Grain size dependence of the yield stress for metals at quasistatic and dynamic loadings

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Abstract
Micro mechanisms of plastic deformation and the defect structure evolution are sufficiently changing with the strain rate increase. It leads to non-monotonic relations between the macroscopic characteristics of metal strength or ductility and the structure parameters such as a grain size. Our simulations predict an inverse Hall-Petch relation for ultrafine-grained metals at extremely high strain rate (above $10^7 s^{-1}$). Mechanisms of the homogeneous nucleation of dislocations and the mechanical twining can effectively decrease the stresses at strain rates up to $10^9 s^{-1}$.

Keywords High strain rates plasticity, Ultrafine-grained materials, Inverse Hall-Petch relation, Grain boundary sliding

1. Introduction

Materials with ultrafine-grained structure (with the grain diameters of several tenth parts of micrometer), as well as nanocrystalline materials, are widely investigated both theoretically and experimentally for the last twenty years [1,2]. This goes in parallel with the development of experimental technic [3], and leads to discover and investigation of some new effects specific for these materials. One of them is an inverse Hall-Petch relation – the decrease of the yield stress at the grain size decrease. All observations of this effect can be divided on two parts: deformation at low strain rates - usually less than $10^{-1} s^{-1}$ [4-6], and the molecular dynamics simulation at extremely high strain rates - usually greater than $10^8 s^{-1}$ [7]. Preparation and experimental investigation of the nanocrystalline materials is very difficult. On the other hand, the molecular dynamics is very limited in application to macroscopic volumes of microcrystalline and coarse grained materials. It does not allow one to define directly the macroscopic characteristics of the material and to carry out simulations of deformation of the macroscopic volumes of substance with realistic strain rates.

For investigation of the internal defect structure influence on the macroscopic strength and ductility one can take some microscopic mechanisms proposed by theoretical investigations or molecular dynamics simulations and to include it in the modeling in the framework of continuum mechanics. Simulation results could be verified by comparison with experimental data. This way, supplemented by the procedure of averaging over the micro-volumes of substance, allows us to monitor the change of the defect structure and its influence on the strength parameters of different metals.

2. Yield strength at low strain rate

The yield strength σ_y is one of the key macroscopic parameters, which determines the strength of the material. It grows with the dislocation density ρ_D increase and the grain size d decrease, which are well-known effects in most polycrystalline metals and alloys. This dependences are expressed by the Taylor [8,9] and the Hall-Petch relations [10,11] for the barrier of dislocations gliding:

$$\sigma_y = \sigma_0 + \alpha G b \sqrt{\rho_D} + k_{HP} \big/ \sqrt{d} \quad (1)$$

Here σ_0 includes an influence of impurities and of the Pierls relief resistance for dislocation gliding; G is the shear modulus, b is the Burgers vector, k_{HP} is the Hall-Petch constant, which is a characteristic of the metal. This relation is exactly satisfied until the grain size in polycrystalline material is higher than 1 μm and at the low strain rates. Influence of the mechanical twinning on the resistance for dislocations gliding can be accounted in the form of the Hall-Petch relation with an average distance between the twins Δ instead of the grain size and with other constant k_{TW} [9].

If we introduce the volume fractions of the dislocations $R = b^2 \rho_D$, the grain boundaries $\eta = 1-\left(1-\delta/d\right)^3 \approx 3\delta/d$ and the twins [12] $F = \left(1+\Delta/2e\right)^{-1}$ then the Eq. (1) takes the next form:

$$\sigma_y = \sigma_0 + k_1 \frac{\sqrt{R}}{b} + k_2 \frac{\sqrt{\eta}}{\sqrt{\delta}} + k_3 \frac{\sqrt{F}}{\sqrt{e}}, \tag{2}$$

were δ and e are the grain width and the twin width correspondently, which are almost constant for the material as well as the Burgers vector. Constants: $k_1 = \alpha G b$, $k_2 \sim \sqrt{3} k_{HP}$, $k_3 \sim k_{TW}/\sqrt{2}$. As the volume fractions are less than unity, the yield stress is limited. Introduction of impurities apparently is the only way to the increase yield stress to the theoretical tensile strength value [13].

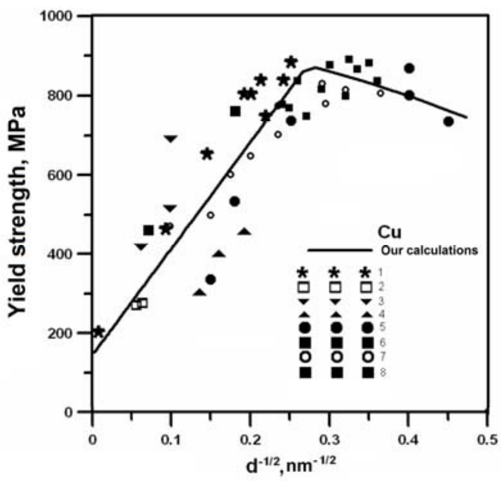

Figure 1 The grain size dependence of the yield strength for copper. Experimental data: 1 – [1], 2 – [17], 3 – [18], 4 – [19], 5 – [4], 6 – [20], 7 – [5], 8 – [6].

In microcrystalline metals ($d < 1\,\mu\text{m}$), it is often observed the abnormal Hall-Petch relation with k_{HP} different from that in the coarse-grained crystal; as a result, slope of the Hall-Petch curve is changing [14]. Therefore, the yield stress does not achieve the value predicted from the Eq. (2). In many nanocrystalline materials with d lesser than 12 nm-15 nm an inverse Hall-Petch relation is observed: the yield strength decreases with the decrease of the grain size [4-6,15]. This effect is often related with the grain boundary sliding as an alternative mechanism of plasticity. As it was shown in [16], there is a barrier resistance stress y_b; it is equal to the doubled external stresses, which must be exceeded for initiating of the grain boundary sliding. It depends on the grain size.

$$y_b = 0.01 \cdot \frac{G}{1-\nu}\left(1-\frac{\delta}{d}\right)^2, \tag{3}$$

where ν is the Poisson ratio of the material, which is slightly varied for different metals. For activation of the grain boundary sliding one need to apply the stress exceeding $\sigma_y = 2y_b$; for copper and iron it is about 1GPa. Therefore, in ultrafine-grained and nanocrystalline materials the plastic flow occurs only at high internal stresses. This model give a good fit with experimental results for different metals [16]. Fig. 1 presents the experimental observation points and the theoretical curve for copper in the Hall-Petch coordinates. One can see an existing of the maximum of the yield strength for grain size of about 12nm. Yield strength here is less than 1 GPa.

3. Yield strength at high strain rates

Micro mechanisms of plastic deformation and defect structure evolution are sufficiently changing with the strain rate increase. The high stain rate experiments demonstrate a deviation from the Hall-Petch relation even for ultrafine grained metals. At these deformation conditions we will define dynamical yield strength of the material through the maximal shear stresses, which is reached during the high-rate deformation. Dynamical yield stress not fully determined by the internal stresses from different obstacles as in the quasistatic deformation conditions. At extremely high strain rate (above 10^6 s^{-1}) it has a sufficiently dynamical nature and defined by dynamics properties of the dislocation and grains gliding, by the kinetics of the dislocation generation and annihilation. For the yield stress definition one must solve a full system of equation which describes the material plasticity as it was done in [21]. This system includes the equations for dislocation and grain boundary plasticity and the continuum mechanics equations.

3.1 Dislocation plasticity model

Theoretical description of the dislocation plasticity one can get using the model proposed in [22]. In monocrystalline metals, dislocations can glide along the limited numbers of slip planes; we shall numerate it by index β . Equation for plastic deformation caused by the dislocation glide [23] can be written as:

$$\frac{dw_{ik}^D}{dt} = -\frac{1}{2}\sum_{\beta}\left(b_i^\beta\ n_k^\beta + n_k^\beta b_i^\beta\right) V_D^\beta\ \rho_D^\beta\ . \tag{4}$$

Here b^β is the Burgers vector of dislocations, ρ_D^β is the scalar density of dislocation (their number per unit square) in glide plane with index β , V_D^β – velocity of dislocations. These parameters fully determine the plastic deformation of the coarse-grained crystals. Velocity of dislocation can be defined from the movement equation [22]:

$$\frac{m_0}{\left(1-\left(V_D^\beta / c_t\right)^2\right)^{3/2}}\frac{dV_D^\beta}{dt} = \left(F_D^\beta \pm \frac{b^\beta Y}{2}\right) - \frac{B(T)V_D^\beta}{\sqrt{1-\left(V_D^\beta / c_t\right)^2}}\ , \tag{5}$$

Here $F_D^\beta = S_{ik} b_i n_k$ is the Pitch-Keller force (it acts on the unit length of dislocation line from the external stresses), Y is the static yield stress of the material, which depends on the dislocation density, the grain size and the presence of different impurities [24]. m_0 is the field mass of dislocation, c_t is transverse sound velocity. The terms with sound velocity allows one to take into account an experimental fact that dislocation velocity is always limited above by the sound velocity. Coefficient of viscous friction $B(T)$ is temperature dependent [25,26]. Eq. (5) had demonstrated a good fit with experimental data for over barrier dislocation gliding at the high rate deformation [22].

For determination of the dislocation density one can write a kinetics equation in the next form [22]:

$$\frac{d\rho_D^\beta}{dt} = \frac{\eta}{\varepsilon_L}\frac{B\left(V_D^\beta\right)^2 \rho_D^\beta}{\sqrt{1-\left(V_D^\beta / c_t\right)^2}} - k_a b\left|V_D^\beta\right|\left(\rho_D^\beta\right)^2 - \frac{\rho_D^\beta\left|V_D^\beta\right|}{d}\ . \tag{6}$$

Here the dislocation source (the first term in the Eq. (5)) has been recorded from the energy-wise consideration; $\eta = 0.1$ is a portion of dissipated power, which is spent on generation of new defects; the energy $\varepsilon_L = 8эB / b$ [25] is required for generation of new dislocations (per unit of length). Annihilation term (the second term in the Eq. (5)) was written similar to [27].

For nanocrystalline materials one has to take into account an additional term in the kinetic equation (5). Dislocation core are being delocalized in the disordered grain boundary material [28], when it reaches any grain boundary [29]. Therefore, dislocation in nanocristalline material has a lifetime, which is equal to the traveling time of dislocation through the grain $d / \left|V_D^\beta\right|$, where d is an average grain size. Corresponding additional term in the right-hand part of the kinetics equation (5) is the next: $-\rho_D^\beta \left|V_D^\beta\right| / d$. The proposed model was verified on the experiments at various high strain rate deformation conditions, including the shock wave propagation in metals [22,30]. Its application demonstrates a good fit with experimental data at minimum adjustable parameters.

3.2 Model for grain boundary sliding

The plastic deformation related with the grain boundary plasticity one can describe similar to the Maxwell model for a highly viscous liquid [31] with the exception of the barrier resistance stress y_b. It means that grain boundaries are elastically deformed during short intervals of time. But when the deformation ceases, shear stresses remain in them, although they are dumped in the course of time, so that after sufficiently long time almost no inertial stress remains in the boundaries, exception of y_b. Viscous force appears in the grain boundaries due to diffusion, which counteracts the sliding of the grains layers relative to each other; it can be characterized by a relaxation time τ. As a result, the plastic deformation caused by the grain boundary sliding can be written in the next form [16]:

$$\dot{w}_{ik}^{gb} = \frac{1}{2G} \sum_\alpha \tau_i^\alpha n_k^\alpha \frac{\Theta\left(\sigma_\tau^\alpha - y_b\right)}{\tau}, \tag{7}$$

where $\Theta(x)$ is a Heaviside function, index α numerates the possible shifting planes of the grains; normal vectors to these planes can be written as n_i^α. Stresses applied to corresponding plane are $\sigma_{ik} n_k^\alpha$ and the stress component, which acts in the tangent direction τ_i to the plane, is equal to the convolution product $\sigma_{ik} n_k^\alpha \tau_i$. We will denote τ_i^α as the direction of the tangent vector corresponding to the maximum shear stresses applied to this plane. Then the maximal shear stress acting on the layer of grains can be represented as $\sigma_\tau^\alpha = s_{ik} n_i^\alpha \tau_k^\alpha$, where s_{ik} is a deviator of stresses. Using a linear approximation, one can obtain the following expression for the relaxation time of grain boundary sliding [16] from data of the molecular dynamics simulation [32]:

$$\tau = \frac{d k_b T}{12 G b \nu_D V_s} \exp\left(\frac{U_s}{k_b T}\right) \tag{8}$$

Activation volume V_s can be estimated as $V_s \sim b^3$. Activation energy U_s has the same order as the activation energy of viscous flow in molten state of the metal [28].
Tensor of the full plastic deformation can be written as

$$w_{ik} = w_{ik}^D + w_{ik}^{gb} \tag{9}$$

4. Simulation results

4.1 Dislocation starvation

At increasing of the strain rate an over-barrier dislocation gliding occurs and the domination resistant force becomes a phonon drag to the gliding dislocations [23]. At the further increasing of the strain rate the main mechanism of strain hardening becomes the dislocation starvation - it is well known phenomena in the field of nanopillars and thin film modeling [33] at rapid deformation condition. A distinction between the bulk material and these nano-crystals is in the cause of the starvation. In nano-crystals there are no ordinary dislocation sources, and the plasticity is usually provided by several entered dislocations and by surface instabilities [33]. In the bulk materials there is relatively large dislocation density and active dislocation sources exist. But the maximal dislocation density can be estimated through critical stress for the Frank-Read sources activation:

$$\sigma_\tau = Gb/L_{FR} \,. \qquad (10)$$

Here b $L_{FR} \sim 1/\sqrt{\rho_D}$ – a base of the Frank-Read source which has the same order as an inverse square root of the total dislocation density ρ_D. Then, for reasonable stresses $\sigma_\tau \sim 2\,\text{GPa}$, the total dislocation density is limited by the value $\rho_D \sim 10^{16} m^{-2}$. On the other hand, the Orowan equation [24] gives:

$$\dot{\varepsilon} = \rho_D b V_D \,. \qquad (11)$$

The dislocation velocity V_D can not exceeded the transverse sound velocity $c_t \approx 3000\,\text{m/s}$. As a result, we obtain the maximal strain rate at which dislocations can theoretically provide the full relaxation of shear stresses: $\dot{\varepsilon} < 10^{10} s^{-1}$. In real metals sufficient part of dislocations consists of immobile dislocations, which is not contributing to plastic relaxation. Our calculations demonstrate that the dislocation starvation takes place already at $\dot{\varepsilon} > 10^7 s^{-1}$. Therefore, even in ultrafine crystals with the grain size of about hundreds of nanometers a sufficient deviation from the Hall-Petch relation takes place at high strain rates, and it is erroneously to extrapolate the molecular dynamics simulation results on microcrystalline material by experimental data obtained at low strain rate.

The dislocation mechanism of stress relaxation is very limited for the strain rates exceeding $10^9 s^{-1}$ because of a dislocation starvation. Figure 2 demonstrates the dislocation starvation in ultrafine-grained copper at the strain rate from $10^7 s^{-1}$ to $10^9 s^{-1}$.

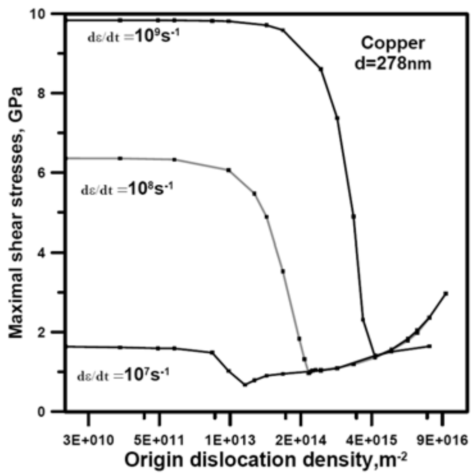

Figure 2 The dependence of the maximal shear stress on the origin dislocation density for copper at extremely high strain rates: 10^7-10^9 s^{-1}.

For origin dislocation densities below $10^{12}m^{-2}$ (an undeformed material) the yield stress is high and it is almost unchanged with the dislocation density decrease. One can see that there is an "optimal" dislocation density which corresponds to the lowest shear stress. It is proportional to the strain rate according to Orowan equation (11). Further increasing of the origin dislocation density results in the increase of the yield strength according to the Taylor hardening low (1). Increasing of the dislocation density during the deformation is almost absent if the origin dislocation density exceeds $10^{14}m^{-2}$, as it was demonstrated by our calculations with use of the Eq.(6) for dislocations kinetics.

4.2 An inverse Hall-Petch relation in ultrafine crystalline copper

Figure 3 presents dependence of the dynamical yield stress on the grain size (in the Hall-Petch coordinates) at strain rates from $2.4\cdot10^{8}s^{-1}$ to $3.5\cdot10^{8}s^{-1}$ with «not optimal» origin dislocation densities. In the coarse grained materials (grain size above 300μm) the Hall-Petch relation is observed.

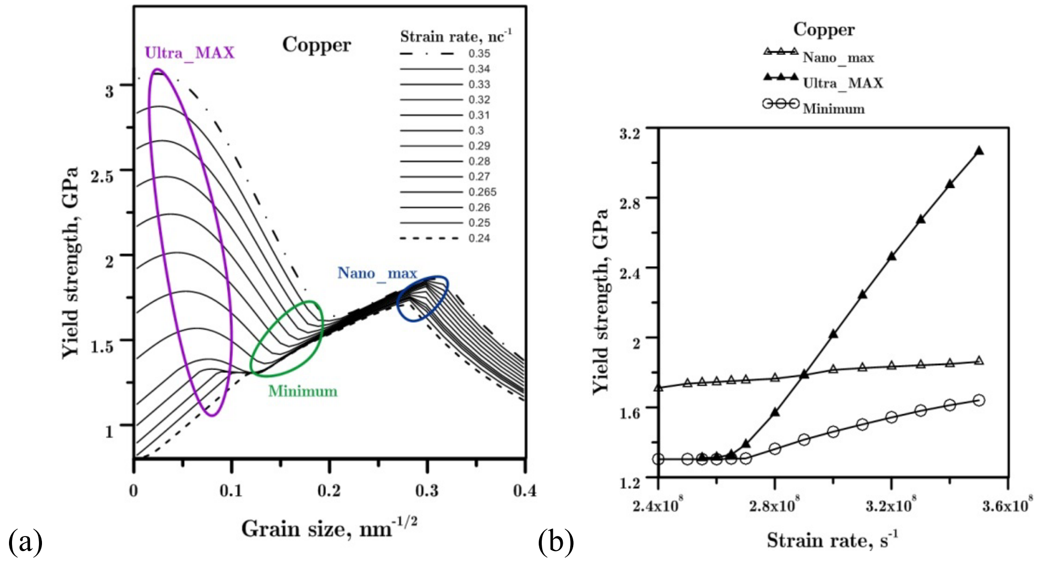

Figure 3 The dependence of the dynamic yield stress on the grain size at different strain rate (a) and on the strain rate at different grain size (b) for copper at extremely high strain rate.

The well-known inverse Hall-Petch relation is also observed for the grain size range <12 nm ($d^{-1/2}$~0.3). But the second maximum of the dynamic yield strength corresponding to the grain sizes of about of hundreds of nanometers appears in this situation. Our calculations demonstrate that at the strain rate above $10^{7}s^{-1}$, the ultrafine-grained copper is stronger to shifting than the nanocrystalline copper. Existence of additional maximum in the ultrafine-grain material is explained by the beginning of the grain boundary sliding and by its contribution into the plastic deformation rate. Figure 3(b) demonstrates a linear growth of the yield strength with increasing of the strain rate. Growth rate is maximal for the ultrafine crystalline metals.

4.3 Yield strength limitations

For all high strain rates the yield strength increases with the strain rate increase. But there are several mechanisms limiting this growth. The homogeneous nucleation dislocation must solve the problem of the dislocation starvation. It can be included as an additional dislocation source in the dislocation kinetics equation (6):

$$\frac{d\rho_D^G}{dt} = 2\pi c_t N, \quad \dot{N} = J_{GD} - \frac{N}{c_s\sqrt{\rho_D}}, \tag{12}$$

where N is a number of homogeneously nucleated dislocation per unit volume. We supposed here that the homogeneously nucleated dislocation loop becomes an ordinary dislocation if its diameter grows up to the mean distance between the dislocations. The nucleation rate of the dislocations per unit volume is equal to [34]:

$$J_{GD} = J_{GD}^{0} \exp\left(-\frac{U_{GD} - \sigma_{\tau} V_{GD}}{kT} \right) \tag{13}$$

For copper activation volume $V_{GD} = 2.7 \cdot 10^{-28}\ \mathrm{m}^3$, activation energy $U_{GD} = 4.67\ \mathrm{eV}$ and the constant $J_{GD}^{0} = 10^{14}\ \mathrm{s}^{-1}$ [34]. Figure 4 demonstrates the dependence of the dynamic yield stress on the strain rate for different dislocation densities. One can see that homogeneously nucleation of dislocation effective for strain rate $10^8 s^{-1}$-$10^9 s^{-1}$. After that efficiency of dislocation gliding mechanism achieve its theoretical limit.

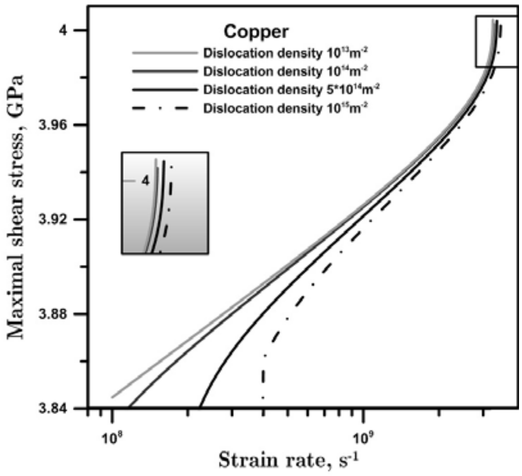

Figure 4 the dependence of the dynamic yield stress on the strain rate for different dislocation densities.

The twinning, as an additional mechanism of plasticity, has to limit the yield strength at extremely high-rate deformations. But our estimates show that efficiency of twinning mechanism is only a few times more than the efficiency of the dislocation plasticity. Therefore, it also decreases stresses in only limited range of the strain rates – less than $10^{10} s^{-1}$.

4. Summary

The yield strength at low strain rate is limited and can be sufficiently increasing to theoretical tensile strength only by the way of impurities introduction. At the strain rates above $10^6 s^{-1}$, the ultrafine-grained metals have the maximum dynamical yield strength (instead of the nanocrystalline metals at the low strain rates). Abnormal and inverse Hall-Patch relations in the ultrafine grained copper were demonstrated by numerical simulations; dislocation starvation effect is related for its explanation. Analogous effect was detected experimentally in tantalum [35] and copper [36]. Mechanisms of the homogeneous nucleation of dislocation and the mechanical twinning effectively decrease the dynamical yield strength at the strain rates $10^8 s^{-1}$-$10^9 s^{-1}$.

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