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Features of high strain rate deformation of aged alloys

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The sliding of an ensemble of edge dislocations under high strain rate deformation of an aged binary alloy is theoretically analyzed. An analytical expression of the dependence of the dynamic yield strength on the dislocation density is obtained. The conditions under which this dependence is nonmonotonic and has a minimum and maximum are obtained. The minimum occurs during the transition from the dominance of dynamic drag of dislocations by point defects to the dominance of drag by other dislocations (Taylor hardening). The position of the maximum corresponds to the value of the dislocation density, at which their contribution to the formation of the spectral gap becomes dominant.

Keywords: dislocations, defects, high strain rate deformation, yield strength.

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1. Introduction

Metal alloys are widely used in various industries, therefore, the study and improvement of their mechanical properties is a very important task [1,2]. The density of dislocations has a significant influence on the formation of these properties. In the case of quasi-static deformation, the dependence of the mechanical properties of alloys on the dislocation density is determined by the Taylor relation [3]. This relation is quite universal and is confirmed by numerous experimental studies [4-10]. However, this dependence is more complex in the case of high strain rate deformation of aged binary alloys. High strain rate deformation is realized both at the stage of processing alloys and manufacturing products, and during their operation [11–16]. At the same time, the strain rate can reach $10^3 - 10^9 \text{ s}^{-1}$, and dislocations move at speeds from tens to hundreds and even thousands of meters per second.

The theoretical description of the evolution of a dislocation ensemble in a deformable crystal has been very successfully implemented in the works of [17-21]. In these works, kinetic equations for dislocation density are formulated, including the processes of generation of dislocations from sources, immobilization, reproduction, annihilation and diffusion of dislocations. This approach is very versatile and effective and has allowed us to obtain excellent agreement with numerous experimental data, in particular, in the field of quasi-static deformation. In the field of high strain rate deformation, the theory of dynamic interaction of structural defects (DID) developed by us can be useful in analyzing a number of important cases [22-27]. In fact, it is a modified string model of Granato-Lukke. It is not as universal as the system of equations [17-21] and does not allow taking into account all specific aspects of plastic deformation. In particular, it does not take into account the processes of annihilation and the origin of dislocations and assumes that the density of dislocations remains constant. But this theory correctly describes the mechanism of dissipation during the supra-barrier movement of dislocations and the effects of collective interaction of structural defects in the dynamic domain. This circumstance made it possible to qualitatively explain a number of experimental dependences, in particular, the dependence of the dynamic yield strength of the alloy on the concentration of the second component, the density of dislocations, and the strain rate. In particular, the linear [28,29], root [30,29] and N-shaped [31,29,25] dependence of this limit on the concentration of dopant, non-monotonic velocity dependence having a maximum of [32,26], non-monotonic dependence was explained of the dislocation density, having a maximum of [33,34] and a minimum of [27,35]. Conditions under which the dependence of the dynamic yield strength on the dislocation density can have both a minimum and a maximum are obtained in this paper.

We will analyze high strain rate deformation of an aged two-component alloy containing the Guinier-Preston zones. These zones appear in alloys at the first stage of aging and play a very important role in the formation of their mechanical properties [36-39]. Let infinite edge dislocations under the action of a constant external stress σ_0 move in planes parallel to *XOZ* with a constant velocity ν in a crystal containing atoms of the second component and the Guinier-Preston zone. The dislocation lines are parallel to the axis *OZ*. The position of the *k*-th dislocation is determined by the function

$$W_k(z,t) = \nu t + w_k(z,t). \tag{1}$$

Here $w_k(x, t)$ is a random variable describing transverse dislocation oscillations that occur when it interacts with chaotically distributed structural defects. The average value of this value over the dislocation length and over the chaotic distribution of defects is zero.

The dislocation slip is described by the following equation

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

Here m — the mass of the dislocation length unit, B the damping constant due to phonon, magnon, electronic or other dissipation mechanisms characterized by a linear dependence of the dislocation drag force on its sliding speed, c — the propagation velocity of transverse sound waves in the crystal, σ_{xy}^p , σ_{xy}^{dis} , σ_{xy}^G — components of the stress tensor generated on the line k of the dislocation, respectively, by point defects (atoms of the second component), other dislocations and Guinier-Preston zones.

Ginier-Preston zone planes are parallel to the dislocation sliding planes, and their centers are randomly distributed in the crystal. We assume that all zones have a radius *R*, the same thickness equal to the diameter of the atom of the second component, the same Burgers vectors $\mathbf{b}_0 = (0, -b_0, 0)$ that are parallel to axis *OY*.

Each dislocation of the ensemble is considered as an elastic string with effective tension and effective mass. These dislocations perform over-barrier sliding in the elastic field of structural defects. The main mechanism of dissipation is the excitation of dislocation vibrations as a result of the interaction of dislocation with structural defects. The effectiveness of such a mechanism was confirmed by the authors of the work [40], who theoretically investigated the over-barrier movement of the dislocation and proved that as a result of interaction with point defects, it experiences strong excitation of its own oscillations. The authors of this work took into account the random nature of the transmission of the moving dislocation of the pulse by individual impurity atoms and calculated the correlation function $G(\tau) = \langle w(z, t)w(z, t + \tau) \rangle$, where the function w(z,t) describes the displacement of a single dislocation site during its oscillations during sliding along the crystal. This correlation function is determined experimentally through the correlation function of inelastic light scattering proportional to it $\langle E(t)E(t+\tau)\rangle$, which can be measured using optical displacement spectroscopy [41]. This experimental method makes it possible to measure field fluctuations through current fluctuations for times less than the characteristic period of dislocation oscillations. According to the authors of the work [40], the amplitude of dislocation oscillations can exceed the amplitude of thermal oscillations by several orders of magnitude. The excitation of natural oscillations occurs the more efficiently, the more

point defects distort the crystal, that is, the amplitude of the oscillations increases with an increase in the mismatch parameter.

The effectiveness of this dissipation mechanism is influenced by the type of vibrational spectrum of dislocation, primarily the presence of a gap in it. The presence of a gap means that the dislocation oscillates in a potential well, which moves along the crystal along with the dislocation. Such a pit may arise as a result of the collective interaction of point defects or other dislocations with a moving dislocation. In this case, the dislocation oscillation spectrum containing the gap Δ has the form

$$\omega^2(q_z) = c^2 q_z^2 + \Delta^2. \tag{3}$$

Let us describe in more detail the collective interaction of point defects with dislocation. According to DID theory, dynamic interaction of defects with a dislocation, depending on the dislocation sliding velocity, can have both a collective nature and nature of independent collisions [23]. Let us denote the time of interaction of the dislocation with the impurity atom as $\tau_{def} = R/\nu$, where R — the radius of the defect, the time of propagation of the disturbance along the dislocation at a distance of the order of the average distance between the defects we denote $\tau_{pr} = l/c$. In the region of independent collisions $v > v_0 = R\Delta_{def}$, the inequality $\tau_{def} < \tau_{pr}$ is fulfilled, i.e. the dislocation element does not experience the influence of other defects during interaction with the point defect. In this region, no gap appears in the spectrum of dislocation oscillations. In the area of collective interaction ($\nu < \nu_0$), on the contrary, $\tau_{def} > \tau_{pr}$, i.e. during the time of interaction of a dislocation with a point defect, this dislocation element manages ,,to feel" the influence of other defects that caused a dislocation shape disturbance. In this region, a gap appears in the dislocation oscillation spectrum, which is described by the following expression [29]

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

In the case of a high density of dislocations, it is their collective interaction with each dislocation that makes the main contribution to the formation of a gap in the spectrum of this dislocation. This is the case for density values $\rho > \rho_0$, where

$$\rho_0 = \frac{\sqrt{n_d \chi^2}}{b^2}.$$
 (5)

Here n_d — dimensionless concentration of atoms of the second component, χ — parameter of their dimensional discrepancy. The spectral gap is described by the following expression [24]:

$$\Delta = \Delta_{dis} = b \sqrt{\frac{\rho M}{m}} \approx c \sqrt{\rho}; \quad M = \frac{\mu}{2\pi (1-\gamma)}, \quad (6)$$

where γ — Poisson's ratio, μ — shift modulus.

The force of dynamic drag of a moving edge dislocation by point defects, according to the DID, will be calculated in the second order of perturbation theory, considering the transverse oscillations of the dislocation in the sliding plane to be small, which are described by the function w(z, t):

$$F = b \left\langle \frac{\partial \sigma_{xy}}{\partial X} w \right\rangle = b \left\langle \frac{\partial \sigma_{xy}}{\partial X} G \sigma_{xy} \right\rangle, \tag{7}$$

where G — Green's function of the dislocation equation of motion. Fourier transform of this function looks like

$$G(\omega, q) = \frac{1}{\omega^2 + i\beta\omega - c^2q^2}; \quad \beta = \frac{B}{m}.$$
 (8)

According to the DID theory, we can write down an equation for contribution of various structural defects to the dynamic yield strength in the following form

$$\tau = \frac{nb}{8\pi^2 m} \int d^3 q |q_x| \cdot |\sigma^d_{xy}(\mathbf{q})|^2 \delta\big(q_x^2 \nu^2 - \omega^2(q_z)\big), \quad (9)$$

where $\omega(q_z)$ — dislocation vibration spectrum, n — volume concentration of structural defects, $\sigma_{xy}(\mathbf{q})$ — Fourier image of the corresponding component of the stress tensor generated by the defect.

The DID theory is in a sense analogous to the theory of the mean field. Each dislocation slides across the crystal, oscillating in a potential well that moves with it and is created by the collective action of other defects — by some average field.

The dynamic yield strength of a binary alloy is equal to the sum of the contributions of the Taylor hardening τ_T , the contribution of the Guinier zones—Preston τ_G and the atoms of the second component τ_d

$$\tau = \tau_T + \tau_G + \tau_d. \tag{10}$$

The component τ_T is proportional to the square root of the dislocation density

$$\tau_T = \alpha \mu b \sqrt{\rho}. \tag{11}$$

where α is a dimensionless coefficient of the order of one.

Next, consider the region of strain rates bounded by the inequality

$$\dot{\varepsilon} < \dot{\varepsilon}_{cr} = \rho b^2 c \sqrt{\rho + \rho_0}. \tag{12}$$

In this area, the dynamic deceleration force of dislocation by Guinier–Preston zones does not depend on the speed of dislocation movement. Accordingly, τ_G does not depend on the strain rate. Let us make numerical estimations. We obtain the critical velocity value $\dot{\varepsilon}_{cr} = 10^8 \text{ s}^{-1}$ for the values $\rho = 5 \cdot 10^{15} \text{ m}^{-2}$, $b = 4 \cdot 10^{-10} \text{ m}$, $n_d = 10^{-4}$, $\chi = 10^{-1}$, $c = 3 \cdot 10^3 \text{ m/s}$.

Taking advantage of the results of the work [22–27], an expression for the contribution of the Guinier–Preston zones is obtained in the following form

$$\tau_G = \frac{D}{\sqrt{\rho + \rho_0}}; \quad D = \mu n_G bR. \tag{13}$$

Here n_G — volume concentration of Guinier–Preston zones.

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Dependence of the dynamic yield strength of a binary alloy on the dislocation density.

The contribution of the atoms of the second component can be described by the following expression

$$\tau_d = \frac{K}{\rho(\rho + \rho_0)}; \quad K = \frac{\mu n_d \chi^2 \dot{\varepsilon}}{b^3 c}.$$
 (14)

Analysis of the expression (10) shows that the dependence of the dynamic yield strength is nonmonotonic and has a minimum and maximum. The graph of this dependence is shown in the figure.

The maximum of this dependence is observed at density values of the order ρ_0 , the position of the minimum is determined by the expression

$$\rho_{\min} = \left(\frac{2\dot{\varepsilon}\rho_0}{\alpha c}\right)^{2/3}.$$
 (15)

We obtain $\rho_0 = 10^{15} \text{ m}^2$, $\rho_{\min} = 10^{13} - 10^{14} \text{ m}^{-2}$ in the studied range of strain rates. The obtained result is consistent with the conclusion of the DID theory: the minimum yield strength is observed when the dominant contribution of defects to the complete inhibition of dislocations is changed, the maximum occurs when the dominant contribution to the formation of the spectral gap is changed. In our case, the minimum occurs during the transition from the dominance of dynamic inhibition of dislocation by point defects to the dominance of inhibition by other dislocations (Taylor hardening). The position of the maximum corresponds to the dislocation density value, at which the dominant contribution of the gap is replaced by the dominant contribution of dislocations.

Both extremes can be observed at a high value of the volume concentration of the Guinier–Preston zones $n_G = 10^{23}-10^{24} \text{ m}^{-3}$ and the change in dislocation density from 10^{11} m^{-2} to 10^{16} m^{-2} . At the same time $n_d = 10^{-4}$, $\dot{\varepsilon} = 10^7 \text{ s}^{-1}$, $\rho_0 = 10^{15} \text{ m}^{-2}$, $\rho_{\min} = 10^{13}-10^{14} \text{ m}^{-2}$.

The results obtained can be useful in analyzing the mechanical properties of aged alloys under conditions of high-energy external impacts.

Conflict of interest

The authors declare that they have no conflict of interest.

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