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Violation of the Taylor relation under high-energy external influences

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Received April 4, 2022

Revised May 5, 2022

Accepted May 6, 2022

The motion of an edge dislocation ensemble in a binary alloy under high strain rate deformation is theoretically analyzed. Within the framework of the theory of dynamic interaction of defects (DID) an analytical expression for the dependence of the dynamic yield stress on the dislocation density is obtained. The conditions for the violation of the Taylor relation under high-energy external influences are determined. The experimentally observed nonmonotonic dependence of the dynamic yield strength on the dislocation density is explained. The minimum of this dependence is due to the competition between the influence of various structural defects on moving dislocations. This minimum takes place during the transition from the dominance of dynamic drag by one type of defects to the dominance of another type defects.

Keywords: dislocations, high strain rate deformation, defects, Guinier-Preston zones, alloys.

DOI: 10.21883/PSS.2022.08.54620.340

High-energy external influences on metals and alloys give rise to high strain rate deformation of these materials, which is realized in such technologically important applications as molding, cutting, punching, high-speed machining, development of shock-resistant materials, piercing of protective shells, impact damage of aircraft and spacecraft and structures, explosion welding, impact on materials by high-power laser pulses, dynamic channel-angular pressing [1–6].

A great number of papers [7–13] have been devoted to influence of dislocation density on formation of mechanical properties of metals and alloys. In process of high strain rate deformation, plastic deformation rate reaches values of 10^3 – 10^9 s⁻¹. Most articles analyze high strain rate deformation using molecular dynamics method, which allows us to study many features of interaction between moving dislocations and other structural defects and visualize effects of dynamic interaction [14,15]. However, this method does not allow us to obtain analytical expressions of dependence of mechanical properties on the plastic deformation rate and characteristics of structural defects, such as concentration, size, and misfit parameter. The theory of dynamic interaction of defects (DID) that we developed allows us to solve a wide range of problems on high strain rate deformation of functional materials within a unified approach and to obtain the above analytical expressions [16–21]. The mechanism of dissipation during dynamic interaction with structural defects consists in irreversible transition of dislocation kinetic energy into energy of its transverse vibrations in the sliding plane. This mechanism turns out to be very sensitive to the type of the dislocation oscillation spectrum of the dislocation, primarily to a gap in this spectrum, since it is

its presence and magnitude that the efficiency of excitation of dislocation oscillations depends on.

The above features lead to the fact that under conditions of high strain rate deformation, the effect of various structural defects on mechanical properties of alloys may differ significantly from their influence during quasi-static deformation. Dynamic effects and such parameter as time of interaction between moving dislocation and structural defect drag it begin to play a significant role. This time depends on both the speed of dislocation movement and the size of the defect it overcomes. If the alloy contains two types of defects significantly differing in their geometric dimensions and, consequently, time of interaction between dislocation and such defects, it leads to the appearance of two maxima on the velocity dependence of dynamic yield strength of such an alloy [20]. Such defects can be Guinier–Preston zones and alloying additives. Another important consequence of such structural defects in an alloy is a change in the nature of the dependence of mechanical properties on dislocation density. As is known, in the case of quasi-static deformation, dependence of yield strength on dislocation density is determined by Taylor relation, according to which yield strength of crystalline metals and alloys is proportional to the square root of the dislocation density [22]:

$$\tau_T = \alpha \mu b \sqrt{\rho}, \quad (1)$$

where μ — shear modulus, ρ — dislocation density, α — dimensionless coefficient of the order of unity, b — modulus of dislocation Burgers vector. Strictly speaking, equation (1) must include a term of sum τ_0 — critical shear stress. However, this term of sum does not depend on dislocation densities, and in cases of high dislocation densities we are

considering it is not essential. Therefore, we, like the authors of papers [23,24], will not take it into account. Taylor relation is quite universal. The authors of [25] observed its fulfillment during high strain rate deformation of copper and steel. Under certain conditions, however, such deformation leads to Taylor relation distortion. Strength of a binary alloy under conditions of high strain rate deformation is determined by force of dynamic drag of dislocations by structural defects. This force depends on which defects make the main contribution to formation of spectral gap and which — directly to development of dynamic resistance of moving dislocation. Dominant influence of these or those defects is determined by their concentration and power. Competition of dynamic interaction of dislocations with various defects significantly complicates the nature of dependence between mechanical properties of alloys and dislocation density. As was shown in [20], when main contribution to drag of the moving dislocations ensemble is made by the Guinier–Preston zones, and the main contribution to formation of a gap in the spectrum of dislocation is made by the collective interaction of dislocations, Taylor relation distortion occurs. Dependence of dynamic yield strength of a binary alloy on dislocation density in this case becomes non-monotonic: root growth is replaced by a decline. The maximum corresponds to the density at which the contribution of collective interaction of dislocations to spectral gap formation begins to exceed the contribution of collective interaction of point defects with moving dislocations.

In this paper, analytical expressions for the dependence of yield strength of metals and alloys on dislocation density for various cases of high strain rate deformation are obtained, and it is shown that this dependence has a non-monotonic character.

Analysis of high strain rate deformation of aged binary alloys will be carried out within the framework of the theory of dynamic interaction of defects (DID) that we have developed. This theory is a modified Granato–Lücke model, where a dislocation is treated as an elastic string with effective tension and an effective mass of field origin. DID theory significantly extends the scope of this model and allows us to explain a number of available experimental data from unified positions, to reveal the generality in physical nature of completely different processes, and to predict a number of new dynamic effects, detection of which can become an incentive to set up new targeted experiments.

As noted above, the main dissipation mechanism in our case is excitation of dislocation oscillations as a result of dislocation interaction with structural defects. Effectiveness of such mechanism was confirmed by the authors of [26], who theoretically investigated dislocation motion in the dynamic velocity region and proved that, as a result of interaction with point defects, it experiences a strong excitation of its own oscillations. The authors of this paper took into account the random nature of the momentum transfer of the moving dislocation by individual impurity atoms and calculated correlation function $G(\tau) = \langle w(z, t)w(z, t + \tau) \rangle$, where

function $w(z, t)$ describes dislocation unit shift when it oscillates while sliding along a crystal. The latter is determined experimentally through its proportional correlation function of inelastic light scattering $\langle E(t)E(t + \tau) \rangle$, which can be measured by optical displacement spectroscopy [27]. The aforementioned experimental method makes it possible to measure field fluctuations through current fluctuations for the times shorter than the characteristic dislocation oscillation period, thus greatly extending the capabilities of traditional optical methods widely used in the experimental study of dislocation structures. According to the authors of [26], amplitude of dislocation excitation may exceed amplitude of thermal oscillations by several orders of magnitude, and excitation of natural oscillations occurs the more effectively the greater the distortion introduced by point defects into the crystal lattice, i.e. increases with increasing misfit parameter.

Let us consider uniform sliding of an ensemble of infinite boundary dislocations under the action of constant external stress σ_0 in a field of structural defects chaotically distributed in the crystal volume. Dislocation lines are parallel to OZ axis, the Burgers vectors are parallel to OX axis, in the positive direction of which the dislocations slide with constant velocity v . Sliding plane of k -dislocation coincides with XOZ plane, and its position is determined by function

$$W_k(y = 0, z, t) = vt + w_k(y = 0, z, t). \quad (2)$$

The term of sum vt describes motion of the dislocation center of mass at velocity v , and function $w(z, t)$ — oscillations of the dislocation element arising from interaction with chaotically distributed defects in crystal structure. Since $w(z, t)$ is a random variable, $\langle w(z, t) \rangle = 0$, where symbol $\langle \dots \rangle$ means averaging over dislocation length and chaotic defect distribution

$$\langle f(r_i) \rangle = \frac{1}{L} \int_L dz \int_V \prod_{i=1}^N f(r_i) \frac{dr_i}{VN}, \quad (3)$$

where V — crystal volume, N — number of defects in a crystal, L — dislocation length. When averaging is performed according to standard procedure, number of defects N and crystal volume V are going to infinity, while their ratio remains constant and equal to the average defect concentration.

Equation of motion of dislocation under study has the form of

$$m \left\{ \frac{\partial^2 W_k}{\partial t^2} - c^2 \frac{\partial^2 W_k}{\partial z^2} \right\} = b [\sigma_0 + \sigma_{xy}^p + \sigma_{xy}^{dis} + \sigma_{xy}^G] - B \frac{\partial W_k}{\partial t}. \quad (4)$$

Here m — mass per dislocation unit length, which, according to [22], is determined by equation

$$m = \frac{\rho_C b^2}{4\pi(1 - \nu)} \ln \frac{L_d}{r_0}, \quad (5)$$

where ρ_C — crystal density, L_d — dislocation length order magnitude, r_0 — atomic distance order magnitude,

γ — Poisson's ratio, B — damping constant due to phonon, magnon, electron or other dissipation mechanisms, characterized by linear dependence of dislocation drag force on its sliding velocity, c — velocity of transverse sound waves in a crystal, σ_{xy}^p , σ_{xy}^{dis} , σ_{xy}^G — components of stress tensor created on the line of k -dislocation accordingly by point defects (atoms of the second component), other dislocations and Guinier–Preston areas.

Dislocation drag in this region is largely determined by energy transfer from the dislocation to various elementary excitations in a crystal, but at high concentrations of impurities and other lattice defects the dynamic interaction of the dislocation with these defects becomes very significant and greatly affects its mobility and crystal properties provided for by dislocation motion.

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

$$F = b \left\langle \frac{\partial \sigma_{xy}}{\partial X} w \right\rangle = b \left\langle \frac{\partial \sigma_{xy}}{\partial X} G \sigma_{xy} \right\rangle, \quad (6)$$

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

$$G(\omega, q) = \frac{1}{\omega^2 + i\beta\omega - c^2q^2}; \quad \beta = \frac{B}{m}. \quad (7)$$

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

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

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

In the case of point defects, we consider them to be dilatation centers and introduce a smooth clipping of their elastic field at a distance of the order of the effective atom radius to eliminate non-physical divergences. Their elimination in our case plays a fundamental role, since correct description of collective effects influence on dislocation dynamics requires taking into account interaction of structural defects at distances of the order of the lattice constant [17]:

$$\sigma_{xy}(r) = \mu r_0^3 \chi \frac{\partial^2}{\partial x \partial y} \frac{1 - \exp(-r/r_0)}{r}. \quad (9)$$

Here r_0 — effective atom radius of the point defect, χ — its dimensional misfit parameter

$$\chi = \frac{r_0 - r_a}{r_a}. \quad (10)$$

Here r_a — effective atom radius of the matrix.

Fourier transform of the stress tensor component we need looks like

$$\sigma_{xy}(\mathbf{q}) = 4\pi\mu r_0^3 \chi \frac{q_x q_y}{q^2} \frac{r_0^{-2}}{q^2 + r_0^{-2}}. \quad (11)$$

After the necessary transformations the equation for contribution of point defects (in particular, atoms of the second component in the two-component alloy) to the value of dynamic yield strength can be reduced to the following form

$$\tau = \frac{2nb\mu^2\varepsilon^2}{m} \iiint d^3q |q_x| \frac{q_x^2 q_y^2}{q^4} \frac{r_0^2}{(q^2 + r_0^{-2})^2} \times \delta(q_x^2 v^2 - \omega^2(q_z)). \quad (12)$$

Since the dissipation mechanism under study is realized due to excitation of dislocation vibrations, it turns out to be very sensitive to the type of dislocation vibrational spectrum, in particular, its efficiency depends on the presence of a gap in the spectrum. A spectral gap means that dislocation oscillates being in a parabolic potential well. Problems about dislocation oscillations in a potential well have been considered by other authors as well, in particular, the problem about dislocation oscillations in Peierls relief. However, within the framework of the theory developed by us, problems on motion of a dislocation making oscillations in a potential well moving along a crystal are solved. Such a well can be created as a result of collective interaction of point defects with a moving dislocation, collective interaction of dislocations of a moving ensemble with each individual dislocation, magnetoelastic interaction of a dislocation with a magnetic subsystem of a crystal, and action of image forces on a dislocation sliding in a near-surface layer. In the above cases, the spectrum of dislocation oscillations looks like

$$\omega^2(q_z) = c^2 q_z^2 + \Delta^2, \quad (13)$$

where Δ — spectral gap, which is equal in order of magnitude to $\Delta = c/L$, where L — characteristic scale of interaction making the main contribution to gap formation. It is the size of this gap that determines the depth of the parabolic potential well, where the sliding dislocation oscillates. The depth of this well, and hence the dynamic behavior of dislocations, can be greatly influenced by high hydrostatic pressure, exposure to which is one of the promising methods to improve properties of functional materials [28].

This paper considers several cases of high strain rate deformation characterized by a non-monotonic dependence of yield strength on dislocation density. One of them is implemented when the collective interaction of point defects with a moving dislocation makes the main contribution both to formation of the dislocation oscillation spectrum and to dynamic drag of dislocations. Contribution of the collective

interaction of alloying additives to spectral gap formation becomes dominant, if the following condition is met

$$n_d > \left(\frac{\rho b^2}{\chi} \right)^2, \quad (14)$$

where n_d — dimensionless concentration of alloying impurity. Numerical estimates show that such a case can be implemented, for example, at $\rho \leq 10^{14} \text{ m}^{-2}$ and $n_d = 10^{-2} - 10^{-4}$.

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 [17]. Let us denote time of dislocation interaction with impurity atom as $r_{def} = R/v$, where R — defect radius, let us denote propagation time of perturbation along a dislocation by a distance of the order of the average distance between defects as $r_{pr} = l/c$. In the region of independent collisions $v > v_0 = R\Delta_{def}$ inequality $\tau_{def} < \tau_{pr}$ is satisfied, i.e. the dislocation element is not affected by other defects during the interaction with the point defect. In this region, no gap appears in the spectrum of dislocation oscillations. In the region of collective interaction ($v < v_0$), on the contrary, $\tau_{def} > \tau_{pr}$, i.e., for the time of dislocation interaction with a point defect, such dislocation element has time to „feel“ influence of other defects that caused dislocation form perturbation. In this region, a gap appears in the dislocation oscillation spectrum, which is described by the following expression [17]:

$$\Delta = \Delta_d = \frac{c}{b} (n_d \chi^2)^{1/4}. \quad (15)$$

Using the results of DID theory and performing the necessary transformations, we obtain in this case the following equation for dynamic yield strength of a binary alloy

$$\tau = \frac{\dot{\epsilon}}{\rho b} \left(\frac{\mu \chi \sqrt{n_d}}{c} + \frac{B}{b} \right) + \alpha \mu b \sqrt{\rho}. \quad (16)$$

Here $\dot{\epsilon}$ — plastic strain rate, B — phonon drag coefficient of dislocation.

The equation obtained is characterized by a non-monotonic dependence of dynamic yield strength on dislocation density at high concentration of alloying additives. In the case under study Taylor relation is distorted. Yield strength decreases to a certain minimum value with increasing dislocation density, after which yield strength begins to increase.

Let us determine dislocation density at which dynamic yield strength has a minimum value. Differentiating equation (16) and setting it to zero, we obtain the required expression for dislocation density

$$\rho_{\min} = \left(\frac{2\dot{\epsilon}}{\alpha \mu b^2} \left(\frac{\mu \chi \sqrt{n_d}}{c} + \frac{B}{b} \right) \right)^{2/3}. \quad (17)$$

With the obtained value of density, contribution of Taylor hardening begins to exceed the contribution of dynamic drag of dislocations by impurity atoms and phonons.

Let us make a numerical estimation. For values $\mu = 5 \cdot 10^{10} \text{ Pa}$, $b = 4 \cdot 10^{-10} \text{ m}$, $n_d = 10^{-2}$, $\chi = 10^{-1}$, $c = 3 \cdot 10^3 \text{ m/s}$, $B = 10^{-4} \text{ Pa} \cdot \text{s}$, $\dot{\epsilon} = 10^6 \text{ s}^{-1}$ we will get $\rho_{\min} = 10^{13} \text{ m}^{-2}$.

Taylor relation is also distorted when the collective interaction of alloying additive atoms with dislocations makes the main contribution to the force of dynamic drag, and the collective interaction of dislocations among themselves dominates in spectral gap formation. Such a situation can be realized at high dislocation density and high plastic strain rate: $\rho = 10^{15} - 10^{16} \text{ m}^{-2}$, $\dot{\epsilon} = 10^8 - 10^9 \text{ s}^{-1}$.

In this case, the gap in the dislocation oscillation spectrum is described by equation [17]:

$$\Delta = \Delta_{dis} = b \sqrt{\frac{\rho M}{m}} = c \sqrt{\frac{2\rho}{\ln(D/l_{dis})}} \approx c \sqrt{\rho};$$

$$M = \frac{\mu}{2\pi(1-\gamma)}, \quad (18)$$

where γ — Poisson's ratio, l_{dis} — average dislocation length, D — a value of order of magnitude of crystal size.

Dependence of dynamic yield strength on dislocation density is also non-monotonic and has a minimum, but decrease in this case is more drastic

$$\tau = \mu \frac{n_d \chi^2}{(\rho b^2)^2} \left(\frac{\dot{\epsilon} b}{c} \right) + \alpha \mu b \sqrt{\rho}. \quad (19)$$

The value of dislocation density corresponding to the minimum value of the dynamic yield strength in this case is determined by equation

$$\rho_{\min} = \left(\frac{4n_d \chi^2 \dot{\epsilon}}{\alpha b^4 c} \right)^{2/5}. \quad (20)$$

A similar dependence can be observed in aged binary alloys containing Guinier–Preston zones. It occurs when the Guinier–Preston zones give the main contribution to dynamic drag, and the spectral gap is formed as a result of the collective interaction of dislocations. This case can be realized at high values of dislocation density and Guinier–Preston zone concentration: $\rho = 10^{15} - 10^{16} \text{ m}^{-2}$, $n_G = 10^{23} - 10^{24} \text{ m}^{-3}$. At the same time decrease of yield strength becomes slower

$$\tau = \mu \frac{n_G b R}{\sqrt{\rho}} + \alpha \mu b \sqrt{\rho}. \quad (21)$$

In the case considered above the force of dynamic drag of dislocations by Guinier–Preston zones has a nature of dry friction, i.e. is independent on dislocation sliding speed and, consequently, of plastic strain rate. Dynamic yield strength becomes minimal at the value of dislocation density

$$\rho_{\min} = \frac{n_G R}{\alpha}. \quad (22)$$

Let us make a numerical estimation. For values $n_G = 10^{23} \text{ m}^{-3}$, $R = 10^{-9} \text{ m}$ we will get $\rho_{\min} = 10^{14} \text{ m}^{-2}$.

If plastic strain rate reaches high values, deviation from Taylor relation is possible even in pure metals. Such situation is possible at values $B = 10^{-4} \text{ Pa} \cdot \text{s}$, $\dot{\varepsilon} = 10^8 - 10^9 \text{ s}^{-1}$, $\rho = 10^{15} - 10^{16} \text{ m}^{-2}$. In this case, dependence of dynamic yield strength on dislocation density has the following form

$$\tau = \frac{\dot{\varepsilon} B}{\rho b^2} + \alpha \mu b \sqrt{\rho}. \quad (23)$$

Such dependence has indeed been observed experimentally [24]. Equation (23) is in qualitative agreement with a similar equation obtained in [24] and differs from it only by a numerical coefficient of the order of unity. At the same time the minimum position is determined by the following value of dislocation density

$$\rho_{\min} = \left(\frac{2\dot{\varepsilon} B}{\alpha \mu b^3} \right)^{2/3}. \quad (24)$$

Let us make numerical estimations. For values $\rho = 5 \cdot 10^{15} \text{ m}^{-2}$, $\mu = 5 \cdot 10^{10} \text{ Pa}$, $b = 4 \cdot 10^{-10} \text{ m}$, $n_d = 10^{-2}$, $\chi = 10^{-1}$, $c = 3 \cdot 10^3 \text{ m/s}$, $B = 10^{-4} \text{ Pa} \cdot \text{s}$, $\dot{\varepsilon} = 10^6 \text{ s}^{-1}$ we will get value of dynamic yield strength $\tau = 10^8 \text{ Pa}$, which by order of magnitude complies with experimental data [24].

The obtained results may be useful in 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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