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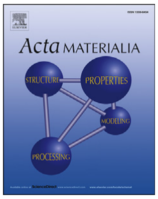

Full length article

Free surface effects on stress-driven grain boundary sliding and migration processes in nanocrystalline materials

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ABSTRACT

The free surface effects on grain boundary (GB) deformation mechanisms mediated by GB sliding and migration processes in nanocrystalline materials are theoretically described. Particular attention is devoted to the specific features of the GB sliding and the cooperative GB sliding and migration processes occurring near free surfaces in nanocrystalline materials. The critical stresses, energies and geometric parameters which characterize the GB deformation mechanisms in question are calculated. The role of the free surface effects in the interpretation of experimental data on the GB sliding and migration processes in nanocrystalline materials is discussed.

1. Introduction

Nanocrystalline (NC) bulk materials, films and micropillars exhibit excellent mechanical properties that are of utmost interest to diverse applications; see, e.g., reviews [1–8]. These properties are inherent to NC materials due to their specific structural features, such as nanoscopic sizes of grains and large amounts of GBs. In particular, the specific structural features critically affect plastic deformation mechanisms in NC materials where conventional lattice slip is hampered or even completely suppressed, while GB deformation mechanisms can intensively operate [1–9]. Indeed, following experimental data, computer simulations and theoretical models, plastic flow in NC materials effectively occurs through such GB deformation mechanisms as GB sliding [10–16], stress-driven GB migration [17–27], cooperative GB sliding and migration process [28–30], twin deformation generated at GBs [31–35], rotational deformation modes carried by GBs [36–44], and GB diffusional creep [45,46].

In NC thin films and NC micropillars, in addition to the nanostructure, free surface effects inevitably come into play and substantially influence plastic deformation processes [6]. Besides, plastic deformation near free surfaces can significantly contribute to overall deformation of bulk NC materials where the onset of plastic flow often occurs at free surfaces. Also, it is worth noting that it is near-surface deformation processes that are typically observed in electron microscopy experiments, providing the most valuable information on the structural transformations associated with plastic flow in solids. At the same time, the theoretical research efforts addressing the free surface effects on plastic deformation in NC materials are limited; see, e.g., previous theoretical models concerning plastic flow through GB rotations near free surfaces [47] and nanotwin generation at free surfaces [48]. In this context, from both fundamental and applied viewpoints, it is highly interesting to understand and describe the free surface effects on operation of GB deformation mechanisms in NC materials. The main aim of this paper is to theoretically examine the free surface effects on stress-driven GB sliding and migration processes that effectively conduct plastic deformation in NC bulk materials, films and micropillars.

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2. Free surface effects on grain boundary sliding in nanocrystalline materials

GB sliding occurs as a dominant GB deformation mechanism in NC materials in diverse conditions [1–6,8,10–16]. For instance, GB sliding plays the key role in superplastic deformation in NC materials [10,12], as with their ultrafine-grained and microcrystalline counterparts [10,49–51].

We now examine the geometric features of GB sliding near the free surfaces of NC bulk materials, films and micropillars. Let us consider a nanocrystalline specimen that has a flat free surface and is subjected to a tensile load σ; see Fig. 1a which schematically presents a two-dimensional section of the specimen. In the following, we will examine the two situations which are different in geometry of GB deformation. In the first situation, GB sliding occurs along a GB that is not connected to the specimen free surface (Fig. 1b,c). In the second situation, GB sliding occurs along a GB that reaches the free surface, and a free surface step is generated due to the GB sliding process (Fig. 1d,e).

Let us consider the first situation where GB sliding occurs along GB AB terminated at triple junction B that initially is at a distance H from the free surface (Fig. 1b,c). Within the model [15], the applied shear stress induces GB sliding that transforms the initial configuration *I* of GBs (Fig. 1b) into configuration *II* (Fig. 1c). GB sliding is assumed to be accommodated, in part, by emission of lattice dislocations from triple junctions (Fig. 1c).

Besides, following Ref. [15], GB sliding leads to the formation of a dipole of wedge disclinations B and D in configuration *II* (Fig. 1c). The disclinations are characterized by the strengths $\pm\omega$ whose magnitude ω depends on the tilt misorientation of the GB BK (assumed to be a symmetric tilt boundary). The arm of the dipole BD – the distance between its disclinations – is to the magnitude s of the relative displacement of grains (Fig. 1c). The magnitude s is also called the GB sliding distance.

Let us calculate the energy change ΔW_1 (per unit disclination length) that characterizes GB sliding. The energy change ΔW_1 can be written in its general form as follows:

$$\varDelta W_1 = W^{dip} + W_{\text{int}}^{dip-\sigma} - A, \tag{1}$$

where W^{dip} is the proper energy of the disclination dipole, $W_{\text{int}}^{dip-\sigma}$ is the energy of its interaction with the applied stress σ, and A is the work spent by the resolved shear stress τ to GB sliding. The shear stress τ is related to the tensile stress σ as $\tau = \sigma\sin(2\alpha)/2$, where α is the angle between GB AB and the tension direction (Fig. 1b).

In the isotropic approximation, the energy ΔW_1 can be calculated using the expressions [52] for both the self-energy of wedge disclinations and the energies of their elastic interaction near a planar free surface as follows:

$$\begin{aligned}\varDelta W_1 = {} & \frac{D\omega^2 s^2}{2}\left\{\ln\frac{R_0}{s} + \cos^2\alpha\right\} - \frac{\sigma\omega\, s(2H + s\cos\alpha)\cos\alpha}{2} \\ & - (\sigma\sin(2\alpha)/2 - \tau_0)ps.\end{aligned} \tag{2}$$

Here $D = G/[2\pi(1-\nu)]$, G is the shear modulus, ν is Poisson's ratio, p is the grain size, τ_0 is the friction stress describing the resistance to GB sliding, and R_0 is the screening length for stress fields created by the disclination dipole. R_0 is in the following relationship with the geometric parameters that specify GB sliding:

$$R_0 = \left(4H^2 + 4Hs\cos\alpha + s^2\right)^{1/2}. \tag{3}$$

In formula (2), the first term describes the proper energy of the disclination dipole, the second term characterizes the energy of its interaction with the applied stress σ, and the third term specifies the work spent by the resolved shear stress to GB sliding.

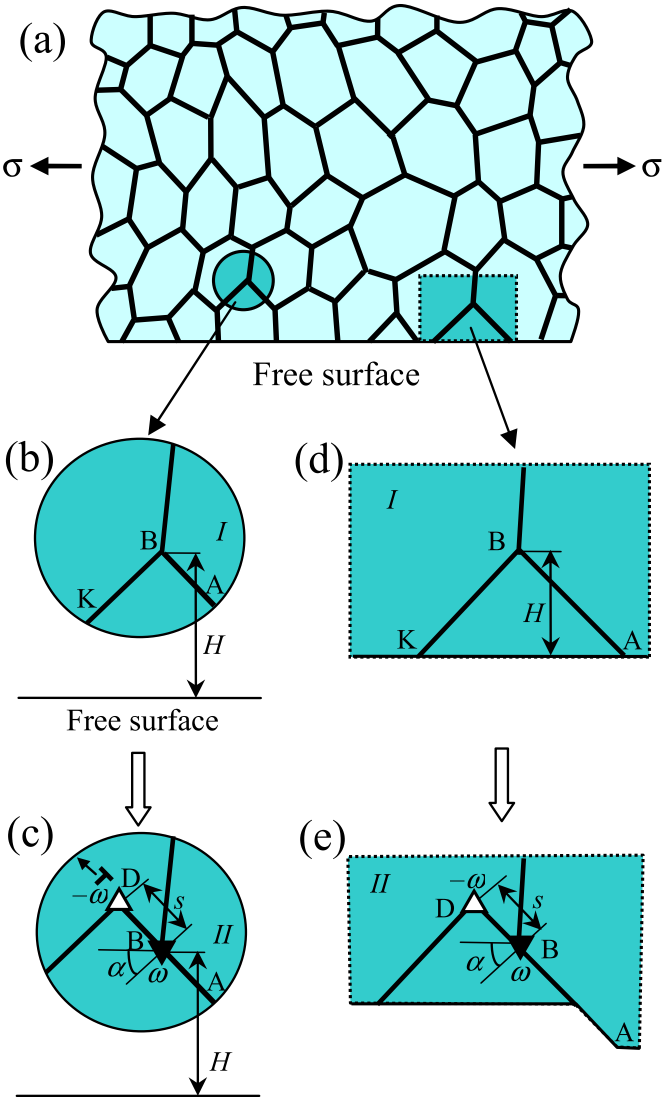

Fig. 1. Geometry of GB sliding near a free surface of a nanocrystalline solid under a tensile load. Figures (b) and (c) illustrate the case where GB sliding occurs along a GB that does not contact the free surface. Figures (d) and (e) illustrate the situation where GB sliding occurs along a GB that reaches the free surface. (a) General view. (b,d) The magnified insets of (a) show the geometry of GBs before GB sliding. (c,e) The magnified insets of (a) present the geometry of GBs after GB sliding. Wedge disclinations specified by strengths ω and $-\omega$ are shown as open and full triangles, respectively.

In the following, we will consider the typical situation where the resistance to GB sliding is negligibly low, that is, $\tau_0 \approx 0$. Also, we will examine disclination configurations whose stress fields are screened by free surfaces, in which case H is smaller than the screening length R_0 of the stress field created by the disclination dipole (R_0 is assumed to be in the range from one to several grain sizes [15]. For disclinations specified by $H > R_0$, the stress fields are screened by other internal defects, the free surface effects are negligibly low, and formula (2) is not correct. The case of $H > R_0$ is beyond the scope of this paper addressing the free surface effects on GB deformation.).

With formula (2), for nanocrystalline Cu, we calculated dependences of the energy change ΔW_1 on the GB sliding distance s. Fig. 2 shows these dependences in the case of nanocrystalline Cu