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Stress-driven migration, convergence and splitting transformations of grain boundaries in nanomaterials

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ABSTRACT

Convergence and splitting transformations of grain boundaries (GBs) migrating under stress in nanocrystalline and ultrafine-grained materials are theoretically described. With the disclination model of GB junctions, the elastic interaction between migrating GBs that mediate plastic deformation and their response to the external stress are examined. A special attention is devoted to convergence of migrating GBs with their immobile counterparts as well as to their following splitting transformations. Equilibrium migration distances, energy and critical stress characteristics for migration of GBs and their various transformations are calculated. In particular, it is theoretically revealed that a GB migrating under a comparatively high shear stress tends to converge with its immobile counterpart and then splits into two new GBs that migrate in opposite directions. We estimated the critical stress for convergence and splitting transformations of GBs and the saturation grain size in metals (Cu and Ni) processed by severe plastic deformation. Our estimates are consistent with the corresponding experimental data reported in the literature.

1. Introduction

The outstanding mechanical properties of nanocrystalline and ultrafine-grained materials (hereinafter called nanomaterials) are crucially influenced by their structure having a mean grain size d as its key characteristic parameter; see, e.g., [1–11]. In particular, yield stress and hardness of metallic materials grow as $d^{-1/2}$ with reduction of the grain size d down to values of the order of 10 nm [1–4,12,13]. These dependences are called the Hall-Petch relationships and, in particular, explain superior strength and hardness exhibited by nanomaterials having nanoscale and ultrafine grains.

Also, owing to the grain size effects, in parallel with conventional lattice slip, grain boundary (GB) deformation mechanisms can effectively operate in nanomaterials [1–4,7–11]. These mechanisms are GB sliding, stress-driven migration of GBs, rotational deformation, GB diffusional creep mode, etc. Among GB deformation mechanisms, of a special interest is the stress-driven migration of GBs (Fig. 1), because it contributes to both plastic flow and grain growth in nanomaterials [14–48], as with their coarse-grained counterparts [49–53]. That is, stress-driven migration of GBs not only carries plastic deformation in nanomaterials, but also is capable of causing pronounced changes in the grain architecture that controls the outstanding mechanical and functional properties of these nanomaterials. In particular, grain growth carried by migrating GBs under stress can result in nano-to-coarse-grained structural transformations in a material, in which case its strength and hardness significantly degrade as plastic deformation progresses.

The previous research efforts [14–48] in the discussed area were focused mostly on GB migration onset and continuous GB evolution (that does not affect GB misorientation) under stress. At the same time, in order to fully understand the role of stress-driven GB migration in both plastic deformation and grain growth in nanomaterials, it is very important to identify and describe dramatic transformations of migrating GBs when they reach immobile GBs and converge with them. Indeed, when a migrating GB at the end of its continuous migration process in a grain meets another GB, it typically losses its individuality and undergoes a “discrete-like” convergence transformation that changes GB misorientation. Such

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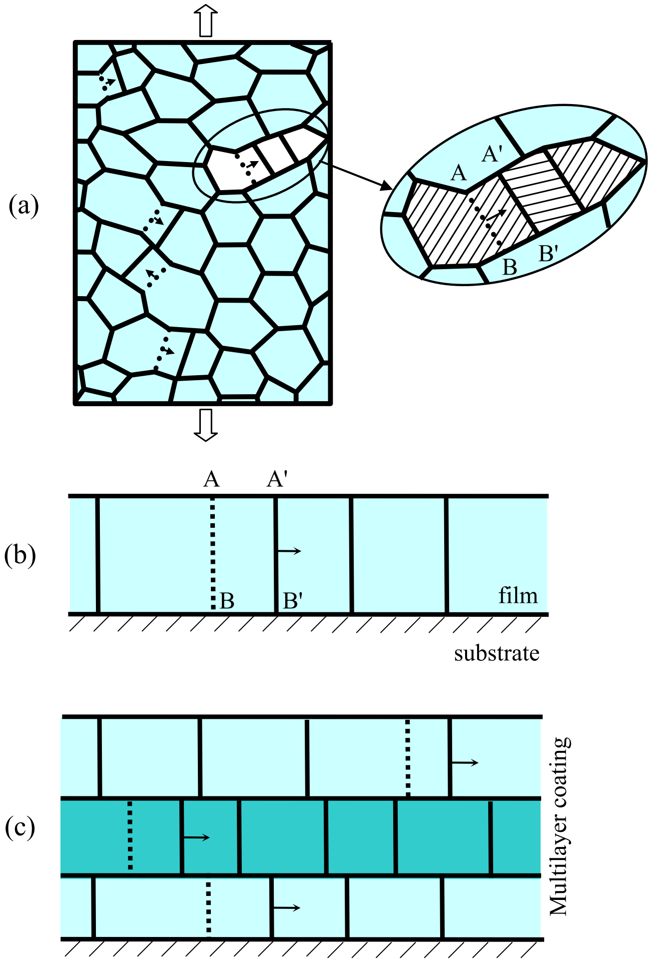

Fig. 1. Stress-driven GB migration in (a) nanostructured bulk material; (b) film with nanoscale or ultrafine grains; (c) multilayered film with nanoscale or ultrafine grains (schematically).

transformations crucially affect or even control both evolution of grain arrangement and GB-mediated deformation processes in nanomaterials under mechanical load. In particular, after a convergence of a migrating GB with its immobile counterpart, the resultant GB either becomes immobile or moves as a whole or splits into two new GBs that can move and/or become immobile (Fig. 2). In doing so, the stress-driven GB migration either is localized within one grain (Fig. 2c) or initiates new migration events and thus expands inducing growth of neighboring grains (Fig. 2d–f) in a mechanically loaded nanomaterial. The main aim of this paper is to theoretically describe convergence and convergence-induced transformations of GBs migrating under stress in nanomaterials.

2. Convergence and splitting transformations of grain boundaries migrating under stress in nanomaterials: geometric aspects

Let us consider the geometry of convergence and splitting transformations of GBs migrating under stress in nanomaterials. In doing so, in order to simplify our analysis, we examine a two-dimensional model arrangement of nanoscale grains with pure tilt GBs (Fig. 2a). This nanoscale grain configuration contains a vertical GB AB that migrates under the shear stress τ in a rectangular grain towards another vertical GB CD CD (Fig. 2a–c). Such a rectangular grain serves as a good model of elongated grains formed in nanomaterials at high plastic strains; see e.g. Refs. [54,55]. Besides, columnar grains with rectangular two-dimensional sections are typical in nanocrystalline/ultrafine-grained films and multilayer coatings fabricated by electrodeposition (Fig. 1 b and c).

When the GB AB specified by tilt misorientation ω_0 migrates under the shear stress τ towards the GB CD (Fig. 2 a–c), the migrating GB keeps its individuality in the sense that its misorientation parameter ω_0 is constant. Namely this process (Fig. 2a–c) was the main subject of previous research efforts addressing stress-driven migration of GBs in bi-crystals and nanomaterials; see, e; g., [12–53]. Instead, here we will focus our examination on the situation where the GB AB at the end of its individual migration under stress meets the GB CD and losses its individuality. More precisely, from a geometric viewpoint, one can distinguish the following transformations of the GBs AB and CD: (i) GBs AB and CD converge resulting in a new immobile GB C_1D_1 (Fig. 2d). (ii) GBs AB and CD converge into a new GB C_1D_1 that migrates (Fig. 2e). (iii) GBs AB and CD first converge forming a new GB which then splits into an immobile GB C_2D_2 and mobile GB C_1D_1 (Fig. 2f). (iv) GBs AB and CD first converge forming a new GB which then splits into two mobile GBs C_1D_1 and C_2D_2 that migrate under stress in the same direction (Fig. 2g). (v) GBs AB and CD first converge forming a new GB which then splits into two mobile GBs C_1D_1 and C_2D_2 that migrate under stress in opposite directions (Fig. 2h). (vi) GBs AB and CD do not converge, but when the migrating GB AB approaches the GB CD, the latter GB starts to migrate in the same direction as the GB AB (Fig. 2i). (vii) When the migrating GB AB approaches the GB CD, the latter GB starts to migrate in the opposite direction so these GBs may meet and converge (Fig. 2 j and k).

The case (vii) in part was examined in paper [56] focused on continuous migration of low-angle GBs that simultaneously start to migrate (Fig. 2k) and do not undergo “discrete-like” convergence and splitting transformation (at which GB misorientations change). Besides, according to Ref. [56], the stresses needed to activate the continuous migration (vii) are extremely large. In the context discussed, the continuous migration (vii) is not significant for extended grain growth, in contrast to the transformations (i) - (vi) whose detailed theoretical analysis (involving changes in GB misorientations) will be presented below.

We now examine the transformations (iv) and (v) illustrated in Fig. 2g and h, respectively. These transformations are basic ones, because other transformations, (i)-(iii) and (vi), under our consideration represent their partial cases. Also, note that the transformations (iv) and (v) are different from each other in only direction of migration of one GB resulted from a splitting transformation (Fig. 2g and h). In mathematical terms, the transformations (iv) and (v) are different in sign of the parameter specifying the position of the GB in question. In the context discussed, for the aims of this paper, it is sufficient to examine the transformation (iv) from the GB configuration shown in Fig. 2a to that illustrated in Fig. 2g. The transformation in fact consists of both the conventional continuous migration from the GB position shown in Fig. 2a to that illustrated in Fig. 2c and the “discrete-like” transformation from the GB configuration presented in Fig. 2c to that shown in Fig. 2g. The conventional migration process (Fig. 2a–c) has been theoretically described in Refs. [18,30]. Therefore, here we will just briefly consider its geometric aspects, while the main analysis will be focussed on the transformation from the GB configuration shown in Fig. 2c to that illustrated in Fig. 2g.

Let the GBs AB and CD in the initial configuration (Fig. 2a) be symmetric tilt boundaries characterized by tilt misorientation angles ω_0 and ω_0', respectively. Also, in its initial state, the vertical GB AB (Fig. 2a) terminates at the GB junctions A and B, which are