8.5 DYNAMICS OF DEFECT-LOADED GRAIN BOUNDARIES UNDER SHEAR DEFORMATION IN α-Fe — L. Yang, F. Gao, H. L. Heinisch, and R. J. Kurtz (Pacific Northwest National Laboratory)

OBJECTIVE

To simulate the dynamics of defect-loaded grain boundaries (GBs) in bcc Fe under shear deformation using molecular dynamics, to study the effects of loaded defects on the motion of grain boundaries, and to explore the interaction of interstitial-loaded GBs with vacancies.

SUMMARY

The defects produced in collision cascades will interact with microstructural features in materials, such as GBs and dislocations. The coupled motion of GBs under stress has been widely observed in simulations and experiments. Two symmetric tilt GBs with a common <110> tilt axis (Σ3 and Σ11) in bcc iron are used to investigate the coupled motion of GBs under shear deformation. Also, we have explored the effect of self-interstitial atoms (SIAs) loading on the GB motion, with different concentrations of interstitials randomly inserted around the GB plane. The simulation results show that the interstitial loading reduces the critical stress of the GB coupled motion for the Σ3 GB. Furthermore, the interstitials and vacancies are inserted randomly at the GB plane and at a distance of 1 nm away from the GB plane, respectively, to understand the self-healing mechanism of GBs under stress. The behavior of the defect-loaded GBs depends on the GB structure. The loaded interstitials in the Σ3 GB easily form <111> interstitial clusters that do not move along with the GB. The vacancies in the Σ3 GB impede the GB motion. However, the interstitials move along with the Σ11 GB and annihilate with vacancies when the GB moves into the vacancy-rich region, leading to the self-healing and damage recovery of the Σ11 GB.

PROGRESS AND STATUS

Introduction

It is known that grain boundaries (GBs) play a significant role in the microstructure evolution and mechanical properties of materials. In irradiation environments, the defects produced in the collision cascades, such as self-interstitial atoms and vacancies, will interact with microstructural features, such as GBs and dislocation cores [1, 2]. Bai et al. observed that the interstitials produced by nearby collision cascades tend to be absorbed into GBs in copper [1], and Vorovikov et al. proposed a radiation damage healing mechanism due to GB motion under stress in tungsten [2]. In general, four typical motions of GBs, in response to shear stresses, are found in many materials, including 1) normal motion (i.e., the process by which a GB moves in its normal direction), 2) relative translation of the grains parallel to the GB plane coupled to normal GB motion (so called coupled motion of GB), 3) relative rigid body translation of the grains along the GB by sliding, and 4) grain rotations [3]. Ferritic steels and alloys are widely used for structural materials in current nuclear fission reactors, and they are proposed as

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candidate materials for plasma facing first wall structural materials in future fusion energy facilities [4]. Campana et al., simulated the influence of displacement cascades on GB structures and their stability in bcc Fe, and found that a cascade near a GB can significantly reduce the critical stress for shearing or migration of the GB [5]. Here, the coupled motion of two tilt GBs in bcc iron with different concentrations of defects are investigated under a shear deformation that is applied parallel to the GB plane and perpendicular to the tilt axis. Also, we have investigated the detailed mechanism for an interstitial-loaded GB to annihilate with vacancies when the GB moves into a vacancy-rich region.

Simulation Methods

Two symmetric title GBs with a common <110> tilt axis (Σ3 and Σ11) are used to investigate the coupled motion of GBs under shear deformation. The simulation cell sizes of Σ3 and Σ11 are 84.20Å × 140.00Å × 80.84Å with 80,240 Fe atoms and 47.5356 Å ×140.00 Å ×40.54Å with 22,600 Fe atoms, respectively. Periodic boundary conditions are imposed along the x and z directions, but fixed boundary conditions are applied along the y direction, where the x, y and z represent the [1-11], [-112] and [-1-10] directions in the Σ3 GB model, and [1-13], [-332] and [-1-10] directions in the Σ11 GB model.

The NVT (constant number of atoms, volume and temperature) ensemble is applied in the present simulations with a time step of 1 fs. To study the effects of loading self-interstitial atoms (SIAs), different concentrations of interstitials are inserted randomly around the GB plane. After the interstitials are inserted, the configuration is quenched to 0 K, followed by a temperature rescaling to the desired temperature for 50 ps. Then, the system is driven by applying a velocity V=1.0 m/s to the atoms in the uppermost region at a given temperature. Temperatures of 0, 100 and 300 K are considered for the Σ3 GB. The corresponding shear stress is calculated according to the method in Ref. 6. The orientation and identification of specific regions of the simulation cell are shown in Fig. 1. The upper part B is used to control the deformation of the sample, where the atoms are displaced along the x direction by a constant increment at each time step, but they are free to move in the yz plane. The atoms in region F are rigidly fixed in their original positions, whereas the atoms in region T are used to control temperature by performing a velocity rescaling on the atoms every 100 time steps according to the difference between the current temperature and the desired temperature.

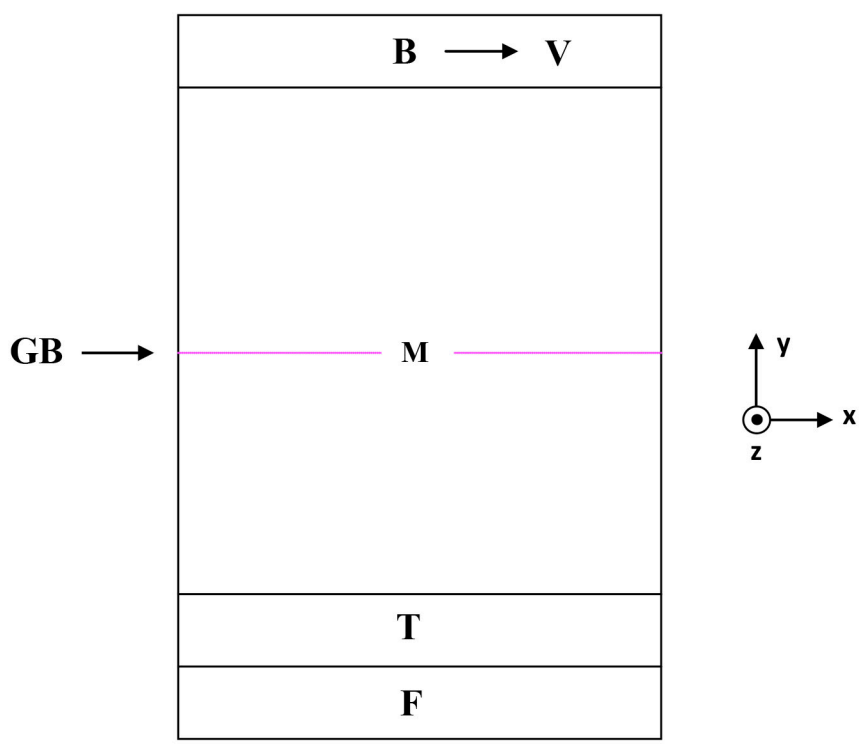

Figure 1. Geometry of the simulation box.

The atoms in the middle region M are free to move. The interstitial concentrations of 10%, 30%, 50%, 70% and 100% are the ratios of the number of interstitial atoms to that of Fe atoms on the GB plane in the Σ3 and Σ11 GBs. The critical stress is averaged by the each critical stress during the 1.0 ns simulation in the GBs. In order to understand the self-healing mechanism in bcc Fe under stress, the interstitials are inserted randomly around the GB plane, and the same amount of vacancies is introduced synchronously at a distance of 1.0 nm away from the GB plane.

Results and Discussion

The motion of the Σ3 and Σ11 GBs without defects under shear deformation was simulated at 0, 100 and 300 K. A coupled GB motion is observed in the two GBs when applying shear deformation along the x direction. After adding the shear deformation, the GB becomes mechanically unstable and jumps to a new position at the critical stress. The shear velocity (*V*) applied to the B region was tested in the Σ3 GB at 300 K, and it was determined that the critical stress required for migration of the GB depends only slightly on the velocity when *V* is varied from 0.1 m/s to 10 m/s, but the GB migration velocity normal to the GB plane is proportional to V. Thus, the velocity of shear deformation of 1.0 m/s was considered in the following studies.

The coupled GB motion is significantly affected by the loaded SIAs. The critical stress at three temperatures for the Σ3 GB as a function of SIA concentration is presented in Fig. 2. During application of the shear deformation, the SIAs migrate easily along the <111> direction, especially at 300 K, and this leads to the formation of <111> clusters. When the GB migrates along the –y direction, the applied stress enhances the motion of the SIA clusters along the x direction (<111>), but they seldom migrate along with the GB. As expected, the critical stress decreases with increasing temperature for a given interstitial concentration. For the three temperatures studied, the critical stress decreases with the loaded SIAs at the concentrations of 10% and 30%, which is due to the fact that the SIAs enhance the GB motion. The critical stress is the lowest at an SIA concentration of 30 %. However, at a concentration of 50% or larger the critical stress increases with increasing SIAs from 30% to 100%. It is found that the SIAs form an extra atomic layer parallel to the GB at a concentration of 100%, although it is not a perfect atomic layer. The critical stress at 100% concentration is lower than the perfect GB, which is due to the fact that the inserted SIAs at this concentration do not form a perfect atomic layer, and some of them are still in interstitial positions. The simulations for the Σ11 GB are now in progress.

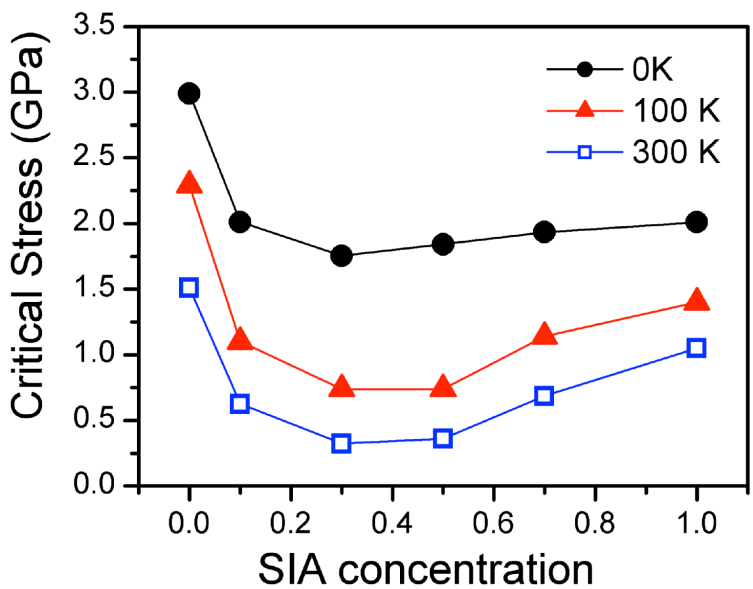

Figure 2. Average critical stress versus the inserted SIA concentration in the Σ3 GB at different temperatures.

Under irradiation, many interstitials created during collision cascades can be absorbed by nearby GBs, leaving the slower vacancies behind in the bulk. To understand the interaction of the interstitial loaded GBs with vacancies, a 10 % concentration of interstitials are inserted randomly around the GB plane and the same amount of vacancies is introduced synchronously at 1.0 nm away from the GB plane. Fig. 3 shows several snapshots of the Σ3 GB configuration simulated at 300 K. It is of interest to note that most of the inserted interstitial atoms accumulate to form <111> clusters during the applied shear deformation, and these clusters can migrate along the <111> direction. When the GB moves toward the vacancy-rich region, only a few Fe atoms migrate to and combine with the vacancies, but the SIA clusters are left behind in the bulk, as shown in the snapshot at 0.6 ns in Fig. 3. Once the GB moves into the vacancy-rich layer, the vacancies are absorbed by the GB, which impedes the GB motion somewhat. Only 8.8% inserted SIAs recombine with vacancies after the GB plane breaks through the layer with vacancies, but the rest of the SIAs form clusters and remain behind in the bulk, as shown in the snapshot at 1.0 ns.

Similar simulations have been performed in the Σ11 GB. The interstitial atoms at a concentration of 20% are loaded into the GB at 300 K. The motion of the interstitials is significantly different from that in the Σ3 GB. Fig. 4 shows several snapshots of the Σ11 GB configuration simulated. It is found that the coupled GB motion in the Σ11 GB is more favorable than in the Σ3 GB. Moreover, the interstitial atoms migrate along with the GB (see Fig. 4 at 0.2 ns). The snapshot at 0.5 ns illustrates that the interstitial atoms almost recombine with the vacancies when the GB moves into the vacancy-rich layer. After the GB sweeps off vacancies in the layer, the atomic configuration almost recovers to a perfect GB structure, except for a few interstitials at the GB plane. This result exhibits a self-healing mechanism in the Σ11 GB under stress, which is different to that in the Σ3 GB. The difference response of the two GBs to defects may be attributed to the different GB structures.

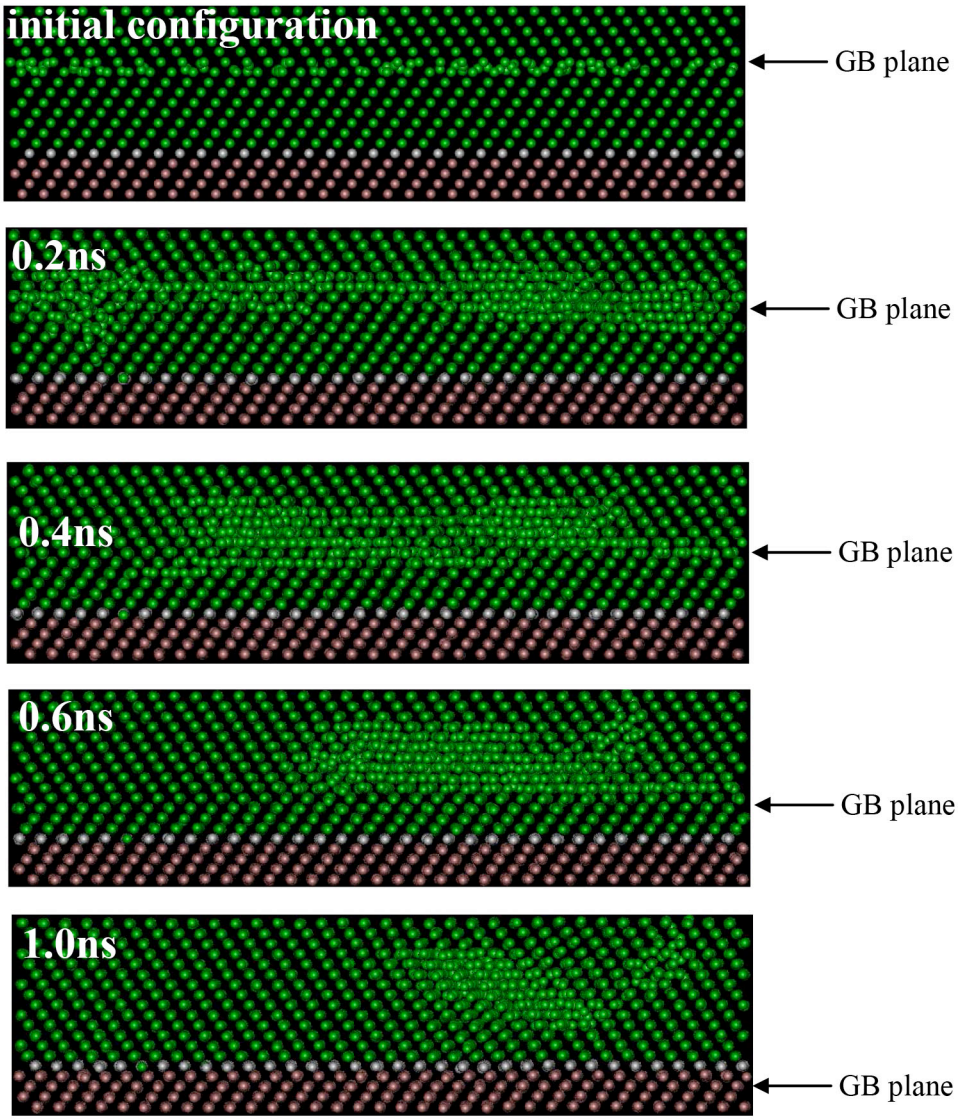

Figure 3. Snapshots of atomic configurations of the Σ3 GB with 10% SIAs and 10% vacancies at 300 K, where the SIAs are originally distributed near the GB plane and vacancies are located on the layer with white spheres.

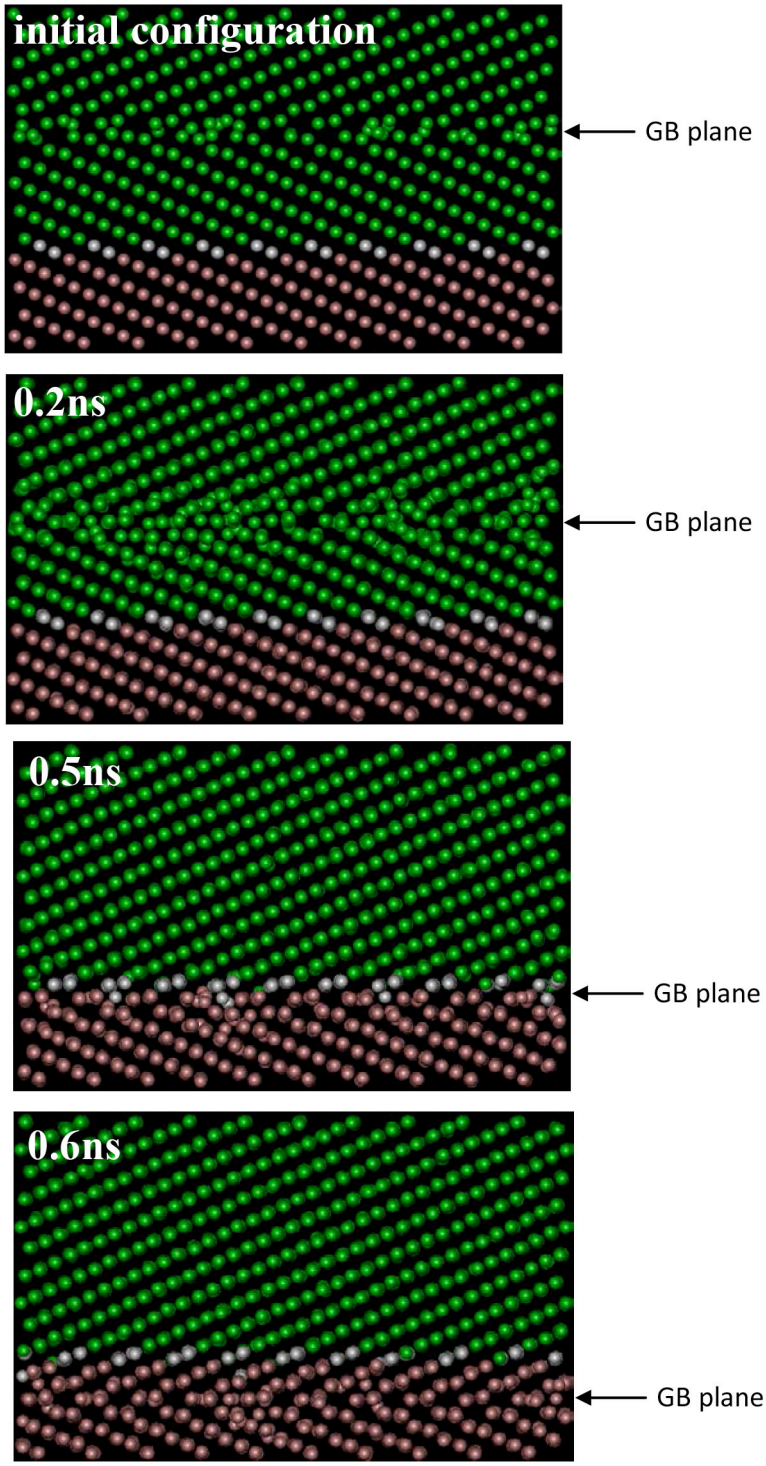

Figure 4. Snapshots of atomic configurations of the Σ11 GB with 20% SIAs and 20% vacancies at 300 K, where the SIAs are originally distributed near the GB plane and vacancies are located on the layer with white spheres.

SUMMARY

The interstitial loading reduces the critical stress of the GB coupled motion in the Σ3 GB of bcc Fe. The behavior of the defects in the GBs depends on the GB structure. The interstitials loaded into the Σ3 GB easily form <111> clusters that remain behind in the bulk when the GB migrates along the direction perpendicular to the GB plane. The vacancies in the Σ3 GB impede the GB coupled motion. However, the loaded interstitials can move along with the Σ11 GB and combine with the vacancies, leading to defect recovery and the self-healing of radiation damage. The self-healing phenomenon is observed only in the Σ11 GB.

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