Materials Science and Engineering A 532 (2012) 245–248

Contents lists available at SciVerse ScienceDirect

Materials Science and Engineering A

journal homepage: www.elsevier.com/locate/msea

A simple mechanical model for grain boundary sliding in nanocrystalline metals

E.N. Borodin*, A.E. Mayer[1]

Department of Physics, Chelyabinsk State University, Chelyabinsk, Br. Kashirinikh str. 129, 454001, Russia

ARTICLE INFO

Article history:
Received 7 June 2011
Received in revised form 12 October 2011
Accepted 23 October 2011
Available online 28 October 2011

Keywords:
Grain boundary sliding
Nanostructured materials
Plasticity
Grain boundaries

ABSTRACT

In this paper we consider grain boundary sliding as a dominant mechanism of plasticity in nanocrystalline metals. A mechanical model for barrier resistance to sliding has been proposed. Characteristic time of plastic relaxation due to grain boundary sliding has been estimated based on molecular dynamics simulation data. At quasi-static deformation yield strength is determined by barrier resistance, and the predicted threshold stresses are in good agreement with experimental data.

1. Grain boundary sliding

Many observations of nanocrystalline metals show that they have equiaxed grain structure [1–3], the same as observed inside shear bands of ultrafine polycrystals [4] at deformation spots. This allows to represent the structure of nanocrystalline material as a close packed lattice of grains. Dislocation plasticity is suppressed in nanocrystals due to intense interaction between dislocations and grain boundaries [5]. Thus collective shifts of grains must be a dominant plastic deformation mechanism [2]. It is also confirmed by molecular dynamics simulations [6,7]. These shifts (or slidings) take place in planes in the directions of maximal shear stresses σ_τ. There are two intrinsic forces that resist the sliding of the grains. The first one is an elastic force from neighbor grains: when a sliding plane shifts on a grain diameter, every grain deforms two neighbor grains in adjacent planes. For this shift to happen shear stress must exceed some threshold value y_b, which is necessary to cause corresponding deformation of neighbor grains; it is the essential condition of activating the grain boundary sliding. An effective force $\sigma_{eff} = \sigma_\tau - y_b$ acts on sliding grains, and the grains start to move when this effective force is above zero. The second force acting on moving grain planes is a frictional force. High angle grain boundaries are most common in nanocrystalline metals. Structure of these boundaries is similar to amorphous phase of metals [1,8]. Therefore, the frictional force corresponds to some viscous deformation in boundaries, as it occurs in a highly viscous liquid.

2. Model for the grain sliding

The Maxwell model of highly viscous liquid [9] suggests that at very short intervals of time material behaves as an amorphous solid, and at long intervals of time – as an ordinary viscous fluid. The equation for time derivative of shear stress takes the following form:

$$\frac{d\sigma_\tau}{dt} = 2G\frac{d\varepsilon}{dt} - \frac{\sigma_{eff}}{\tau}, \tag{1}$$

where t is the time, ε the macroscopic shear deformation, G the shear modulus, and τ the relaxation time.

In [10] we combined dislocation dynamics [11] for plasticity in grains and the Maxwell model (Eq. (1)) for plasticity at the grain boundaries; high strain rates have been analyzed in [10]. This approach gave satisfactory description for high strain rate deformation of copper and for the abnormal Hall–Petch relation observed in nanomaterials [12,13]. But the key parameter of this model – the Maxwell relaxation time τ – was substituted in [10] as an empirical parameter. In this paper we develop our previous approach by proposing a mechanical model for resistance threshold y_b of grain sliding and by estimating of the relaxation time. For the last point we use equation proposed in [12,14], which is based on molecular dynamics simulation data.

From Eq. (1) one can write $\sigma_{eff} = 2G\tau\dot{\varepsilon}$ for steady conditions $\dot{\sigma}_\tau = 0$. Condition $y_b \ll \sigma_\tau$ is commonly satisfied at high strain rate (10^8–10^9 s^{-1}), which is usual in molecular dynamics simulation; it leads to:

$$\sigma_\tau \simeq \sigma_{eff} = 2G\tau\dot{\varepsilon}. \tag{2}$$

* Corresponding author. Tel.: +7 351 799 71 61; fax: +7 351 742 09 25.
E-mail addresses: elbor7@gmail.com (E.N. Borodin), mayer@csu.ru (A.E. Mayer).
[1] Tel.: +7 351 799 71 61; fax: +7 351 742 09 25.

0921-5093/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.msea.2011.10.086

Table 1
Activation parameters for different metals [12,15].

Metal	Cu	Ni	Al
V_s (10^{-30} m^3)	17.4	16	27
U_s (eV)	0.246	0.268	0.185
ν_D(10^{12} s^{-1})	6.46	7.19	8.12
τ/d, 10^{-2} s m^{-1}	0.38	0.53	0.04

Condition $\dot{\sigma}_\tau = 0$ means that the plastic deformation rate is equal to macroscopic strain rate $\dot{\varepsilon} = \dot{\varepsilon}_P$. According to [12,14], plastic deformation rate in steady conditions can be expressed as

$$\dot{\varepsilon}_p = \frac{6b\nu_D}{d}\exp\left(-\frac{U_s}{k_bT}\right)\mathrm{sh}\left(\frac{\sigma_\tau V_s}{k_bT}\right), \quad (3)$$

where b is the Burgers vector, ν_D the Debye frequency, U_s and V_s the activation energy and volume, k_b the Boltzmann constant, T the temperature and d is an average grain size of a material.

Taking inverse function of (3) we have:

$$\sigma_\tau = \frac{k_bT}{V_s}\mathrm{arcsh}\left(\frac{\dot{\varepsilon}_p d}{6b\nu_D}\exp\left(\frac{U_s}{k_bT}\right)\right). \quad (4)$$

Decomposition of the hyperbolic sine in Taylor series gives us:

$$\sigma_\tau \approx \frac{dk_bT}{6b\nu_D V_s}\exp\left(\frac{U_s}{k_bT}\right)\dot{\varepsilon}_p - \frac{k_bT}{6V_s}\left(\frac{d}{6b\nu_D}\exp\left(\frac{U_s}{k_bT}\right)\right)^3\dot{\varepsilon}_p^3 + \cdots. \quad (5)$$

Comparing Eqs. (2) and (5) we conclude that the first term in this expansion is the coefficient $2G\tau$. Hence, we have the relaxation time of the grain boundary sliding:

$$\tau = \frac{dk_bT}{12Gb\nu_D V_s}\exp\left(\frac{U_s}{k_bT}\right). \quad (6)$$

This comparison also shows that the Maxwell model (Eq. (1)) is valid than the second term and the higher terms in Eq. (5) are less than the first term. For values $U_s = 0.2$ eV (Table 1), $T = 300$ K, $b = 3\times10^{-10}$ m, $\dot{\varepsilon}_p = 10^9$ s^{-1}, $\nu_D = 10^{13}$ s^{-1} and $d = 10^{-8}$ m we have that the first term 15 times more than the second.

Molecular dynamics simulations [3,12] show that several processes take place at grain boundaries simultaneously: for example, there are a large number of uncorrelated atomic slip events and free volume migration. Activation parameters, U_s and V_s, must take into account all of these processes; therefore, they can only be found by an empirical way. Activation volume can be estimated as $V_s \sim b^3$. We take the activation energy of grain boundary sliding U_s from [5] for nickel. It has the same order of magnitude as activation energy of viscous flow in molten state of the metal [15]. Activation parameters for copper and aluminum have been fitted by comparison with MD simulation results. Parameters of the model are collected in Tables 1 and 2.

It follows from the data of Tables 1 and 2 that the relaxation time τ is of the order of 10^{-9}–10^{-10} s. At the constant strain rate ($\dot{\varepsilon} = \mathrm{const}$), the following solution of Eq. (1) can be written:

$$\sigma_\tau(t) = y_b + 2G\tau\dot{\varepsilon}\left(1 - \exp\left(-\frac{t}{\tau}\right)\right), \quad (7)$$

which is valid for the initial condition $\sigma_\tau(0) = y_b$. It means that the finite rate of shear stress relaxation in grain boundaries is significant for strain rates exceeding 10^5 s^{-1} ($y_b/G \sim 0.01$, see further Eq. (16)), which are typical for molecular dynamics simulations [3,5] and shock wave experiments. For quasistatic deformations with creep strain rates 10^{-5}–10^{-2} s^{-1} we can take into consideration only the threshold stresses y_b.

Table 2
Predicted barrier stress and shear modulus values for different metals.

Metal	Cu	Ni	Al	Fe	Pd	Au
y_G (GPa)	0.6	1.23	0.4	1.2	0.8	0.47
G (GPa)	42	76	26	78	51	28.5

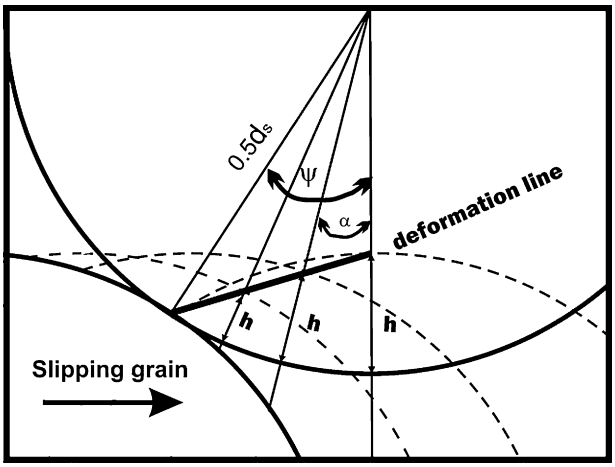

Fig. 1. The deformation of neighbor grains: slipping grain is situated in the bottom left corner and it moves to the bottom right corner of the picture, static neighbor grain is above it. Position of slipping grain at different times is shown by dotted lines. "Deformation line" crosses all points in which maximal deformation (h) of both grains is reached. α is a current angle between the direction to center of slipping grain and vertical line. For $h = 0$ contact angle $\alpha = \psi$.

3. The threshold stress

For a precise definition of the threshold stress y_b we should consider, how a sliding grain deforms its neighbor grains (Fig. 1), which are assumed to be spherical. The distance between the "deformation line" (see Fig. 1) and the neighbor grain boundary is the maximal grain deformation h. Introducing the maximal angle before deformation ψ and the actual angle in deformation process α between point of contact and downwards direction (see Fig. 1), one can obtain:

$$h = \frac{d_s}{2}\left(1 - \frac{\cos\ \psi}{\cos\ \alpha}\right), \quad (8)$$

where d_s is the diameter of the slipping sphere.

For close packed structure $\psi = \pi/6$. According to [9], the radial elastic force acting on a deformed sphere is

$$F = \frac{d_s^2}{\sqrt{2}}\left(1 - \frac{\cos\ \psi}{\cos\ \alpha}\right)^{3/2}\frac{G}{3(1-\nu)}, \quad (9)$$

It is important to mention that in calculation an average grain size d is used; it includes grain boundary width δ, therefore, $d_s = d - \delta$ in (8). Grain boundary thickness δ is about 1 nm. When the maximal values of h (at $\alpha = 0$) become comparable with δ, the acting force tends to zero. Projection of this force on sliding direction is:

$$F_z = \zeta(\alpha)\frac{G}{1-\nu}(d-\delta)^2, \quad (10)$$

where

$$\zeta(\alpha) = \frac{\sin\ \alpha}{3\sqrt{2}}\left(1 - \frac{\cos\ \psi}{\cos\ \alpha}\right)^{3/2}. \quad (11)$$

For close packed structure ($\psi = \pi/6$) maximum $\zeta(\alpha)$ is reached at 15°; it corresponds to $\zeta_{\max} = 2.06\times10^{-3}$. The threshold stress acting on the sliding grains from two neighbor grains is then equal to

$$y_b = \frac{2F_z^{\max}}{(\pi/4)d^2}. \quad (12)$$