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Atomic rearrangements at migration of symmetric tilt grain boundaries in vanadium

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ABSTRACT

The paper reports on a molecular dynamics study of atomic rearrangements and migration of symmetric tilt grain boundaries in a vanadium crystallite under shear load specified as constant-velocity displacements of its faces parallel to the boundary plane. The study shows that such grain boundaries migrate normal to their plane with a high velocity and that this velocity depends on their structure and on the shear rate. The migration is jump-like, involves a periodic rise and drop of internal stress, and represents a sequence of specific self-consistent structural rearrangements in grain boundary regions.

1. Introduction

Grain boundaries (GBs) occupy a large volume in nanocrystalline materials and greatly contribute to their unique properties. The migration of GBs under mechanical load can substantially change the physical and mechanical properties of such materials, and many studies are conducted to establish the mechanisms of this migration [1]. One of the most efficient methods of studying the grain growth in polycrystals is computer simulation. As has been found [2], some types of GBs can migrate with anomalously high velocities in shear-loaded fcc materials and can change their structure. Thus, to stabilize and control the internal structure of materials, it is important to identify and study the mechanisms responsible for GB migration.

According to a molecular dynamics simulation [3], the motion of a grain boundary normal to its plane often causes tangential grain displacements such that the lattice intersected by the boundary is involved in shear deformation. If shear stresses act on the boundary, its normal displacements can cause one of the grains to grow by absorbing the other. The way of GB migration along the normal depends on the direction of applied shear stress.

Under high-rate shear load, certain of the symmetric tilt GB regions can experience dynamic vortex motion of atoms through their self-consistent collective displacements on scales of several lattice parameters both in the loading direction and in the GB plane [4,5]. Such vortex atomic displacements, though individually small, provide anomalously high GB velocities and can rearrange the structure of grains to the structure of their neighbors.

Molecular dynamics data are available on the migration of tilt GB triple junctions with ⟨1 1 1⟩ and ⟨1 0 0⟩ misorientation axes in nickel [6]. The data suggest two migration mechanisms: for low-angle boundaries ⟨1 0 0⟩, it is the motion of paired GB dislocations with a change of dislocations-partners, and for tilt boundaries ⟨1 1 1⟩, it is the motion of such dislocations in combination with pairs of GB dislocations having common glide planes. Because the activation energy of the second mechanism is relatively low, the mobility of boundaries ⟨1 1 1⟩ is much higher than that of boundaries ⟨1 0 0⟩.

As has been shown [2], four main types of GB displacements are possible under external shear load: (1) coupled motion in which the grain boundary is displaced normal to its plane, leading the growth of grains through “dissolving” the others; (2) combined motion which causes grains to translate parallel to the GB plane and shift normal to it; (3) rigid-body translation of grains relative to each other; and (4) rotation of grains with a change of their orientation to the GB plane.

In conventional theories of capillarity-driven grain growth, the velocity of GBs is determined by their curvature and energy [7]. However, such theories cannot explain many experimental and computation results, e.g., high rates of growth [8], rotation [9], and sliding of grains [10]. It should be expected that in bicrystals under shear, not only collective vortex motions of atoms can provide high velocities of plane GBs [5]. Due to the symmetry of grains relative to GBs, a certain sequence of structural rearrangements in GB regions can provide mechanisms for migration, and their features will undeniably depend on the GB structure.

On the atomic scale, the motion of low-angle symmetric tilt GBs is provided by collective glide of parallel edge dislocations under Peach–Koehler forces [3,4] such that shear strains arise in the region

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intersected by them and cause coupled lateral grain displacements. For high-angle symmetric tilt GBs, the atomic mechanisms of motion are still poorly understood [11].

It should be noted that most of the related studies concern fcc metals, and those considering the mechanisms of GB migration in bcc materials are scanty and so are the data on their atomistic research. Here we study the atomic mechanisms of coupled motion of high-angle symmetric tilt grain boundaries in bcc vanadium under high-rate shear loading.

2. Research techniques

Our molecular dynamics simulation was performed for a shear-loaded vanadium crystallite in LAMMPS software [12]. The interatomic interactions were described by a many-body potential calculated using the embedded atom method in the Finnis–Sinclair approximation [13]. The choice of vanadium was due to the wide use of its alloys as structural materials [14,15]. The model crystallite was shaped as a parallelepiped containing about 40,000 atoms (Fig. 1). The *X* and *Z* axes were assigned periodic boundary conditions. The conditions at the crystallite edges in the *Y* direction corresponded to the regions of grips 1.5 nm thick. The *Y* and *Z* coordinates of grip atoms during loading were fixed. The initial crystallite temperature was 300 K. The crystallite contained a symmetric tilt grain boundary (3 1 0)[0 0 1] or (2 1 0)[0 0 1] modeled by a gamma-surface minimization algorithm [16]. The grip velocity along the *X* direction was varied from 1 to 100 m/s. The computation results were visualized in OVITO software [17].

3. Results

The calculations demonstrate that the model GBs move with a high velocity under shear load. Fig. 2 shows the position of the (3 1 0)[0 0 1] grain boundary at different points in time for a grip velocity of 1 m/s. The GB velocity is determined by the shear rate and by the GB structure, and increasing the shear rate increases the GB velocity. At the shear rates considered, the average velocity of the (2 1 0)[0 0 1] grain boundary ranges from 3 to 280 m/s, and that of (3 1 0)[0 0 1] is lower, ranging from 2 to 180 m/s.

Note that periodic boundary conditions prevent the rotation of grains. Since GB is symmetrical, the grains have the same shear moduli parallel to GB. Consequently, the grip movements do not produce any volume driving forces. Stresses caused by grip movements can initiate the GB motion if it leads to a shear deformation of the crystallite. The GB migration is due to a coupling effect. The direction of the GB displacement depends only on the crystallographic parameters of the boundary. This statement completely agrees with computer calculations of the features of the GB migration in crystallites reported elsewhere [18,19].

The elastic stress during shear loading rises and relaxes periodically. Noteworthy is that the GB motion has a clearly defined jump-like character due to the crystallinity of the material. When the stress is relaxed, the GB velocity increases rapidly, reaches its maximum, and decreases almost to zero, as evidenced by the curves in Fig. 3(a). Such stop-and-go motion is characteristic for symmetric tilt GBs in fcc metals [3]. The activation of coupled GB motion requires a certain critical shear stress. If the stress is lower than critical, no GB motion occurs. In our study, the stress reveals a linear time dependence during its rise and relief, suggesting that no structural defects are generated in the deformed crystallite. According to our thorough analysis, any lattice defects like, e.g., vacancies, are absent in the regions passed by the grain boundaries, which agrees with other research data [3] and with the conclusion that the displacement of high-angle symmetric tilt GBs is unrelated to dislocation mechanisms [18,19].

It should be noted that those atomic planes which are far from the grain boundary also reveal periodic motion in the normal direction

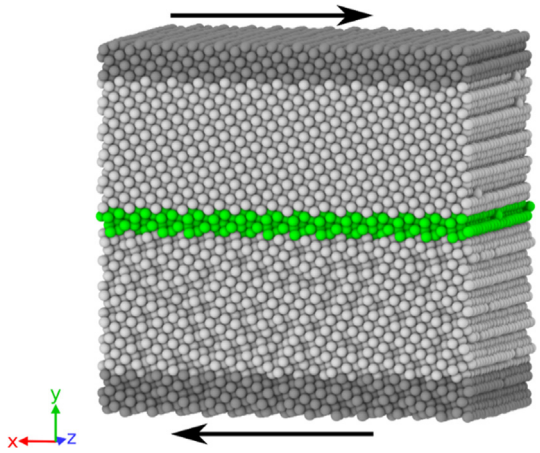

Fig. 1. Initial crystallite structure and its loading pattern: green – (2 1 0)[0 0 1] grain boundary region; dark gray – grips; arrows – shear directions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

(Fig. 3(b), red[1] curve) due to the crystallinity of the material and constant grip velocity. However, their jump-like motion is less pronounced compared to the atomic planes near the boundary (Fig. 3(b), blue curve). The dip on the blue curve for the grip position between 0.15 and 0.35 nm owes to the grain boundary passing through the corresponding plane.

According to the calculations, the grain boundaries (3 1 0)[0 0 1] and (2 1 0)[0 0 1] differ greatly in atomic rearrangements responsible for their migration. The boundary (2 1 0)[0 0 1] is displaced due to atomic rearrangements in three atomic planes: in two planes forming the boundary and in the plane of the upper grain adjacent to them, which are marked by green and blue colors, respectively, in Fig. 4(a)–(c). Under shear loading, the blue plane is rearranged into the structure of the lower grain (Fig. 4(b)), resulting in atomic displacements in the *YZ* plane to a value of about 0.08 nm (Fig. 4(c)). The atomic plane of the upper grain is rearranged into the structure of the lower grain through three successive displacements in different directions. At a shear rate of 1 m/s, each displacement takes about 3.6 ps. The values of these three displacements are equal to about 0.07, 0.03, and 0.06 nm, and the result is that atoms of the blue plane consistently occupy the positions of atoms of the upper and then of the lower GB plane, and finally go to the lattice of the lower grain (Fig. 4(a)–(c)).

The grain boundary (2 1 0)[0 0 1] migrates through more complex atomic rearrangements compared to the boundary (3 1 0)[0 0 1]. As can be seen from Fig. 3, each stress drop causes specific rearrangements in eight atomic planes (Fig. 4(d)): five belong to the boundary (dashed) and three belong to the upper grain (red, green, and blue). After each rearrangement, three GB planes transform into the structure of the lower grain and three planes of the upper grain transform into the GB structure. Let us analyze how the colored planes are rearranged into the structure of the lower grain. The rearrangement takes about 200 ps. During this time, the resulting *YZ* components of atomic displacements for the red, blue and green planes are about 0.07, 0.01, and 0.08 nm, respectively. Note that the rearrangement of the colored planes to the structure of the lower grain involves three GB displacements each with a duration of 4.0 ps. After the first GB displacement, we have the red, green and blue planes shifted by 0.02, 0.04, and 0.03 nm, respectively. As a result, the considered atomic planes of the upper grain become a part of the grain boundary (Fig. 4(e)). After the first displacement, the red and green planes are shifted such that they have the same *Y* coordinate. After the second displacement, the red and green planes

[1] For interpretation of color in Fig. 3, the reader is referred to the web version of this article.