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# Uniaxial stress-driven coupled grain boundary motion in hexagonal close-packed metals: A molecular dynamics study

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**Abstract**—Stress-driven grain boundary (GB) migration has been evident as a dominant mechanism accounting for plastic deformation in crystalline solids. Using molecular dynamics (MD) simulations on a Ti bicrystal model, we show that a uniaxial stress-driven coupling is associated with the recently observed 90° GB reorientation in shock simulations and nanopillar compression measurements. This is not consistent with the theory of shear-induced coupled GB migration. In situ atomic configuration analysis reveals that this GB motion is accompanied by the glide of two sets of parallel dislocation arrays, and the uniaxial stress-driven coupling is explained through a composite action of symmetrically distributed dislocations and deformation twins. In addition, the coupling factor is calculated from MD simulations over a wide range of temperatures. We find that the coupled motion can be thermally damped (i.e., not thermally activated), probably due to the absence of the collective action of interface dislocations. This uniaxial coupled mechanism is believed to apply to other hexagonal close-packed metals.


*Keywords:* Grain boundary motion; Interface dislocations; Deformation twinning; Molecular dynamics; Titanium

## 1. Introduction

The strength and ductility of materials are inherently governed by their microstructure. In crystalline metals, for example, the mechanical properties are often associated with the way that dislocations interact with grain boundaries (GBs). Classically, one would expect an increase in the yield stress for small grain sizes (possessing a higher density of grain boundaries) to follow the Hall–Petch relation, in which the strength scales with the reciprocal square root of grain size [1–3]. However, as the structural scale reduces from the micrometer to the nanometer range, GB-mediated plasticity mechanisms (such as atomic shuffling, GB sliding and GB rotation [4–7]) are believed to be enhanced due to increasing GB density and suppression of dislocation activation [8,9]. Therefore, an improved understanding of the GB-based plastic deformation process is critical for the design of desirable mechanical properties.

Among possible GB-based mechanisms, shear-driven coupled GB migration has been observed to be dominant in both experiments [10–12] and molecular dynamics (MD) simulations [5,13,14]. Although most studies have focused on face-centered cubic (fcc) (e.g. Cu [5], Ni [12], Al [15]) and hexagonal close-packed (hcp) metals (e.g. Mg [11,16]), it is believed that such coupling is responsible for stress-driven GB motion and stress-induced grain growth in nanocrystalline materials in general. During the coupled GB motion, the boundary produces shear deformation of the lattice and causes relative translation of the grains parallel to the GB plane. The coupling effect can be characterized by a coupling factor $\beta = V_{//}/V_n$, where $V_{//}$ is the in-plane translation and $V_n$ is the normal boundary displacement. It has been shown that such coupling depends not only on the GB crystallography (for perfect coupling, $\beta = 2\tan(\theta/2)$, where $\theta$ is the tilt angle and $\theta < 90°$) but also on the GB velocity, temperature, etc. [5,17]. For instance, the shear-driven coupling factor can decrease with increasing temperatures, and the GB migration mechanism changes to rigid sliding (coupling disappears) at high temperatures [17].

Atomic computer simulation studies on fcc bicrystals reveal that such shear-driven coupled GB migration can be considered as a dislocation line mediated plastic deformation process. In symmetrical low-angle GBs (LAGBs), the mechanism of shear-driven coupled GB migration is known to be the collective glide of parallel edge dislocations, forming the GB, in response to the Peach–Koehler forces imposed by the shear stress $\tau$. The shear deformation of

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the region traversed by the dislocations leads to a coupled lateral translation of the grains [17]. In high-angle GBs (HAGBs), however, the pure dislocation model is no longer applicable. Nevertheless, it was found that shear-driven coupling still exists at low temperatures. Theoretical studies have indicated that the coupled GB motion in HAGBs can be interpreted as a composite action of mobile interfacial dislocations and localized atomic shuffling [18]. However, due to the limited number of slip systems available for dislocation glide in hcp metals, the evolution of dislocation-mediated plasticity is slow and deformation twinning (DT) has been thought to occur as a major rate-limiting factor. Therefore, the DT assisted GB migration is prevalent in hcp metals [19]. For example, Zhang et al. noted that deformation twinning dominates the $[10\bar{1}0]$ tilt GB motion in magnesium, whereas the coupling is in agreement with the theory of shear-driven coupled GB motion [20].

Recently, a new mechanism for GB motion, where the lattice orientation across the GB differs by 90°, was reported in simulations of hcp-Ti single crystals undergoing shock compression normal to its prismatic plane [21]. This boundary migration process is modeled as a transformation-like lattice reorientation accompanied by a collective action of dislocations and deformation twins. This is in contrast to the 90° GB in fcc metals (such as $\{1\,1\,2\}$ boundaries), where shock compression cannot induce the GB normal motion, only the emission of Shockley partial dislocations [22,23], and no lattice reorientation occurs. Experimentally, a similar boundary motion mechanism was observed in submicron single-crystal Mg undergoing compression along the same crystallographic orientation ([0 0 0 1]) [24]. Although the reorientation mechanism is similar to shear-driven coupled GB motion in HAGBs, it is not clear how it relates to the conventional mechanism of shear-coupled grain boundary motion. Therefore, of fundamental interest is (1) to understand how this lattice reorientation mediated GB migration couples to external stress, and to (2) investigate how the coupling of this mode compares (in properties such as temperature dependence) to the shear-driven GB migration.

In this study we investigate the grain boundary motion in hcp metals using MD methods. Our simulations on $[10\bar{1}0]$ orientated Ti bicrystals, where the lattice orientation across the GB differs by 90°, show that the GB motion is coupled to a uniaxial stress, and not to the shear as proposed by the theory of shear-driven coupled GB migration. We describe in Section 2 the simulation methodology used to study the uniaxial stress-driven GB motion. In Sections 3 and 4, we determine the atomic mechanisms of GB motion and the underlying reason for the uniaxial stress-driven coupling effect. In addition, the geometrical factors, such as GB inclination and GB misorientation (non-90° GB) that are associated with the GB motion are also discussed. Similar to the shear-driven coupling factor, we define a new parameter to describe the uniaxial stress-driven coupling, and analyze the influence of temperature on the coupling parameter, further demonstrating a distinct coupling characteristic from the shear-driven GB motion. Finally, the main results and conclusions are summarized in Sections 5.

## 2. Simulation methods

The atomic interactions of the pure Ti model system studied are described by the interatomic potential developed by Zope and Mishin [25]. The potential accurately reproduces physical properties that are important in the context of this study. In particular, they predict accurate values of the elastic constants and stacking fault energies, as well as twin boundary energies.

A GB was created by constructing two separate crystals with desired crystallographic orientations and joining them along a plane normal to the $y$-direction, as shown in Fig. 1. Periodic boundary conditions were applied in the $x$- and $z$-directions parallel to the GB plane. In the $y$-direction, the grains were terminated at the free surfaces. Each grain has an approximate cubic shape. Two 1.5 nm thick slabs at the top and bottom of the box (Fig. 1a) contain atoms with relative positions frozen to those of the perfect lattice. These are used to impose a compression or tensile stress on the GB. Typical samples contain 1.74 million atoms with dimensions $L_x = 23.6$ nm, $L_y = 37.5$ nm and $L_{z=}34.7$ nm.

Prior to the MD simulation, the block was uniformly expanded by the thermal expansion factor at the selected simulation temperatures. This expansion was intended to eliminate thermal stresses inside the grains. The equilibration MD runs were performed in the NPT ensemble (N, P and T denote the number of atoms, hydrostatic pressure and absolute temperature, respectively), with a Nosé–Hoover thermostat [26] and a Parrinello–Rahman barostat [27]. After the temperature reached the target value, the GB was equilibrated by an isothermal anneal for a few hundred picoseconds. The equilibration was followed by a production run in which the upper surface layer was moved parallel to the $y$-direction with a strain rate of $\sim 10^8\ s^{-1}$. A 1 fs time integration step was used throughout this study. All the simulations performed in this study employed the LAMMPS (large scale atomic/molecular massively parallel simulator) code [28], and the atomic configurations visualized by ATOMEYE [29].

To investigate the GB mobility and the variation with the change in temperature, the GB velocity is extracted from the average positions of the front interface. The position of the GB is determined by utilizing the bond-angle distribution related order parameter (ADOP) developed by Ackland and Jones [30], i.e. the position of the grain boundary corresponds to a jump in the order parameter number when the ADOPs for each atom are plotted as a function of the $y$-position of the simulation box.

## 3. Results

### 3.1. Grain boundary motion under uniaxial loading with normal (90°) interface

#### 3.1.1. Compression-driven GB migration

Previous studies [21] have linked the 90° lattice reorientation process to uniaxial compression (shockwave loading or nanoindentation). Here we focus on the evolution of the grain boundaries accompanying the lattice reorientation under uniaxial compression. An ideal 90° GB model with crystallographic orientations, $(10\bar{1}0)_{Grain2}$// $(0001)_{Grain2}$ // interface plane and $[1\bar{2}10]_{Grain1}$// $[1\bar{2}10]_{Grain2}$ is constructed as shown in Fig. 1b. The quasi-static compression stress is applied to the GBs by displacing the fixed atoms of the upper slab downwards with a constant velocity $v_n = 0.1$ A $ps^{-1}$. The compression-induced GB motion at 30 K is illustrated in Fig. 2. After the initial elastic deformation,