8.2 NUCLEATION OF HE BUBBLES AT A LOW-ANGLE GRAIN BOUNDARY IN α-FE —

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OBJECTIVE

To study the nucleation of He bubbles at the Σ73b low-angle grain boundary in α-Fe using the newly developed Fe-He potential and to compare the results with those previously obtained for the Σ3 GB.

SUMMARY

In a fusion reactor environment He is produced at high rates in steels by nuclear (n, α) transmutation reactions. Understanding the deleterious effects of He, especially the nucleation of He bubbles at GBs in steels, is one of the most important issues in nuclear fusion technology. The accumulation of He atoms and nucleation of He bubbles in the Σ3 <110> {112} GB in α-Fe have been previously studied [1] using molecular dynamics with our newly developed Fe-He potential [2]. It was found that the accumulation of He atoms, the formation of He bubbles, and the evolution of the GB structure all depend on the local He concentration and temperature. In order to broaden understanding of the effects of GB structure on the accumulation of He atoms and the nucleation of He bubbles in α-Fe the interaction of He with the ∑73b<110>{661} GB in α-Fe is currently being investigated using the same methodology as that used for our earlier studies of He in the Σ3 GB. It is found that in the ∑73b GB at low He concentrations most He atoms migrate to the GB dislocations in a very short time, and they can move along the GB dislocation lines at high temperatures. He atoms seldom congregate to form clusters in the ∑73b GB, even at 800 K, compared to clustering in the Σ3 GB. Emission of an Fe self-interstitial atom (SIA) caused by a single He is observed at 300 K, while it occurs for the clusters containing at least four He atoms at 600 K in the Σ3 GB and higher temperatures. At a local He concentration of 5 % (as defined within 20 Å from the GB), a large number of He clusters are formed. The nucleation of He bubbles is more significant at higher temperatures in the ∑73b GB, while it depends only slightly on the temperature in the Σ3 GB. Most of the He clusters are distributed along the GB dislocation lines in the ∑73b GB at low temperatures, forming platelet like configurations. At a 10 % local He concentration, a large number of SIAs are created, which results in the propagation of GB dislocations along the <112-1> direction.

PROGRESS AND STATUS

Introduction

The effect of helium on first wall structural materials has been widely recognized as one of the most crucial material issues in nuclear fusion reactors, because the synergistic interaction of large amounts of helium with the existing and radiation-induced defects and microstructures in materials can significantly degrade their mechanical properties. Multi-scale modeling, especially including the atomic scale, provides a basis to obtain insight into general understanding of the complex radiation damage process. As an important part of this modeling, molecular dynamics (MD) methods, including improved interatomic potentials, have been widely employed to study the atomic-level processes of defects controlling microstructural evolution in advanced ferritic steels.

The new interatomic potential for Fe-He interactions [2] used in the present studies is based on the electronic hybridization between Fe *d*-electrons and He *s*-electrons. This potential was used previously to investigate the nucleation of He clusters and bubbles, the emission of SIAs from the He clusters, and the formation of dislocation loops in bulk α-Fe, as well as to study the effects of these phenomena on microstructural changes at 800 K [3]. That investigation found that a cluster of four He atoms is able to push an iron atom into an interstitial position, creating a He_4V cluster and a SIA. Small He clusters and SIA can migrate in the matrix, but He-vacancy (He-V) clusters are immobile on accessible molecular dynamics time scales. At low He concentrations SIA clusters (or loops) are attached to He-V clusters, while at high He concentrations He-V cluster-loop complexes with more than one He-V cluster are formed. Also, the accumulation of He atoms and nucleation of He bubbles in Σ3 <110> {112} GB of α-Fe have been previously studied using molecular dynamics [1], which provides a good reference to compare with the current study of the accumulation of He atoms and the nucleation of He bubbles in the ∑73b<110>{661} GB.

Simulation Methods

In the present simulations we investigate the nucleation and formation of He clusters in the ∑73b <110> {661} low angle GB in α-Fe, which contains intrinsic GB dislocations. The model consists of 48,000 Fe atoms in a block of size 103.50 Å × 70.00 Å × 80.76 Å. 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 <112-1>, <-616> and <101> directions in the GB model, respectively, as indicated in Figure 1. The interatomic potentials for Fe-Fe, Fe-He and He-He interactions are the same as those used in Ref. 2

The NVT (constant number of atoms, volume and temperature) ensemble is chosen in the present simulations with a time step of 1 fs. Initially the simulation cell is quenched to 0 K at constant pressure with the molecular statics (MS) approach, and then the stress field of the Σ73b GB is determined. It is found that the stress is distributed within about 20 Å of the GB core, with a maximum value of about 10 GPa. He atoms are inserted at random positions within the stressed region near the GB at local He concentrations of 1 % (72 He atoms), 5 % (359 He atoms) and 10 % (718 He atoms), which are the ratios of the number of He atoms to those Fe atoms within the considered stressed region. After He insertion, the cell was again quenched to 0 K to obtain a minimum energy configuration, followed by a temperature rescaling to the required temperature and relaxation for 1 ns. Three temperatures of 300 K, 600K and 800 K are considered.

RESULTS AND DISCUSSION

After randomly inserting 1 % He into the region within 20 Å of the ∑73b GB core, a simulation was performed at 300 K. Within a very short time almost all the He atoms aggregate at the ∑73b GB dislocations, but few He clusters are formed in the GB, especially as compared to He clustering in the Σ3 GB. Some He atoms can move along the ∑73b GB dislocation lines at high temperatures, and clustering of He up to only He_3 is observed to form even at 800 K. In contrast, a few He_6 clusters are formed in the Σ3 GB, as shown in Figure 1, where the upper image shows a view parallel to the tilt axis and the lower image shows a view normal to the GB plane. This suggests that the probability of forming He clusters may be limited in the GBs with higher excess volumes: these calculations are in progress. Emission of a SIA by a single He replacing an Fe atom is observed at 300 K, but this is a rare event, while it occurs for the clusters with four He atoms at 600 K and higher temperatures in the Σ3 GB.

MD simulations of the Σ73b GB with a 5 % He concentration were performed for 1 ns. The final atomic configurations at 300 K and 800 K are shown in Figure 2, from which it is clearly seen that some large He clusers are formed, especially at the higher temperature. It is of interest to note that at 300 K almost all the He atoms are distributed along the GB dislocation lines and all He clusters exhibit longitudinal platelet like shapes along the dislocation lines. However, at 800 K more large He clusters are formed near the GB plane, and most of them have spherical shapes. During the simulations at 800 K, it is clearly seen that the He atoms in clusters accumulate into spherical shapes to minimize the surface energy of the clusters at high temperatures. A number of SIAs are emitted from the clusters, and they collect near the GB dislocation cores.

When the He concentration increases to10 %, He atoms rapidly diffuse to the GB plane at all temperatures considered, and they form many large He clusters with platelet-like structures. The sizes of the He clusters obviously increase with increasing temperature. Helium clusters are distributed almost uniformly near the GB at 600 K and higher temperatures, as shown in Figure 3. It is clear that most He clusters do not have spherical shapes, which is different from the clustering at the He concentration of 5 % (see Figure 2b), which may be associated with the smaller size of the clusters at low concentrations. A large number of SIAs are created by the nucleation of He bubbles. It is of interest to note that those SIAs prefer to aggregate at the dislocation cores in the GB, causing these dislocations to climb along the <112-1> direction (see insets I and II in Figure 3), and that the propagation is more significant at higher temperatures. This phenomenon is different from that in the Σ3 GB for the same He concentration, where the SIAs reconstruct to form an extra atomic layer above the original GB plane, leading to GB climb along the <-112> direction.

CONCLUSION

He accumulation and the nucleation of He clusters (bubbles) in S73b GBs in α-Fe are studied using molecular dynamics, and the results are compared with results previously obtained for the S3 GB. It is clear that the evolution of the GB configurations, the accumulation of He atoms and the nucleation of He bubbles all depend on the He concentration, temperatures and the GB configurations. At a 1% He concentration, most He atoms migrate to the GB dislocation lines in a very short time, but in the Σ73b GB they seldom congregate to form clusters, even at 800 K, especially as compared to those in Σ3 GB. At higher He concentrations a large number of He clusters are formed, and the nucleation of He bubble is more significant at higher temperatures in ∑73b GBs, while it slightly depends on the temperature in Σ3 GBs. Most of the He clusters are distributed along the GB dislocation lines in the ∑73b GB at low temperatures, forming platelet like structures. It is also observed that a large number of SIAs are emitted from the clusters at a 10 % He concentration, which results in the climb of the GB dislocations along the <112-1> direction.

REFERENCES

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[2] L. Yang, H. Q. Deng, F. Gao, H. L. Heinisch, R. J. Kurtz, S. Y. Hu, Y. L. Li, and X. T. Zu, submitted to *Nuclear Instruments and Methods B.*

[3] F. Gao, H. Q. Deng, H. L. Heinisch, and R. J. Kurtz, *J. Nucl. Mater.* **418** (2011) 115.

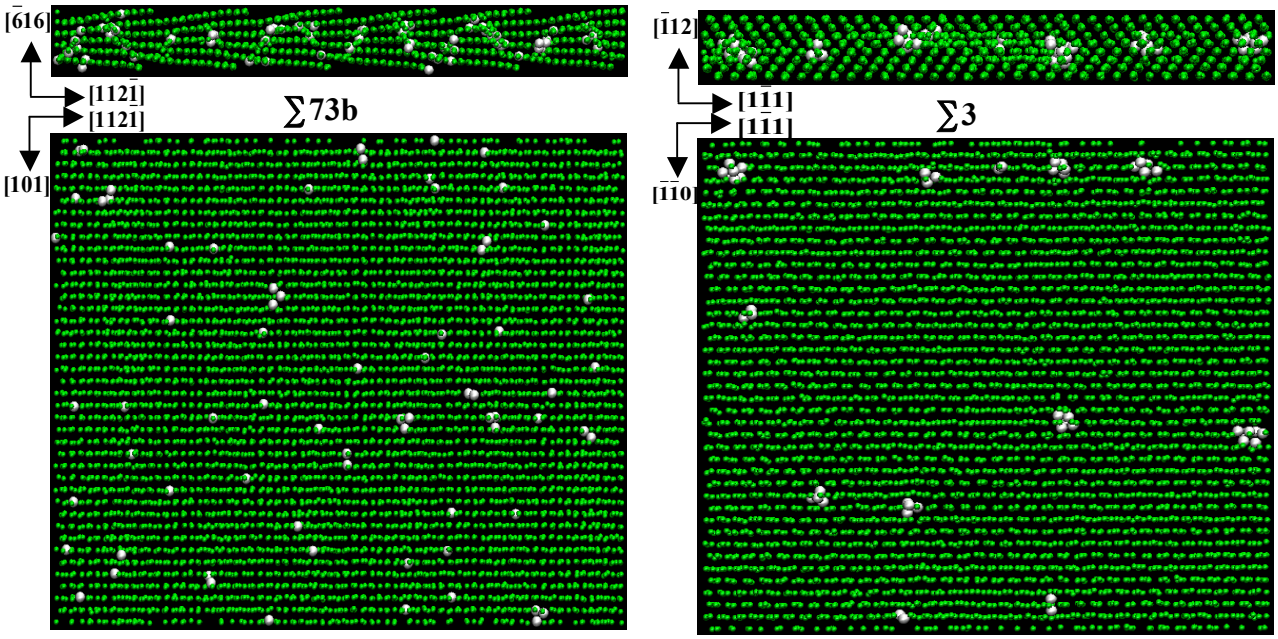

Figure 1. Final atomic configurations with a 1 % He concentration at 800 K in α-Fe: (a) Σ73b GB and (b)Σ3 GB.

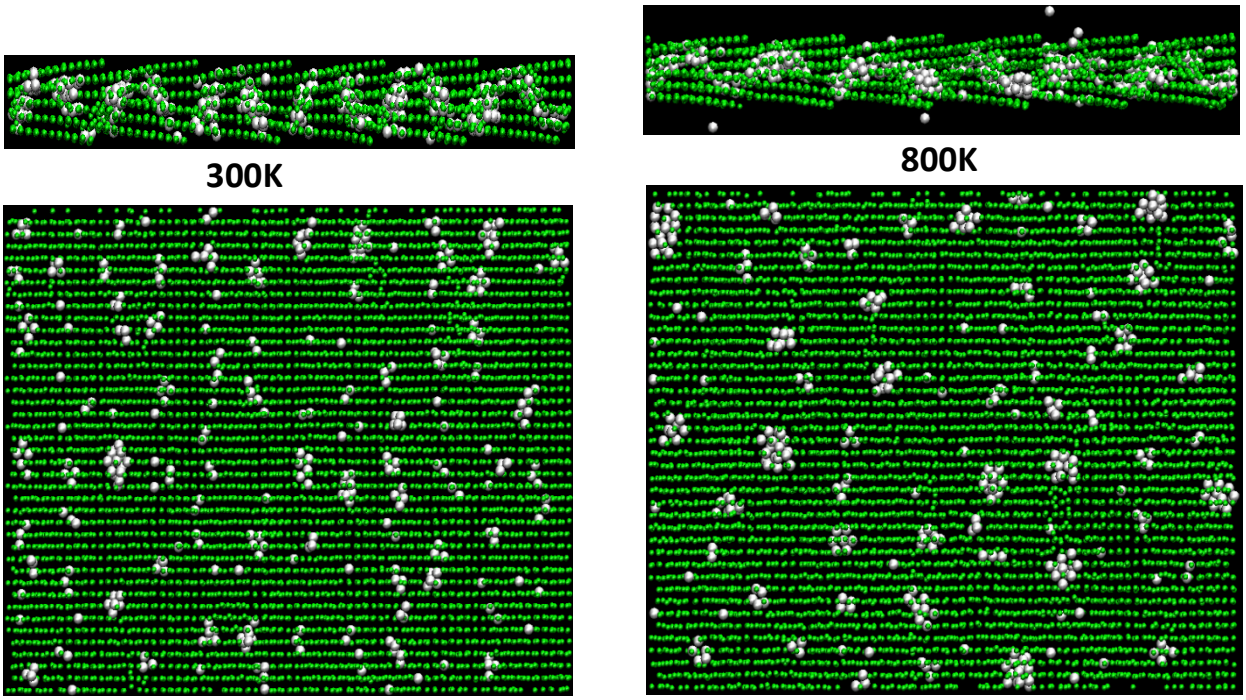

Figure 2. Final atomic configurations of Σ73b GB with a 5 % He concentration in α-Fe at: (a) 300 K and (b) 800 K.

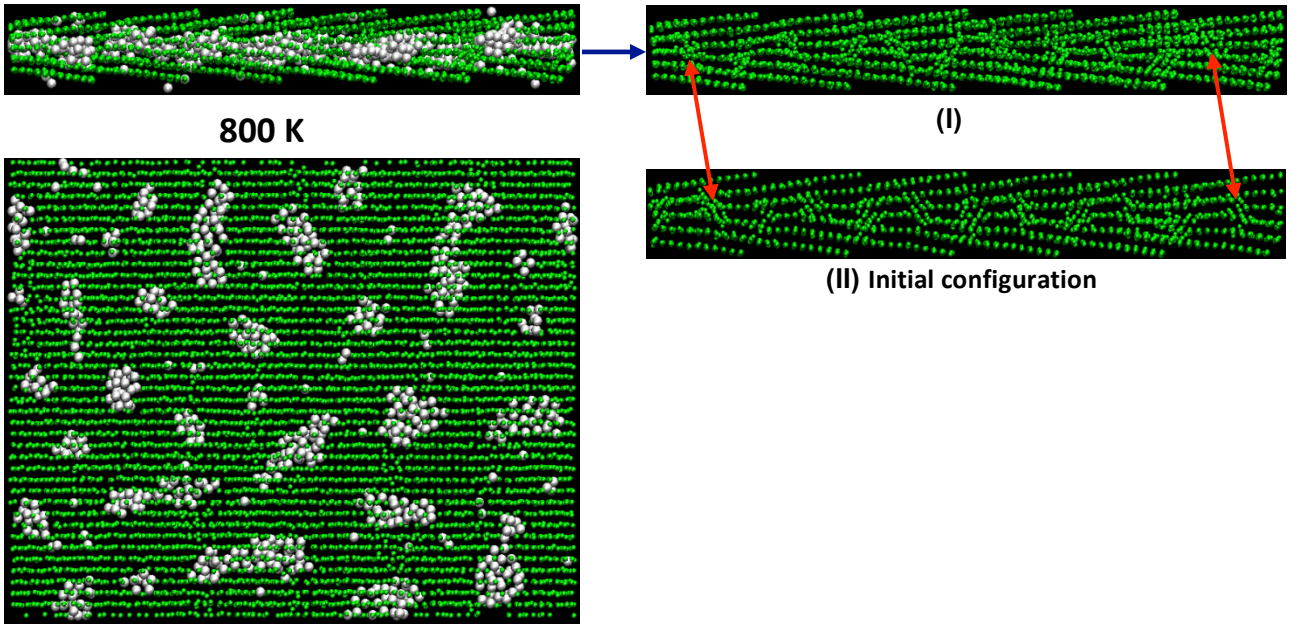

Figure 3. Final atomic configurations of Σ73b GB with a 10 % He concentration at 800 K in α-Fe. The He atoms are omitted from the inset figures I and II.