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# Stress-driven migration of grain boundaries and fracture processes in nanocrystalline ceramics and metals

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**Abstract**

Theoretical models are suggested that describe the effects of stress-driven migration of grain boundaries (GBs) on both the formation of nanoscale cracks (nanocracks) and the growth of comparatively large cracks in deformed nanocrystalline ceramics and metals. The GB migration under consideration is driven by the applied stress, carries plastic flow and produces quadrupoles of disclination defects in nanocrystalline materials. The disclinations create high local stresses capable of initiating the formation of nanocracks. In this paper, the conditions at which the formation of nanocracks is energetically favorable are theoretically described. The external stress values needed to initiate nanocrack formation near the disclinations in nanocrystalline metals (Al and Ni) with the finest grains and nanoceramics ($Al_2O_3$) are estimated. In addition, we estimated the effect of the stress-driven migration of GBs on the growth of pre-existing, comparatively large cracks in nanocrystalline Ni with the finest grains.


*Keywords:* Grain boundary migration; Disclinations; Fracture; Nanocrystalline microstructure; Modelling

## 1. Introduction

Nanocrystalline ceramic and metallic materials exhibit outstanding mechanical properties due to the nanoscale and interface effects [1–6]. In particular, interfaces – grain and interphase boundaries – crucially influence plastic flow and fracture processes in nanocrystalline materials (NCMs) specified by large volume fractions occupied by these interfaces. For instance, following experimental data [7–9], computer simulations [10] and theoretical models [11,12], cracks in mechanically loaded nanocrystalline ceramics and metals often nucleate at and grow along interfaces. During plastic deformation, grain boundaries (GBs) in NCMs serve as sources of partial lattice dislocations and twins [13–18] and effectively conduct such deformation modes as GB sliding [19–21], Coble creep [22,23], triple junction diffusional creep [24] and rotational deformation [25–29]. Furthermore, recent experimental observations [30–45] and computer simulations [46–48] have indicated that GB migration and grain growth processes intensively occur in mechanically loaded ultrafine-grained materials and NCMs. For instance, Gianola et al. [39] observed room temperature grain growth in nanocrystalline Al films in the course of their plastic deformation at quite high levels of applied stress. The yield stress was in the range 91–116 MPa, and the ultimate tensile strength was in the range 149–190 MPa [39]. These values are much larger than those (<50 MPa) characterizing plastic deformation in conventional coarse-grained polycrystalline Al. Furthermore, Gianola et al. [39] observed significant grain growth only in highly stressed regions, including the areas near the tips of slowly growing cracks. On the basis of their experimental data, Gianola et al. [39] concluded that grain growth occurs through the stress-induced GB migration at high local stresses. Farkas et al. [48] reported simulation results showing GB motion in nanocrystalline Ni with an ultrasmall grain size of 5 nm. In their molecular dynamics and

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empirical potential simulations at room temperature, plastic flow and associated GB motion occurred at a high stress level of 2.5 GPa. These simulations indicate that high applied stresses are needed to initiate GB migration in NCMs. Farkas et al. [48] observed GB mobility for distances up to 2.5 nm, or half the grain size.

Stress-driven GB migration is treated as a special deformation mechanism operating in NCMs (for a detailed discussion, see review article Ref. [5]). A very similar process of stress-driven GB migration occurs in bicrystals [49–54]. In doing so, the stress-driven migration of a GB in a bicrystal is coupled to shear deformation of the crystal lattice traversed by the migrating GB. For instance, GB migration coupled to shear in Al bicrystals has been observed in experiments [53,54]. In these experiments, the applied stresses were quite small (<1 MPa). The theory of the stress-driven GB migration coupled to shear deformation in bicrystals was developed by Cahn et al. [50–52]. Its basic statements are in good agreement with both experimental data [53,54] and the results of computer simulations [51,52,55,56] of the migration of low- and high-angle symmetric tilt boundaries in bicrystals. In addition, the coupling of GB migration and shear has been confirmed by computer simulations [57] of GB sliding through the motion of GB dislocations in a Fe bicrystal. In these simulations, the glide of dislocations has been shown to result in coupled motion of the boundary in directions parallel and perpendicular to itself.

Stress-driven GB migration processes coupled to shear in bicrystals are different from those in NCMs and coarse-grained polycrystals due to the difference in their geometric features (e.g. [58,59]). The shear coupled to GB migration in a bicrystal is easily accommodated by a change of the bicrystal shape, in which case the stress needed to initiate the migration process is low. At the same time, the crystal region where the shear coupled to GB migration occurs in a nanocrystalline solid commonly represents an internal region in the solid, and the shear is strongly hampered by the surrounding material. In Ref. [58], the stress-induced GB migration in a nanoscale grain of a nanocrystalline metal was briefly described as a special deformation mode accommodated by the formation of wedge disclinations (rotational defects creating internal elastic strains and stresses). It was theoretically shown that, if shear coupled to migration of a GB occurs in a NCM, it produces a quadrupole of wedge disclinations at the edges of the region traversed by the migrating GB [58].

The presence of disclinations and other defects serving as internal stress sources in NCMs crucially influences their fracture behavior (for a review, see Ref. [60]). In this context, of particular interest are the effects of the stress-driven GB migration and associated formation of disclinations on fracture processes in NCMs. The main aim of this paper is to suggest theoretical models that describe the effects of GB migration (coupled to shear and formation of disclinations) on both the formation of nanocracks (Section 4) and growth of pre-existing, comparatively large cracks (Section 5) in deformed nanocrystalline ceramics and metals. These theoretical models are based on the results of both the geometric consideration of the stress-driven GB migration in NCMs (Section 2) and the brief analysis of the brittle fracture behavior exhibited by nanocrystalline metals with the finest grains (Section 3).

## 2. Geometry of stress-driven migration of GBs in NCMs

The geometric features of the stress-driven GB migration are very important for understanding its effects on fracture processes in NCMs. In Ref. [58], the GB migration geometry in NCMs was briefly discussed. In this section, we consider in detail the geometry of stress-driven GB migration (coupled to shear and accommodated by the formation of disclinations) in NCMs and compare it with the geometry of such a migration process in bicrystals. Following Refs. [50–52], the stress-driven migration of a GB in a bicrystal is coupled to shear deformation of the crystal lattice traversed by the migrating GB and results in a change of the bicrystal shape (Fig. 1). In the framework of the theory [50–52], the ideal coupling (in the absence of GB sliding) is described by the linear relationship $v_{\parallel} = \beta v_n$, where $v_{\parallel}$ and $v_n$ are the velocities of the relative grain translation and normal GB motion, respectively, and $\beta$ is the coupling factor. In face-centered cubic (fcc) crystals, for symmetric tilt boundaries with misorientation angles ranging from 0° to 90°, there is a positive and a negative branch of coupling, at which the coupling factor $\beta$ is positive and negative, respectively [50–52]. For instance, [0 0 1] symmetric tilt GBs in copper show positive coupling if the GB tilt angle ranges from 0° to approximately 35°, and negative coupling if the GB tilt angle ranges from approximately 35° to 90° [52]. The coupling factor is related to the GB tilt misorientation $\omega$ as follows [51,52]: $\beta \approx 2\tan(\omega/2)$ and $\beta \approx -2\tan(\pi/4 - \omega/2)$ in the positive and negative branches of coupling, respectively.

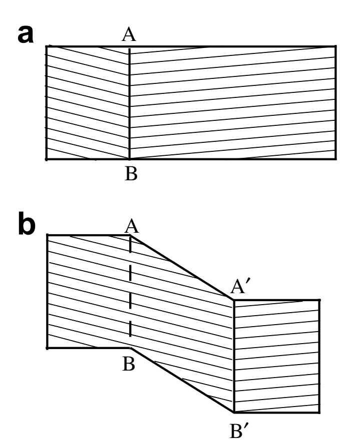


Fig. 1. Stress-driven migration of a tilt boundary in a deformed bicrystal. (a) and (b) depicts the initial and final state, respectively. The boundary migration results in a shear of the area traversed by this boundary. The shear is accommodated by a change in the bicrystal shape.