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Nonequilibrium grain boundaries and their relaxation under oscillating stresses in columnar nickel nanocrystals studied by molecular dynamics

Ayrat A. Nazarov*, Ramil' T. Murzaev

Institute for Metals Superplasticity Problems, Russian Academy of Sciences, 39 Stepan Khalturin st., Ufa 450001, Russia

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ABSTRACT

Atomic structure of columnar nickel nanocrystals with [1 1 2] column axis having nonequilibrium grain boundaries (GBs) containing extrinsic grain boundary dislocations (EGBDs) and its evolution under oscillating stresses are studied by molecular dynamics method. Energy of GBs as a function of the degree of nonequilibrium is evaluated. It is found that under loading by symmetrically oscillating stresses the nonequilibrium GBs generate lattice dislocations, which travel across the grains and are absorbed by opposite GBs thus resulting in a relaxation of the structure, long-range stress fields and the energy of GBs.

1. Introduction

One of important processes occurring during cold plastic deformation of polycrystalline materials is the accumulation of dislocations in grain boundaries (GBs), which act as strong barriers for slip [1–7]. This process results in the formation of extrinsic grain boundary dislocation (EGBD) arrays, which induce long-range stress fields and cause an enhanced latent energy [7,8]. GBs containing EGBDs are commonly called nonequilibrium GBs [3,7–9]. The nonequilibrium structure of GBs can significantly change their diffusion coefficient [10–14], the yield stress of polycrystals [15] and other properties.

Nonequilibrium GBs have been shown to be typical elements of the structure of bulk nanostructured materials processed by severe plastic deformation (SPD) methods [16–21]. Rybin and co-workers [22,23] studied the structure of materials after large plastic strains and developed the concept of mesodefects, which accumulate in GBs due to the trapped dislocations. They found that these defects were not only the consequence of plastic deformation but also determined the basic mechanism of grain subdivision during this process. Namely, misorientation mismatches at triple junctions due to EGBDs result in the formation of junction disclinations, whose relaxation occurs by the formation of new grain boundaries. Basing on the concepts developed by Rybin, earlier we proposed dislocation and disclination models of nonequilibrium GB structure in UFG materials [18–21]. These models allowed us to estimate the internal stress fields and excess energies in these materials and qualitatively explain their mechanical and diffusion properties [24,25].

The nonequilibrium GB structure is not stable and at elevated temperatures relaxes resulting in the diminishing of internal stresses and excess energy [16,17]. Theoretical models of this process of grain boundary recovery process were proposed in [26–28].

Annealing is a very common but not the only treatment that leads to a relaxation of nonequilibrium defect structures in deformed materials. Recently, it has been shown that ultrasonic treatment (UST) can result in a significant recovery of GBs in UFG metals processed by SPD [29–36]. After UST with moderate amplitudes of oscillating stress (around 50 to 100 MPa) the microstructure of UFG nickel is characterized by better defined, straight GBs that is an indication on their equilibrium structure. Microstrains measured by X-ray diffraction and excess energy release measured by differential scanning calorimetric method decrease after UST with certain amplitudes. The relaxation of nonequilibrium GB structure under ultrasound results in an increase of the thermal stability of microstructure and enhancement of ductility of UFG nickel without a loss in the strength achieved due to SPD.

The phenomenon of ultrasound-assisted structure recovery has been addressed by two-dimensional dislocation dynamics simulations [34–36], which have shown that in a polycrystal containing triple junction disclinations and randomly distributed lattice dislocations exposed to the action of oscillating stresses the GBs absorb dislocations in a way, which results in a cancellation of the junction disclinations, i.e. GB recovery through GB-lattice dislocation interaction is possible. However, in UFG materials lattice dislocations can be not available in quantities enough for a compensation of the GB defects and one should think of possible sources of dislocations.

Direct studies of the structure, energy and kinetics of nonequilibrium GBs, their mechanical properties and behavior under

* Corresponding author.
E-mail address: aanazarov@imsp.ru (A.A. Nazarov).

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different influences are possible by molecular dynamics simulations. A few kinds of a nonequilibrium GB structure in bicrystals and nanocrystals have been studied atomistically in several works [37–39]. In these works, the nonequilibrium state was created by introducing either random local shifts of GB atoms from their equilibrium positions [37] or free volumes by removing some GB atoms [38], or in the process of a construction of initial structures [37,39]. However, these kinds of nonequilibrium are essentially different from that caused by EGBDs, since they induce only short range internal stresses, whereas the EGBDs result in long-range stresses. While the short range stresses can relax by a local reconstruction of the GB atomic structure involving local diffusion or athermal displacements of atoms comparable to interatomic distances, those induced by EGBDs can relax only by their elimination from GBs requiring diffusion to the distances comparable to the grain size [26–28] or athermal processes of dislocation emission.

Quite recently, we have carried out molecular dynamics simulations of the behavior under oscillating stresses of a nonequilibrium GB containing a disclination dipole in bicrystalline nickel [40–42]. These simulations have shown that under a sinusoidal applied tension–compression stress the GB emits lattice dislocations, which travel across the grains and sink at free surfaces of the bicrystal. When the sign of the applied stress changes, these dislocations do not come back to the GB, since the dislocations are generated under the combined effect of internal stress field of the disclination dipole and applied stress, when the latter acts on the same direction. That is, an asymmetric process of lattice dislocation generation and GB recovery occurs under a symmetrically oscillating stress.

In the cited works, the free surfaces of the bicrystal were ideal sinks for dislocations emitted from the GBs and it is not clear, if this mechanism of GB recovery will be operating in a bulk polycrystal. Therefore, the aim of the present paper is to demonstrate that the unilateral process of nonequilibrium GB structure relaxation by lattice dislocation emission is a common mechanism of recovery in plastically deformed metals. For this, we develop a model nanocrystal of nickel, selected GBs of which contain EGBDs introduced by a special construction method. For different degrees of nonequilibrium, i.e. quantities of EGBDs, we determine the structures and excess energies of nanocrystals at temperatures 0 and 300 K and study their evolution during the action of an oscillating uniaxial tension–compression stress.

2. Computational details

2.1. Initial system construction

A columnar nickel nanocrystal having the column axis [1 1 2] will be used for simulations. This system is very convenient to analyze the interaction between lattice dislocations and GBs, since it allows the slip of only edge dislocations with a Burgers vector $\frac{1}{2}\langle 1\,1\,0\rangle$ and lines parallel to $\langle 1\,1\,2\rangle$ on a slip plane $\{1\,1\,1\}$. Bicrystals with $\langle 1\,1\,2\rangle$ tilt GBs have been extensively studied, for example, by Shimokawa et al. [43].

A computational cell containing a model nanocrystal is schematically presented in Fig. 1(a). The cell contains four grains, which have a common crystallographic axis [1 1 2], the direction of which coincides with that of the $z-$ axis. The grains have a regular hexagon-shape cross section with an edge a. Maximum size of the hexagons, $d = 2a$, will be taken as the grain size. Grains 1 and 2 have orientations of slip planes parallel to xOz and yOz planes, respectively. Taking the orientation of grain 1 as a reference, grains 3 and 4 are rotated to angles $\pm\,\alpha = \pm\,20^{\circ}$ to form a symmetric high-angle tilt GB between them.

In order to construct a nanocrystal with equilibrium GBs, the grains were directly filled in by atoms belonging to properly oriented crystal lattices. The system thus obtained was checked to find the pairs of too close atoms in GB regions. In these pairs, one of the atoms was eliminated to avoid too strong repulsive interactions during the start of simulations.

To initialize the structures with nonequilibrium GBs, the

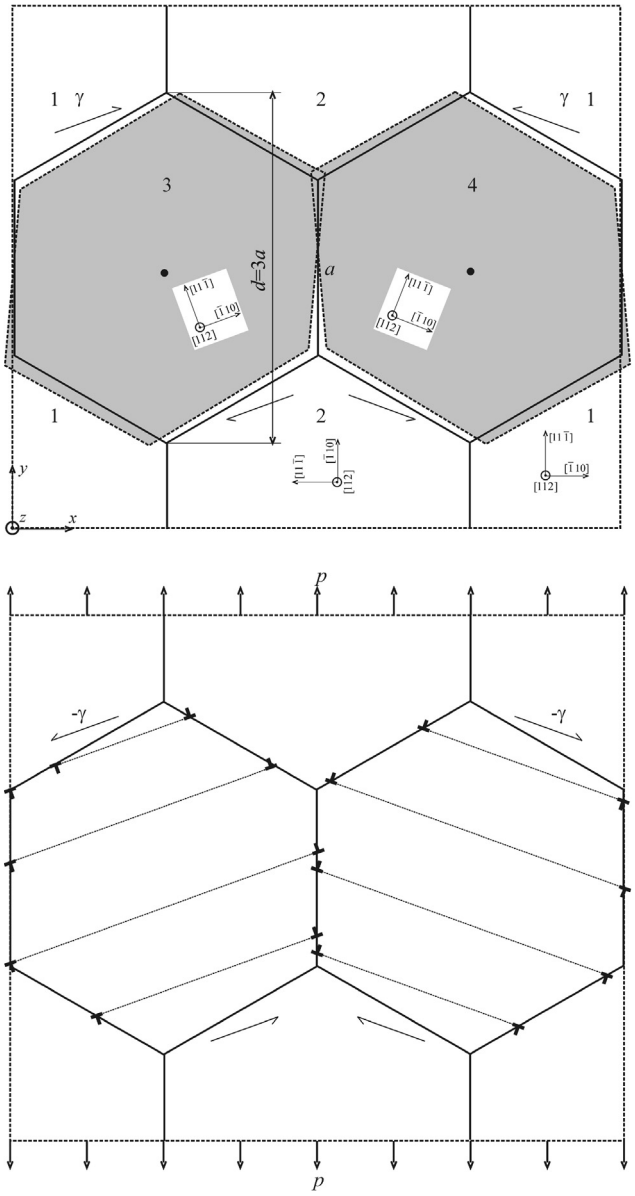

Fig. 1. Construction of the computation cell for columnar f.c.c. nanocrystals with a [1 1 2] axis and nonequilibrium GBs.

construction method proposed in [44] is used. This method is based on shear strain of selected grains of the nanocrystal in order to introduce EGBDs into its boundaries. It is done as follows.

Assume that grains 3 and 4 of the model under consideration are free. Apply them simple shear strains γ in opposite directions by an imaginary slip of dislocations in $(1\,1\,\bar{1})$ slip planes so that the grains are distorted into the regions highlighted by a grey color in Fig. 1(a). The dislocation slip retains the ideal atomic structure of the lattice thus the grains will consist of a perfect lattice. However, the slip is limited to the volumes of the original grains and results in a formation of dislocations at their borders. In order to form these dislocations, one should now apply simple shears of opposite signs to the perfect grains occupying the gray regions.

As a result of this procedure, EGBDs will form in the boundaries of the deformed grains as schematically shown in Fig. 1(b). However, the geometrical procedure alone will not immediately form EGBDs having localized cores and it will require a relaxation of the structure. If one starts an energy minimization without precautions, the pairs of opposite signed dislocations will be attracted to each other and immediately