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Dislocation emission from deformation-distorted grain boundaries in ultrafine-grained materials

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Emission of lattice dislocations from grain boundaries (GBs) specified by deformation-distorted structures with periodic fluctuations of misorientation in deformed ultrafine-grained (UFG) materials is theoretically described. It is theoretically revealed that (i) the dislocation emission from deformation-distorted GBs is significantly enhanced as compared to that from structurally equilibrated GBs; and (ii) the enhancement effect depends on the parameters specifying the deformation-distorted GBs. The influence of deformation-distorted GBs as dislocation sources on the tensile ductility of UFG materials is discussed.

Keywords: Nanomaterials; Ductility; Grain boundaries; Dislocations; Deformation

Ultrafine-grained (UFG) materials, which exhibit unique mechanical and functional properties, have been the subject of intense research efforts motivated by their wide range of applications (e.g. [1–10]). For instance, UFG materials often have very high strength, which is attractive for a range of structural applications [1–6]. In addition, although strong UFG materials at ambient temperatures typically exhibit disappointingly low tensile ductility, there are several examples of such materials which show simultaneously high strength and good ductility (e.g. [11–14]). UFG materials possessing this combination of the mechanical characteristics represent "ideal materials" for many technologies.

The outstanding mechanical properties of UFG materials are crucially influenced by their specific structural features (UFG structure, deformation-distorted GBs, etc.) responsible for the specific features of lattice slip in these materials. Hence, it is experimentally well documented (see Refs. [6,11] and references therein) that grain boundaries (GBs) in UFG materials play a critical role in their plastic flow, which effectively occurs through emission of lattice dislocations from GBs, non-stop dislocation slip in grain interiors and consequent dislocation trapping at GBs. In doing so, GBs serve as dominant sources and sinks for lattice dislocations in UFG materials. This is in contrast to conventional coarse-grained metals and alloys where lattice dislocations are generated and accumulated mostly in grain interiors, but not at GBs. In the context discussed, there is great interest in understanding the physical nature of the specific role of GBs as effective dislocation sources in UFG materials, in contrast to coarse-grained polycrystals.

In general, since GBs in UFG materials produced by severe plastic deformation (SPD) methods typically have deformation-distorted structures, which by definition contain high-density ensembles of extrinsic dislocations trapped at GBs [1,15,16], it is logical to expect that such deformation-distorted structures strongly influence the ability of GBs to emit dislocations. However, very few theoretical examinations focussing on the dislocation emission process (critically important for the deformation behavior of UFG materials) have been reported. In fact, dislocation emission from GBs in UFG and

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nanocrystalline solids with fines grains was described as the emission of dislocations from either equilibrium tilt GBs (that have constant misorientation parameters along their planes) [17–20] or locally distorted GBs (that contain extra dislocations with the same Burgers vectors and are characterized by local changes in GB misorientation parameters) [21–24]. At the same time, all these models [17–24] are questionable in the case of UFG materials.

Let us consider lattice dislocation emission from deformation-distorted GBs in a bulk nanostructured solid under a mechanical load. The solid consists of ultrafine grains divided by GBs. For simplicity and definiteness, hereinafter we will examine the lattice dislocation emission from low-angle tilt boundaries composed of lattice edge dislocations in this solid. The results of our theoretical analysis can be extended to the more general situation with high-angle GBs.

Within our model, we consider deformation-distorted GBs as those containing both "equilibrium" and "non-equilibrium" edge dislocations (Fig. 1). The equilibrium dislocations of each deformation-distorted GB have Burgers vectors $\boldsymbol{b}$ and are arranged in a regular wall configuration (Fig. 1a) providing a constant contribution θ to the GB tilt misorientation. The angle θ is related to the period p of the wall of dislocations and their Burgers vector magnitude b as $\theta \approx b/p$ [25].

The non-equilibrium dislocation array of a deformation-distorted GB provides fluctuations of the GB tilt misorientation along the GB (Fig. 1b,c). We consider non-equilibrium dislocations as periodically arranged perfect edge dislocations having positive and negative Burgers vectors **b** and –**b**, respectively (Fig. 1b,c). For simplicity, we assume that the non-equilibrium dislocations of a GB form a periodic structure consisting of finite dislocation walls with alternating orientations of

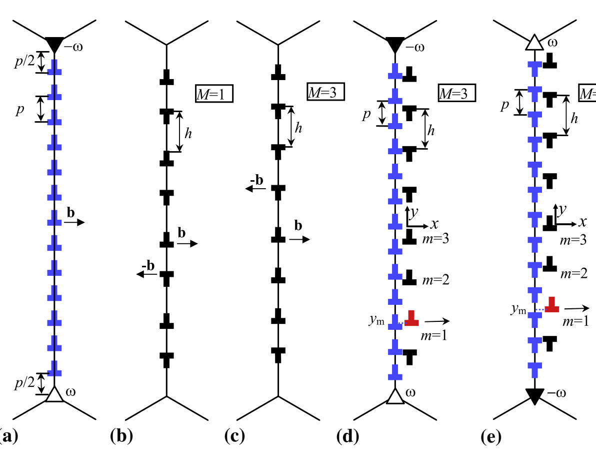

Figure 1. Dislocation structures of deformation-distorted grain boundaries. (a) Equilibrium dislocations belonging to a deformation-distorted grain boundary. They represent perfect edge dislocations that form a wall configuration terminated by triple junctions. (b,c) Configurations of non-equilibrium dislocations in a deformation-distorted grain boundary. (d,e) Emission of non-equilibrium dislocations from a grain boundary. (d) The emitted non-equilibrium dislocation has the same sign as the equilibrium dislocations. (e) The sign of the emitted non-equilibrium dislocation is opposite to that of the equilibrium dislocations.

dislocation Burgers vectors (Fig. 1b,c). So, the non-equilibrium dislocation structure consists of segments, each containing M dislocations, and dislocations signs within one segments are the same, while dislocation signs in neighboring segments are different (Fig. 1b,c). The total number of non-equilibrium dislocations in the GB is $2MN_1$, where N_1 is a positive integer. The sum Burgers vector of all the non-equilibrium dislocations of the GB is equal to zero, and the GB tilt misorientation periodically fluctuates around its mean value θ determined by the equilibrium dislocations (Fig. 1d,e).

Thus, our model describes the GBs with deformation-distorted structures which contain extra dislocations with various Burgers vectors and are specified by "globally" fluctuating misorientation parameters (Fig. 1d,e). Let us calculate within our model the critical (minimum) stress for dislocation emission from a deformation-distorted GB. To do so, for definiteness, we examine the emission of non-equilibrium dislocations (Fig. 1d,e).

Let us consider a GB containing both equilibrium and non-equilibrium dislocations (Fig. 1e). We introduce a Cartesian coordinate system (x, y) with the origin at the center of the GB (Fig. 1e). Let the number of equilibrium dislocations be $2N+1$. Then the component σ_{xy}^{eq} of the total stress field created by the equilibrium dislocations with the Burgers vectors $-\boldsymbol{b}$ (Fig. 1e) is calculated using, in particular, the expression for the stress fields of individual dislocations [26] in an isotropic infinite solid. Our analysis shows that the stress σ_{xy}^{eq} created by the nearest dislocation wall (at a distance of the order of several periods of the dislocation wall or smaller) depends on N very weakly, and even for $N=2$ it practically coincides with the stress field created in the limiting case of $N \to \infty$ (see Supplementary Material (Sec. A)). Therefore, hereinafter, we will consider this limiting case. In doing so, we find: $\sigma_{xy}^{eq} = -D\omega\tilde{x}g(\tilde{x}, \tilde{y})$, where $D = G/[2\pi(1-\nu)]$, G is the shear modulus, ν is the Poisson's ratio, $\tilde{x} = x/p$, $\tilde{y} = y/p$, and:

$$g(x, y) = \frac{2\pi^2(\cos(2\pi y)\cosh(2\pi x) - 1)}{(\cos(2\pi y) - \cosh(2\pi x))^2}. \quad (1)$$

Now let us calculate the stress σ_{xy}^{neq} created by non-equilibrium dislocations. This stress is calculated by the summation of the stresses created by individual dislocations with the Burgers vectors **b** and –**b** in an isotropic infinite solid. Our analysis shows that the stress σ_{xy}^{neq} depends very weakly on the parameter N_1 characterizing the number $2M(2N_1+1)$ of non-equilibrium dislocations in the wall (see Supplementary Material, Sec. B). Therefore, we employ the expression for the stress σ_{xy}^{neq} for the limiting case of $N_1 \to \infty$. As a result, we find:

$$\sigma_{xy}^{neq} = -\frac{\beta^2 D\omega\tilde{x}}{4M^2}\sum_{k=1}^{M} f\left(\frac{\beta\tilde{x}}{2M}, \frac{y - y_0 + h/2}{2Mh}, s_k\right) \quad (2)$$

where $\omega = b/p$, $\beta = p/h$, $s_k = (2k-1)/(4M)$, $f(x, y, s_k) = g(x, y - s_k) - g(x, y + s_k)$, and $y = y_0$ is the coordinate of a non-equilibrium dislocation having a neighboring non-equilibrium dislocation of opposite sign. (In Fig. 1e, such a dislocation is labeled by $m = 1$.)

Let us consider the emission of a non-equilibrium dislocation with the Burgers vector **b** from the GB in