects.

$$\sigma_{xz}^i = D\frac{x(x^2-(z-L)^2)}{(x^2+(z-L)^2)^2}. \quad (9)$$

The sum of the stresses produced by this dislocation and its image vanishes at the free surface, except for its component σ_{xz}. The additional term required to satisfy the boundary conditions is found by carrying out simple but fairly cumbersome calculations using the method described in [9]. The result is

$$\sigma_{xz}^0 = D\frac{2x((z-L)^4+6zL(z-L)^2-2zLx^2-x^4)}{(x^2+(z-L)^2)^3}. \quad (10)$$

It is easy to verify that $\sigma_{xz}^d + \sigma_{xz}^i + \sigma_{xz}^0 = 0$ at the $z = 0$ plane and, therefore, the boundary condition is satisfied. Thus, the additional stress exerted on the dislocation because of the presence of the free surface is given by

$$\sigma_{xz}^s = \sigma_{xz}^i + \sigma_{xz}^0 = D\frac{x((z-L)^4+12zL(z-L)^2-4zLx^2-x^4)}{(x^2+(z-L)^2)^3}. \quad (11)$$

It is easily seen that, at the unperturbed dislocation line, this stress is zero ($\sigma_{xz}^s = 0$ at $x = 0$); i.e., the presence of the surface does not cause forces acting on the straight edge dislocation in the glide plane parallel to the surface. However, the surface changes the spectrum of dislocation vibrations. In order to find this spectrum, as in [6], we write the equation of motion (2) in the dislocation center-of-mass system and expand $\sigma_{xz}^s(vt + w; y)$ in powers of the small parameter w/L

$$\sigma_{xz}^s(vt+w; y) \approx -D\frac{w}{4L^2}. \quad (12)$$

Taking the Fourier transform, we find the vibration spectrum to be

$$\omega^2 = c^2 p_y^2 + \Delta^2, \quad \Delta = \frac{b}{L}\sqrt{\frac{M}{2m}} \approx \frac{c}{L}. \qquad (13)$$

Thus, the problem of an edge dislocation gliding in a plane parallel to the surface is equivalent in some sense to the problem of motion of a pair of dislocations considered in [6]. In this case, the pair is formed by the dislocation and its image.

Using the results obtained in [8], we write the drag force exerted on the dislocation by surface impurities for two extreme cases. If $L\Delta \ll v$, the drag force is given by

$$F = \frac{n_s b^2 \mu^2 \varepsilon^2 R^6}{mcvL^3}. \qquad (14)$$

In our case, the condition $L\Delta \gg v$ cannot be satisfied because $L\Delta \approx c \gg v$. In the case of $L\Delta \ll v$, the drag force is

$$F = \frac{n_s b^2 \mu^2 \varepsilon^2 R^6}{mc}\left(\frac{\Delta^9 L^3}{v^{11}}\right)^{1/2} \exp\left(-\frac{2L\Delta}{v}\right). \qquad (15)$$

In order to estimate this force, we write Eq. (15) in the form

$$F \approx n_0 \varepsilon^2 \mu b \left(\frac{R}{L}\right)^3 \left(\frac{c}{v}\right)^{11/2} \exp\left(-\frac{2c}{v}\right) = n_0 \varepsilon^2 \mu b \left(\frac{R}{L}\right)^3 \exp\left(-\frac{2c}{v} + \frac{11}{2}\ln\frac{c}{v}\right). \qquad (16)$$

where $n_0 = n_s R^2$ is the dimensionless surface density of point defects. From analyzing the dependence of expression (16) on the dislocation velocity, it follows that, as the velocity increases to $v = (4/11)c$, the drag force increases and then begins to decrease. Since our model is valid only for $v \ll c$, the drag force increases with the dislocation velocity over the entire velocity range studied and reaches a maximum at $v \approx 10^{-1}c$. Let us estimate the maximum value of the drag force. Using typical values $\varepsilon \approx 10^{-1}$, $\mu \approx 5 \times 10^{10}$ Pa, $b \approx 3 \times 10^{-10}$ m, the dimensional density $n_0 \approx 10^{-2}$, $L \approx 10R$, and $v \approx 10^{-1}c$, we obtain $F_{max} \approx 10^{-6}\exp(-7)$ N/m. The value of the preexponential factor does not exceed the drag force due electrons, i.e., it is very small, and the exponential factor makes the drag force negligible. Thus, the mechanism of dislocation drag involving the excitation of dislocation vibrations by surface impurities is blocked; i.e., the free surface does not produce a force acting on a dislocation in the glide plane but it prevents dislocation vibrations in this plane.

The results of this study can be useful in analyzing the plastic properties of nanocrystals.

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