Article

Annihilation Mechanism of Low-Angle Grain Boundary in Nanocrystalline Metals

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Abstract: Due to the high density of grain boundaries (GBs), nanocrystalline metals possess superior properties, including enhanced strength, work hardening, and fatigue resistance, in comparison to their conventional counterparts. The expectation of GB migration is critical for grain coarsening and GB annihilation in these materials, significantly affecting the polycrystalline network and mechanical behavior. Here, we perform molecular dynamics (MD) simulations on gold (Au) nanocrystals containing multiple parallel arranged GBs, with a focus on the investigation of annihilation mechanisms of low-angle grain boundaries (LAGBs). It is observed that the shear-coupled motion of LAGBs, consisting of dislocations, gives rise to their preliminary migration with the reduced separation distance between GBs. With subsequent GB motion, the LAGBs encountered with neighboring GBs, and can be annihilated by various mechanisms, including dislocations interpenetration, dislocations interaction, or dislocations absorption, depending on the specific configuration of the neighboring GB. These findings enhance our understanding of GB interactions and shed light on the controlled fabrication of high-performance nanocrystalline metals.

Keywords: nanocrystalline metals; grain boundary; plastic deformation; GB annihilation; molecular dynamics simulation

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1. Introduction

Nanocrystalline materials, with a high percentage of GBs, are widely attractive for various engineering applications due to their enhanced strength and ductility with respect to their coarse-grained polycrystalline counterparts [1,2]. For metallic components subjected to complex mechanical and thermal loading conditions, such as high-speed lightweight aircraft wings in turbulent air [3,4], microstructural stability has to be considered. Although strategies for improving fatigue and corrosion resistance have been proposed [5,6], these materials typically exhibit softening-induced failure, associated with dislocation exhaustion or low-angle grain boundaries (LAGBs) disappearance [1,7,8]. In general, the softening behavior and ductility are strongly related to the deformation mechanisms. Specifically, GB-mediated deformation mechanisms, such as GB sliding [9,10], GB migration [11], or grain rotation [12], are prevalent and at least partly linked with GB annihilation in metallic nanocrystalline materials [13]. A variety of studies have been focused on the mechanical response of individual GBs [14,15], however, the nanocrystalline networks, consisting of multiple GBs, may exhibit different kinetic behaviors [16,17], which was rarely studied. The plastic deformation behavior in polycrystals, involving cooperative motion and interactions of parallel GBs or GB junctions [18,19], plays an important role and must be taken into account in practice.

GB annihilation, associated with strain softening, was generally observed during deformation and may result from GB motion (particularly migration and/or sliding), dislocation-GB interaction [20], grain rotation [21], self-mechanical annealing or thermally-activated GB diffusion [22], etc. [23]. If the boundaries move toward each other sufficiently, they can combine to form a different GB, finally giving rise to GB annihilation. Various investigations showed that during the thermal process or cyclic mechanical loading, the GBs began to migrate and annihilate, resulting in a significantly altered GB network [21]. Moreover, grain microstructure vanishes because of the disappearance of a large number of GBs [24]. However, the dynamical atomic process of GB annihilation was still unclear. Through computer simulations, detailed atomistic information about statics and dynamics can be obtained so as to systematically explore the mechanism of GB annihilation.

In this work, we employed MD simulation on Au nanocrystals with two parallelly arranged GBs to investigate the atomistic process of LAGB annihilation. We found that the deformation mechanism that governs the annihilation behavior of the LAGB depends on the initial GB structure. The difference in shear-coupled migration rates between neighboring GBs gives rise to a reduced separation distance between GBs, leading to accelerated GB migration. As the migration continued, the two GBs merged through dislocation interpenetration, interaction, or absorption for different GBs. The annihilation of LAGBs alters GB structures and contributes to grain coalescence. Our findings provide insights into GB-governed plasticity in nanocrystalline materials.

2. Materials and Methods

MD simulations were carried out on Au tricrystals with a total of ~140,000 atoms using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS, Sandia National Laboratories, Albuquerque, NM, USA) [25] and the embedded atom method (EAM) potentials for Au [26]. Cylindrical tricrystal models with a diameter of 10 nm and a total height of 30 nm (10 nm height for each grain) were created by constructing three separate crystals with respective crystallographic orientation and joining them along the axial direction. GBs with different misorientations were generated by tilting grains around the $\langle 110 \rangle$ axis. Three boundary layers of atoms at the top and bottom of the system were fixed as rigid slabs. The remaining dynamic atoms were allowed to adjust their positions in a Nose-Hoover thermostat at 300 K. Free boundary conditions were applied parallel to the GB plane. To obtain the equilibrated GB structure, the system was relaxed for 20 ps first and energy minimized with a conjugate-gradient algorithm. During the shear loading, samples were under the canonical ensemble (NVT) at 300 K. A constant shear velocity of $v = 1 \text{ m s}^{-1}$ parallel to the boundary plane was applied on the rigid slab of the top grain. A velocity profile with a linear gradient from 0 to 1 m s^{-1} was assigned to the dynamic atoms along the axial direction. (Details shown in Supplementary Figure S1) The time step of the MD simulations was 2 fs, and the total simulation time was 3 ns. The average vertical displacement of the GB atoms was recorded as the GB migration displacement. Ovito (OVITO GmbH, Germany) [27] was used to visualize the bicrystal model, and the common neighbor analysis was employed to identify the dissociation of the GBs during the simulations. Atoms with FCC, hexagonal close-packed (HCP) and disordered structures were marked in blue, red, and cyan, respectively.

The atomic von-Mises stress is defined as:

$$\sigma_{\text{von-Mises}} = \sqrt{1/2[(\sigma_x - \sigma_y)^2 + (\sigma_x - \sigma_z)^2 + (\sigma_z - \sigma_y)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{xz}^2)]} \quad (1)$$

where $\sigma_x, \sigma_y, \sigma_z, \tau_{xy}, \tau_{yz}, \tau_{xz}$ are the six independent components of the Virial stress tensor. The stress tensor components per atom were obtained by dividing the energy by atomic volume during loading.

3. Results

3.1. Annihilation at Low-Angle Grain Boundaries

A series of well-defined tri-crystals, comprising two GBs (Figure 1a,b), permits a much more unambiguous study of the structure evolution and further the dynamic deformation mechanisms of GB annihilation in polycrystals. Figure 1c shows a typical relaxed structure with a diameter of 10 nm and a height of 30 nm. Two $[110]$ tilt GBs (denoted as GB₁ and GB₂) with misorientations of 10° and 10° parallel to each other. The signs of misorientations are defined in Figure 1b, where plus represents an anti-clockwise misorientation of the upper grain relative to the corresponding bottom grain and minus is the opposite. Shearing (Figure 1d–f) was imposed on the sample with a direction parallel to the GBs. The structure of the considered low-angle tilt GBs can be represented by a set of periodically located Shockley partial pairs (Figure 1k), thus the migration of GBs is the movement of the wall of the dislocation pairs. Shear loading initially activated GB migration at different rates for GB₁ and GB₂ because GB₁ possessed stronger mobility compared with GB₂ (Figure 1d). As this process developed, two GBs approached each other, resulting in a reduction of the separation distance between GBs and shrinkage of G2. While the two GBs got closer and closer, quick merging and annihilation of initial GBs were observed. During the merging process, GB₁ instantly moved upward, while GB₂ reversed the direction of motion, i.e., move downward, to the same position, leading to a full annihilation of G2 (Figure 1d,e). The newly recombined GB₃, as a single wall of dislocations with the misorientation of 20° (Figure 1k), steadily migrated in the subsequent shear process (Figure 1f).

Figure 1. Low-angle grain boundaries (LAGBs) annihilated at LAGBs. (a) Schematic showing the set-up of the cylindrical tricrystal sample in this work. (b) The definition of misorientation sign. (c,g) The initial constructed Au nanocrystal, which contained two parallel LAGBs, denoted as GB₁ and GB₂. The misorientations of GB₁ is 10° and of GB₂ is 10° in (c) while -10° in (g), respectively. (d) Upon shearing, the two GBs migrated upward at different rates, resulting in a GB spacing reduction. (e) GB dislocation pairs interpenetrated, giving rise to a new GB. (f) The newly formed GB, denoted as GB₃, migrated upward in subsequent shearing. (h) Upon shearing, GB₁ migrated upward while GB₂ migrated downward. (i) While the two GBs meet, GB dislocation interacted. (j) GB annihilation with left vacancies and dislocations. (k,m) Enlarged structure in (c,f,g,i) showing detailed GB structures before and after annihilation. (l) Migration distance of GB₁ and separation distance between two GBs versus shear displacement. The deformation snapshots of (c–e,g–i) were highlighted by black diamonds. Atoms with FCC, HCP and disordered structures were marked in blue, red, and cyan, respectively. Scale bars: 2 nm.

To further explore the annihilation mechanisms between LAGBs, additional MD simulation was carried out by altering the misorientation of GB₂ (Figure 1b), while fixing the misorientation of GB₁. For GB₂ with a misorientation of -10° , the G1 and G3 possess the same orientation but with some shifting/transition along the GB plane (Figure 1g,m). Upon shearing, the two GBs moved toward each other, engendering the shrinkage of G2 (Figure 1h). As the GB closer to another one, the interaction force between neighboring disassociated dislocation partials grew rapidly. Interaction of dislocations in the same slip planes generated an elongated extended dislocation (Figure 1h). Subsequently, the extended dislocations shrank instantly and finally annihilated (Figure 1i). We found the initial straight GBs became convexly curved towards G2 during migration, probably induced by the non-uniform distribution of stress at the GBs and the annihilation of the internal GB dislocations relaxed stresses, while the stationary boundary GB dislocations fixed the GB. After dislocation pairs interaction and fully annihilation, a single crystal formed with some left-behind vacancies and residual dislocations (Figure 1j,m).

During the above shearing process, GB positions were recorded, and both migration distance of GB₁ and separation distance between GB₁ and GB₂ were measured (Figure 1l, details shown in Supplementary Tables S1 and S2). Attention was first focused on the initial migration of GB₁ for models with different GB₂, identical and unchanged migration-shear displacement coupling were shown during their motion till the time moments close to GB meeting. The coupling factors were estimated to be 0.24, somewhat larger than the theoretical value calculated based on the shear migration geometrical model [15]:

$$\beta = 2 \tan\left(\frac{\theta}{2}\right) \sim 0.175 \quad (2)$$

The variation between simulation and theory may result from temperature [14], free surface [28], GB structure [15], etc. Then, a sharp transition of GB migration rates was found at a separation distance of ~ 6 nm, which suggests the mutual attraction between GBs effectively accelerated the merging process. In the case of FCC materials, the annihilation distance between edge dislocations can be approximated as $6b$, where b is the Burgers vector of dislocations [29] (~ 3 nm for disassociated dislocations). The difference may be induced by lateral dislocations, stress, or temperature.

Dislocation analysis and stress contribution evolution observations were further carried out to explore detailed atomic dynamics during annihilation. For GB₂ with the misorientation of 10° , the Burgers vectors of GB dislocations were $b_1 = 1/6[-1 \ -2 \ -1]$, $b_2 = 1/6[1 \ -1 \ -2]$, while the Burgers vectors of dislocations, compromised of GB₁, were $b_3 = 1/6[-1 \ -2 \ -1]$, $b_4 = 1/6[1 \ -1 \ -2]$ (Figure 2a). Stress contribution showed severe concentration at GB₂ while highly mobile GB₁ migrated to partly release stress (Figure 2e). The increasing attraction with the reduction of GBs separation distance accelerated the migration of GB₁ and reversed the migration direction of GB₂ (Figure 2b). Dislocations spacing of GB₁ and GB₂ were initially four (111) atom layers. After dislocations crossing (Figure 2b), dislocation spacing turned to be one (111) atom layer (Figure 2c). Accompanied with the shrinkage of stacking faults (Figure 2d), stress was released in G2 and concentrated at GB₃ to further activate the migration of GB₃ (Figure 2f).

For GB₂ with the misorientation of -10° , the Burgers vectors of GB dislocations were, $b_1 = 1/6[1 \ 1 \ 2]$, $b_2 = 1/6[-1 \ 2 \ 1]$, while $b_3 = 1/6[1 \ -2 \ -1]$, $b_4 = 1/6[-1 \ -1 \ -2]$, respectively (Figure 2g). A perfect annihilation occurred to the opposite dislocation pairs ($b_2 = -b_3$), locating at the same slip planes. In contrast, the annihilation of the dislocation pairs at the adjacent planes generated some vacancies at the meeting area (Figure 2h). Immediate annihilation of trailing partials occurred with stacking fault eliminated, inducing the merging of GB₁ and GB₂ and further coalescence of G1 and G3 (Figure 2i). However, dislocations near the surface cannot be removed and would glide in subsequent deformation (Figure 2j). Due to the annihilation of GBs, stress was released and re-concentrated at the residual vacancies and dislocations (Figure 2k,l).

Figure 2. Atomistic dynamics and stress contribution evolution during LAGBs annihilation at LAGBs. (a–d) Simulation snapshots showing GB₁, with a misorientation of 10°, annihilated at GB₂, with a misorientation of 10°. (a) The two LAGBs consist of disassociated dislocation pairs, denoted as dislocations 1–4. (b,c) Dislocation pairs glided and interpenetrated into the gaps. (d) After the dislocation pairs are arranged in a row, the stacking faults shrink. (e,f) The atomic von-Mises stress contribution of (a,d), showing increased stress concentration at GBs after GB annihilation. (g–j) Simulation snapshots showing GB₁, with a misorientation of 10°, annihilated at GB₂, with a misorientation of −10°. (g) The two LAGBs consist of disassociated dislocation pairs, denoted as dislocations 1–4. (h,i) Opposite dislocation partials interacted, and the two GBs merged. (j) While GB₁ fully annihilated, there left some dislocations and vacancies. (k,l) The atomic von-Mises stress contribution of (g,j), showing increased stress concentration at vacancies after GB annihilation. Scale bars: 2 nm.

3.2. Annihilation at High-Angle Grain Boundaries

High-angle grain boundaries (HAGBs), with low mobility, act as a barrier for the dislocation glide, leading to a dislocation impediment [30]. To understand the mechanism of the impediment and annihilation of LAGBs at HAGBs, we carried out additional simulations for GB₂ with a misorientation of 30° (Figure 3a) and −30° (Figure 3e). During the whole shearing process, GB₂ stayed at the initial positions while GB₁ migrated upward and approached GB₂ (Figure 3b,f). With continued loading, the leading partials (Figure 3i,k) were absorbed and trailing partials were attached to GB₂ with stacking-fault ribbons connecting (Figure 3c,g). Eventually, GB₂ absorbed all dislocation pairs, i.e., GB₁. The rearrangement of atoms at GB₂ resulted in GB structures modification and generating new GBs (Figure 3i,k). The newly formed GB₃ were still immobile during the subsequent shearing (Figure 3d,h). Quantitative measurement showed a consistent initial coupling factor of 0.22 and critical transition GB separation distance of ~5 nm (Figure 3j, details shown in Supplementary Tables S3 and S4).

Detailed GB annihilation processes and stress contributions are shown in Figure 4. The un-uniform migration of GB₁ resulted in curved GB structures (Figure 4a,g) and different local separation distances between GB₂ and GB₁ segments. The immobile GB₂ bore much more stress concentration compared with GB₁ (Figure 4e,k). In response to the localized stress at GB₂, the foremost leading partial dislocation annihilated and dissociated into GB dislocations at GB₂, leaving the corresponding trailing partial attached to GB₂ (Figure 4b,h). Then, the trailing partial glided into GB₂ and annihilated at GB₂, accompanied with other leading partials approached GB₂ (Figure 4c,i). With all dislocation pairs, compromised of GB₁, annihilated at GB₂ one by one, the structures of HAGBs were altered with increasing or decreasing misorientations (Figure 4d,j). Stress concentrated severely at GB₃ and free surface, while completely released in G1 (Figure 4f,l).

Figure 3. LAGBs annihilated at high-angle grain boundaries (HAGBs). (a,e) The initial constructed Au nanocrystal contained two parallel GBs. The misorientation of the low-angle GB, denoted as GB₁, was 10° and the high-angle GB, denoted as GB₂, was 30° in (a), while −30° in (e), respectively. (b,f) Upon shearing, GB₁ migrated upward and approached GB₂, resulting in a GB spacing reduction. (c,g) The leading partials, denoted as LP in (i,k), were absorbed, leaving the trailing partials, denoted as TP in (i,k), attached to GB₂ with stacking-fault ribbons. (d,h) GB₁ fully annihilated at GB₂, generating new GBs, denoted as GB₃. (i,k) Enlarged structure in (a,d,e,h) showing detailed GB structures before and after annihilation. (j) Migration distance of GB₁ and separation distance between two GBs versus shear displacement. The deformation snapshots of (a–c,e–g) were highlighted by black diamonds. Scale bars: 2 nm.

Figure 4. Atomistic dynamics and stress contribution evolution during LAGBs annihilated at HAGBs. (a–d,g–j) Simulation snapshots showing GB₁, with a misorientation of 10°, annihilated at GB₂, with a misorientation of 30° and −30°, respectively. (a,g) The LAGB (GB₁) consists of disassociated dislocation pairs, which brings about high mobility. (b,h) Leading partials of GB₁ annihilated at GB₂, leaving the corresponding trailing partials attached to GB₂. (c,i) The trailing partials glided into GB₂ and annihilated. (d,j) While all dislocation pairs at GB₂, the LAGB (GB₁) fully annihilated at GB₂. (e,k) The atomic von-Mises stress contribution of (a) and (g), showing severe stress concentration at GB₂ and slight stress concentration at GB₁ before GB annihilation. (f,l) The atomic von-Mises stress contribution of (d,j), showing released stress in G1 after GB annihilation. Scale bars: 2 nm.

Taken together, these results provide important insights into the annihilation mechanisms of LAGBs, which are strongly dependent on the GB structures. Further quantitative analysis, including migration distance of GB₁ and separation distance between two GBs, suggested an almost consistent migration rate of GB₁ and critical accelerating separation spacings between GBs before meeting, which can give deep insight into GB-dominated plasticity.

4. Discussion

With applied force, the motion of GBs within a polycrystal is inevitably impeded by other grains and GB junctions, generally generating grain rotation. Multiple grain rotations bring the orientation of abutting grains closer together, which reduces the GB misorientation angles and even eliminates the GBs, leading to the coalescence of smaller grains [12,21,31]. However, previous observations also showed that LAGBs were activated to migrate steadily before being annihilated [32,33], different from grain rotation mediated GB annihilation. Moreover, the shear-coupled GB migration was believed to have contributed to grain shrinkage and GB annihilation [11,34,35]. The shrinkage of grain, accompanied by the simultaneous growth of neighboring grains, is observed to occur commonly in various materials during plastic deformation under tension [36], shear [11], or indentation [37], finally resulting in statistical grain coarsening. Here, our results showed the high mobility of LAGBs may contribute to a GB annihilation and preferential growth/shrinkage of the corresponding grains.

Stress-assisted migration behavior of individual LAGBs was widely studied. LAGBs were traditionally described in terms of dislocation arrays, and shear stresses were generally thought to influence and activate LAGBs by coupling to the individual dislocations in these arrays [32,38,39]. However, the deformation dynamics of polycrystals, consisting of multiple embedded GBs, especially the coordinated behavior between GBs, are still unknown. With a tri-crystal model system, we studied the annihilation behavior of LAGBs at neighboring GBs, including LAGBs (Figures 1 and 2) and HAGBs (Figures 3 and 4). Grain and GB annihilation have resulted from inconsistent structure-dependent shear-coupled migration rates of GBs. During the encountering annihilation process, dislocation pairs interpenetrated and arranged in a row or merged at LAGBs with leaving-behind defects, while they were absorbed one by one at HAGBs (Figure 5).

Figure 5. Schematic showing the annihilation mechanisms of LAGBs depending on the specific configuration of the neighboring GBs. The GBs are found to merge and finally annihilate through dislocation interpenetrating for LAGBs with the same migration direction initially. GBs annihilated through dislocation interaction for LAGBs with the opposite migration direction initially. The left vacancy and residual dislocations are indicated by dots and 'T'. Meeting with HAGBs, LAGBs annihilated through GBs absorption. Red arrows at the right of GB planes indicate the migration direction under right shear.

Apart from GB structures, other factors should be taken into account to describe proper GB annihilation in polycrystals. For instance, GBs are always dragged by junctions or impurities and cannot migrate until the junctions or impurities are unpinned [40,41]. Especially in high defective metals, the pre-existing defects, such as vacancies and intersti-

tials, will cause jogs formation or the distortion of planes and further alter the deformation mechanisms [42,43]. Furthermore, grain rotation is a deformation mechanism related to GB annihilation, which is often observed to occur during plastic deformation. The coupling effect between grain rotation and GB migration can be particularly important to examine. More investigations should also be carried out in future work on various structures of GBs under different loading conditions.

5. Conclusions

In summary, atomic-scale annihilation mechanisms of LAGBs encountering neighboring GBs with applied shearing stress have been studied in Au tri-crystalline models using MD simulations. It is revealed that LAGB kept a consistent migration rate in the early stage. As the separation distance between the GBs decreases, the migration of the LAGB possessing higher mobility accelerates. The GBs are found to merge and finally annihilate through dislocation interpenetrating and interaction for LAGBs or absorption for HAGBs (Figure 5). LAGBs annihilated at neighboring GBs alter the GB network and contribute to grain coalescence. The motion and annihilation of GBs observed in our simulation are calling for experiments, such as TEM studies on GB annihilation. These findings may provide insights into the control of polycrystalline networks in nanocrystalline metals further assist the design of reliable metallic nanocomponents for high-performance nanodevices.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/met12030451/s1>, Figure S1: Schematic showing the set-up and loading profile.; Table S1: Migration distance of GB1 and separation distance between two GBs versus shear displacement for 10° LAGB annihilated at 10° LAGB; Table S2: Migration distance of GB1 and separation distance between two GBs versus shear displacement for 10° LAGB annihilated at −10° LAGB; Table S3: Migration distance of GB1 and separation distance between two GBs versus shear displacement for 10° LAGB annihilated at 30° HAGB; Table S4: Migration distance of GB1 and separation distance between two GBs versus shear displacement for 10° LAGB annihilated at −30° HAGB;

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