8.3 Dynamics of Helium-Loaded Grain Boundaries under Shear Deformation in α-Fe —

F. Gao, L. Yang, H. L. Heinisch and R. J. Kurtz (Pacific Northwest National Laboratory)

OBJECTIVE

To simulate the motion and behavior of helium-loaded grain boundaries (GBs) in bcc Fe under shear deformation using the molecular dynamics simulation method. Here, we report preliminary results on the effects of helium on coupled migration and relative translation of a S3 GB at 300 K.

SUMMARY

Helium produced in the fusion nuclear environment will interact with microstructural features in materials, such as GBs and dislocations. At elevated temperatures helium at GBs can significantly influence creep-rupture properties by enhancing cavity formation and lowering GB cohesive energy. Grain boundary sliding can lead to stress concentrations at GB triple junctions and hard precipitates in the GB plane that may be sufficient to nucleate cavities. Here we explore the effects of helium on coupled GB migration and sliding under an applied shear stress. The Σ3 symmetric tilt GB with a <110> rotation axis in bcc iron was selected for study. The method for exploring helium effects on GB motion involved randomly inserting different concentrations of helium atoms around the GB plane and then applying a shear stress parallel to the GB plane at 300 K. We reported previously [1] that, in the absence of helium, the critical stress to induce coupled GB migration and sliding occurred at 300 K was 1.5 GPa. The current simulations show that when helium is present the critical stress for coupled GB motion, and the GB migration velocity are both reduced. When the GB helium concentration is low, most single helium atoms and small helium clusters migrate along with the GB. However, at high helium concentrations clusters easily form that remain behind in the bulk when the GB migrates away from its original position.

PROGRESS AND STATUS

Introduction

The behavior of He in Fe has been investigated widely [2-7], because in the fusion reactor environment high levels of insoluble He is generated in steels due to nuclear (n,α) transmutation reactions. Experimental results and atomistic calculations demonstrate that grain boundaries (GBs) act as sinks to trap He atoms in α-Fe. It is known that GBs play a significant role in the microstructure evolution and mechanical properties of materials. The nucleation of He bubbles at GBs in a ternary (Fe-15Cr-15Ni) austenitic steel after He implantation was investigated by Lane and Goodhew [2] using transmission electron microscopy (TEM), while Randle [3] investigated the interaction mechanisms of He bubbles with GBs in an austenitic steel using TEM. Dynamical interaction of He bubbles with GBs in Fe and Fe-9Cr was also studied by *in situ* electron microscopy and thermal desorption spectroscopy (TDS) [4]. In addition, the molecular dynamics (MD) method has been extensively employed to study the atomic-level processes of He behavior at GBs in bcc Fe. We have previously studied the diffusion mechanisms of He interstitials and di-He clusters at GBs in α-Fe using MD simulations [5].

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Of the four typical motions of GBs in response to shear stresses [7] it is the relative translation of the grains parallel to the GB plane (i.e., sliding) coupled with migration normal to the GB plane that we focus on in this study. The combination of GB sliding and migration is referred to as coupled GB motion in this report. In our previous work, the coupled motion of two tilt GBs (Σ3 and Σ11) in bcc iron with different concentrations of vacancy and self-interstitial point defects was investigated under a shear stress applied parallel to the GB plane and perpendicular to the tilt axis [1]. We also investigated the detailed mechanisms for a self-interstitial atom (SIA) loaded GB to annihilate with vacancies when the GB moves into a vacancy-rich region. We found that the SIA loading reduced the critical stress for coupled GB motion in a Σ3 GB [1]. The behavior of the point defect loaded GB depended on GB structure. The interstitials in the Σ3 GB easily formed <111> clusters that remained behind in the bulk when the GB migrated. Vacancies in the Σ3 GB impeded coupled GB motion. In contrast, interstitials were found to move along with the Σ11 GB and recombine with nearby vacancies, leading to defect recovery and healing of radiation damage. It should be noted that this healing phenomenon was observed only in the Σ11 GB. In the present work, the effects of He on the motion of GBs under shear deformation in bcc Fe is studied at room temperature. The behavior of helium in the GB is further analyzed.

Simulation Methods

Details of the simulation methods were reported previously [1]. Briefly, the simulation cell size for the Σ3 GB was 84.20 Å × 140.00 Å × 80.84 Å with 80,240 Fe atoms. Periodic boundary conditions were imposed along the x and z directions, which were parallel to the GB plane. Fixed boundary conditions were applied along the y direction, which was normal to the GB plane. The x, y and z axes in the model correspond to the [1-11], [-112] and [-1-10] directions, respectively in crystal coordinates.

The NVT (constant number of atoms, volume and temperature) ensemble was used in the present simulations with a time step of 1 fs. To study the effects of He, different concentrations of interstitial He were inserted randomly within the GB plane. After the He atoms were inserted, the system was quenched to 0 K, followed by a temperature rescaling to 300 K for 50 ps. Then, applying a shear stress to selected atoms in the model drove the loaded GB. The orientation and identification of the specific regions of the simulation cell are shown in Reference 1. Helium concentrations of 5%, 10%, 20%, and 30% (the number He atoms were 34, 68, 136 and 204, respectively) were investigated. The percentage of He atoms was taken as a fraction of the Fe atoms on the GB plane.

Results and Discussion

Coupled GB motion is observed when shear stress is applied along the x direction. Once the applied shear stress is increased to a critical value, the GB becomes mechanically unstable and migrates to a new position. Figure 1 shows several snapshots of the Σ3 GB with a 5% He concentration. It is of interest to note that some inserted interstitial He atoms accumulate to form small clusters after application of the shear stress. When the GB migrates in the –y direction, most single He atoms and small He clusters move along with the GB. This result is probably due to binding of He to the GB, even though that binding is relatively weak for this GB. However, in our previous work, we found that SIAs migrate easily along the <111> direction and form <111> clusters at 300 K [1]. When the GB migrates in the –y direction, the applied stress

enhances the motion of the SIA clusters along the x direction (<111>), but they seldom migrate with the GB. The present work suggests that He affects coupled GB motion. After applying a shear stress for 0.7 ns, the GB has migrated 7 atomic layers in the –y direction, which is smaller than the 9 atomic layers for the same system without He under the same simulation conditions.

Simulations of higher He concentrations (10%, 20%, 30%) were also performed. Figure 2 shows several snapshots of the Σ3 GB with 20% He. Initially, the He atoms are randomly distributed on the GB plane, as shown at 0.0 ns in Figure 2. After applying the shear stress, most He atoms have aggregated to form clusters near the GB plane within 0.2 ns. With increasing simulation time, we found that some large He clusters formed near the GB plane. For example, the largest He cluster consists of 17 He atoms at 0.7 ns. When the GB moves in the –y direction, only a few He clusters migrate along with it. Most He clusters remain behind in the bulk. This is shown in the snapshot at 0.7 ns in Figure 2, where the GB plane has migrated 6 atomic layers along the –y direction. From these results, along with those at the 5% He concentration, it is noted that the GB migration velocity is impeded by the He atoms and decreases with increasing He concentration. Similar to our previous observation [1], a large number of SIAs are emitted from these large He clusters. These SIAs distribute at the peripheries of the He-V clusters, and form interstitial loops.

The critical shear stress causing coupled GB motion is significantly reduced by the presence of He. The shear stress as a function of time for different helium concentrations at 300 K in the Σ3 GB is presented in Figure 3. It is of great interest that the critical stress decreases with increasing He concentration, and the GB migration velocity of the system with He atoms also decreases with increasing He concentration, as described above. For a system without He, the GB plane migrates three atomic layers but, for a system with He, the GB moves only one or two layers. This may be due to the draggling effect of the He clusters, reducing the ability for coupled motion of GBs.

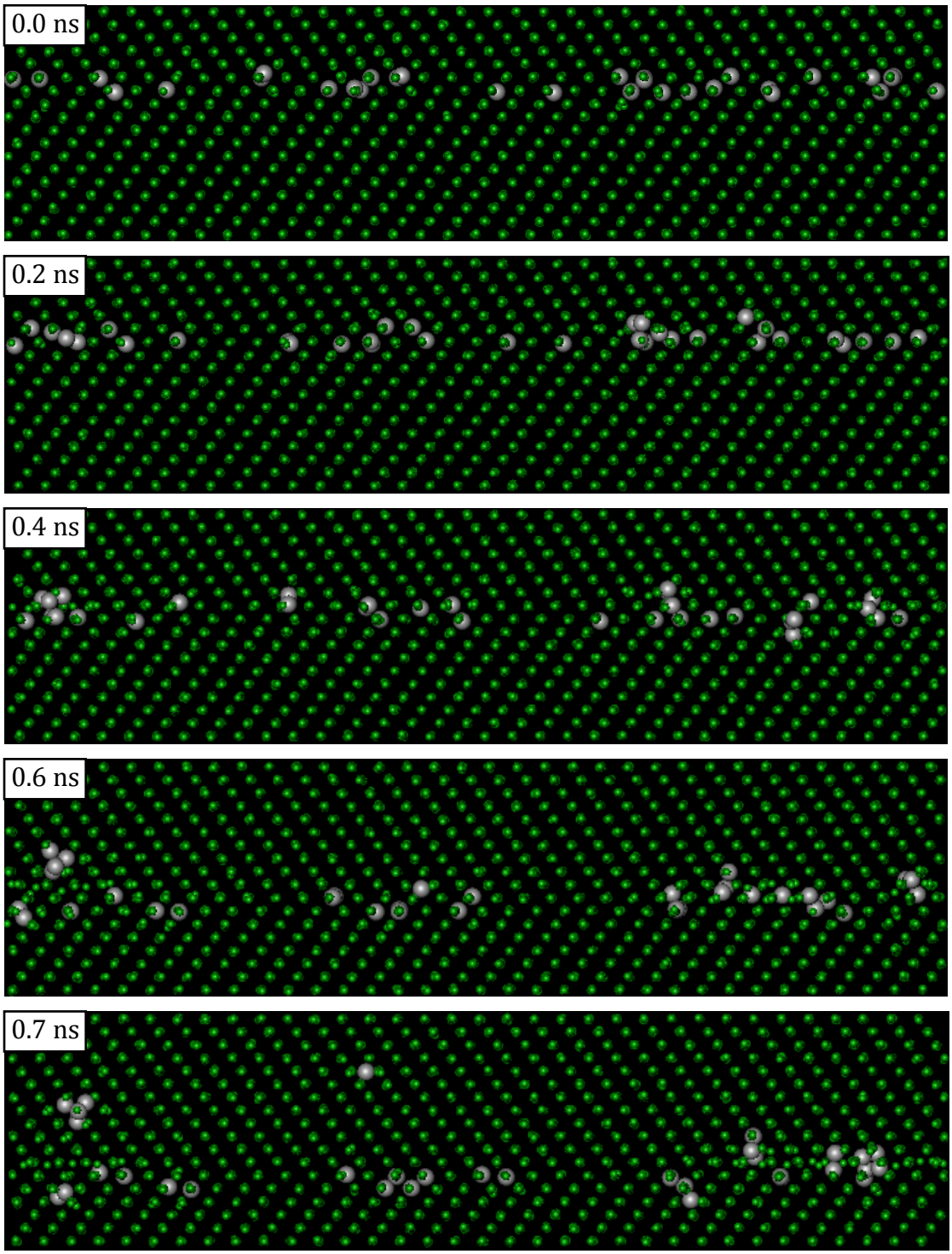

Figure 1. Several snapshots showing Σ3 GB migration at 300 K for a 5% He concentration.

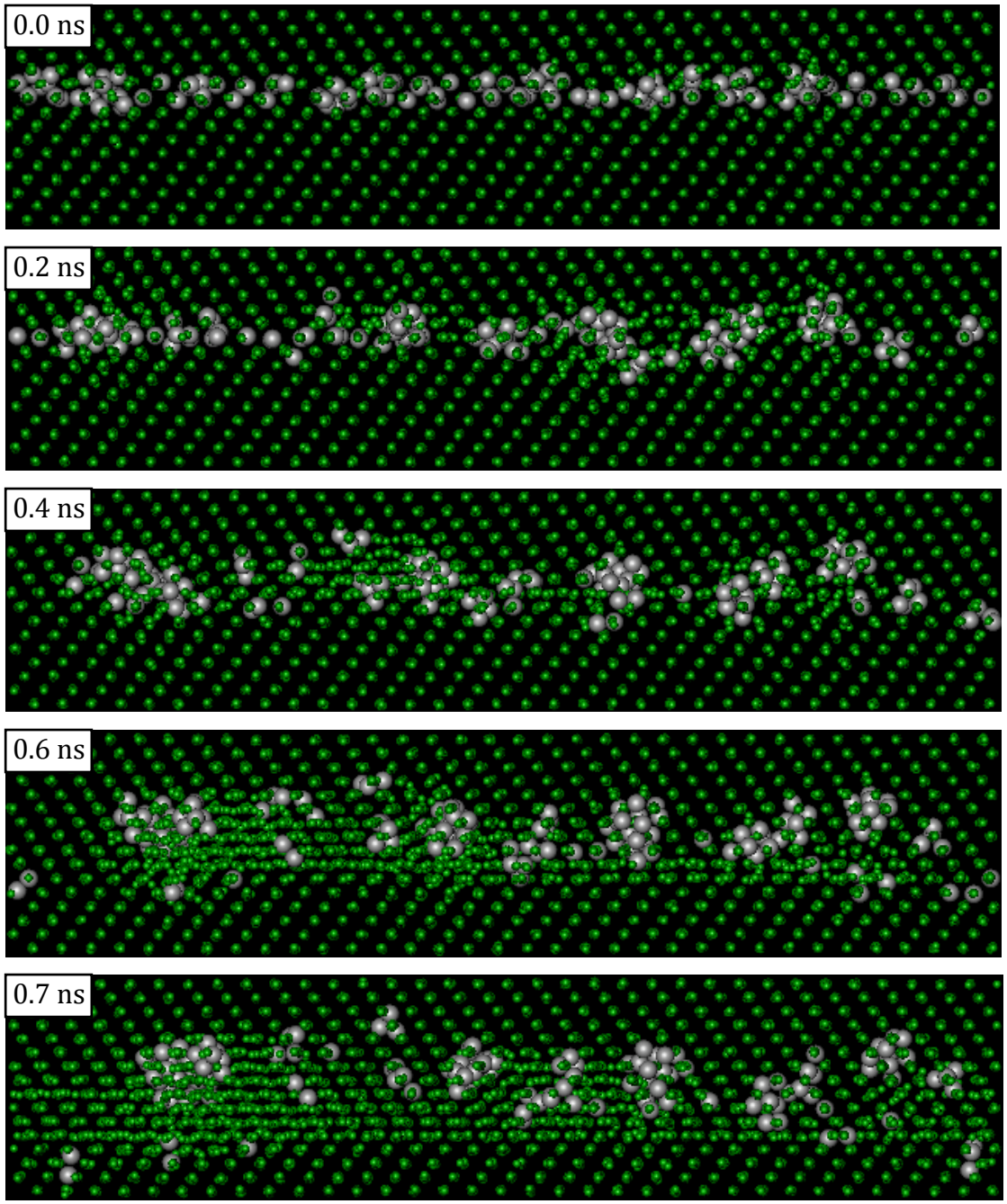

Figure 2. Several snapshots showing Σ3 GB migration at 300 K for a 20% He concentration.

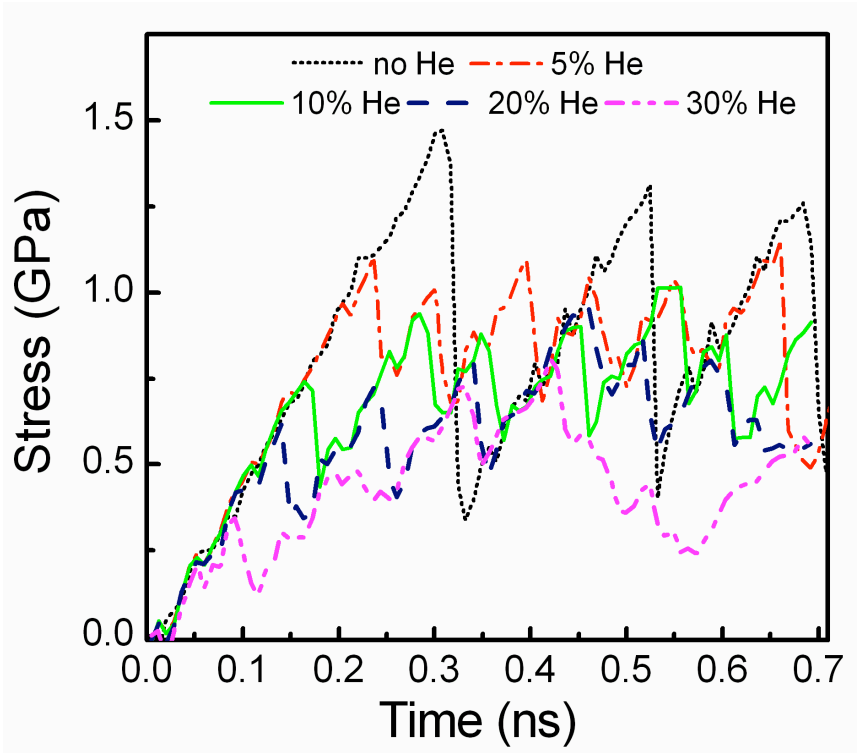

Figure 3. Shear stress as a function of simulation time for different He concentrations at 300 K in the Σ3 GB.

SUMMARY

Helium atoms inserted randomly into a Σ3 GB were found to affect the coupled motion of that boundary. At a 5% He concentration, most single He atoms and small He clusters migrated along with the GB. However, at higher concentrations He atoms easily form clusters that spontaneously emit SIAs. These He-V clusters remain behind in the bulk when the GB migrates normal to the GB plane. Interstitial He reduced the critical stress for coupled motion of the Σ3 GB in Fe at 300 K.

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