7.2 Atomistic Studies of Helium Bubble Nucleation at Grain Boundaries in α-Fe —

L. Yang, F. Gao, H. L. Heinisch and R. J. Kurtz (Pacific Northwest National Laboratory)[1]

OBJECTIVE

To simulate the nucleation and growth of He bubbles at grain boundaries (GBs) in α-Fe using the newly developed Fe-He potential and to study the evolution of the GB structures due to the accumulation of He atoms and the nucleation and growth of He bubbles.

SUMMARY

Experimental results and atomistic calculations demonstrate that GBs act as sinks to trap He atoms in α-Fe. The nucleation and growth of He bubbles at GBs are likely to determine the extent of embrittlement which is potentially one of the most serious material problems related to the development of fusion power. The nucleation of He bubbles in the bulk and at GBs in α-Fe have been previously studied [1-3] using molecular dynamics with our newly developed Fe-He potential [4]. It was found 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. In the bulk of α-Fe, the computational results showed that complexes consisting of a dislocation loop with helium-vacancy (He-V) clusters are formed at high He concentrations [2]. In order to understand the formation and evolution of interstitial dislocation loops due to the growth of He bubbles in the helium-rich vacancy-poor situation, the clustering of He and the growth of He bubbles at two GBs in α-Fe is currently being investigated. It has been found that within the S3 GB, when the size of a He cluster is large enough, a 1/2 <111> dislocation loop is formed, accompanied by the emission of the dislocation loop. However, in the S73b GB the sequential insertion of He atoms induces the emitted self-interstitial atoms (SIAs) to rearrange at the core of the inherent dislocation, leading to the propagation of the dislocation along the [-1 -1 12] direction. The small He bubbles form longitudinal shapes along the dislocation line in the S73 GB, a shape commonly observed at GBs in experiments.

PROGRESS AND STATUS

Introduction

It is well known that helium atoms are expected to be produced at a high rate by (n, α) transmutation reactions in a fusion reactor first wall under irradiation. Because of the extremely low solubility of He in materials, a high concentration of helium will tend to be trapped at defects, such as vacancies, dislocations, and grain boundaries (GBs), which leads to void swelling and produces low-temperature intergranular embrittlement, surface roughening, blistering, and premature creep rupture at high-temperatures. These phenomena can significantly degrade the mechanical properties of materials. Therefore, understanding of the He accumulation and the growth of He bubbles both in the bulk and GBs are of fundamental importance within a fusion reactor environment. Atomistic studies of the nucleation and growth of He bubbles within the Σ3 and Σ73b GBs in α-Fe are being performed. In the present simulations the pair interaction and

[1]This work was supported by the U.S. Department of Energy, Office of Fusion Energy Sciences. PNNL is operated by Battelle Memorial Institute for the U.S. DOE under Contract DE-AC-06-76RLO 1830.

the many-body function for Fe−Fe interactions are those of Ackland [5], while the pair potential for He−He interaction is the Aziz potential [6]. The new Fe−He potential developed at PNNL [4] is used to describe the Fe−He interaction. This set of potentials was used previously to investigate the nucleation of He clusters and bubbles in the bulk and at the GBs in α-Fe, and the formation and evolution of defects, as well as to study the effects of these phenomena on microstructural changes [3]. That investigation found 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. It is of interest to note that <100> dislocation loops are directly formed at the peripheries of these large He clusters in the Σ3 GB at 600 K and 800 K. At high He concentrations, the large number of SIAs that are emitted can rearrange to form an extra atomic plane within the Σ3 GB, resulting in the self healing of the deformation induced by He accumulation and the GB climbing along the [-112] direction. However, a large number of SIAs emitted by He atoms can cause the climb of the GB dislocations along the $[\bar{1}\bar{1}12]$ direction in the ∑73b GB, and the climb is more significant with increasing temperature. In the bulk, at low He concentrations SIA clusters (or the dislocation loops that are formed from the SIA clusters) 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. In the work mentioned above [2], He atoms were inserted at random positions within the bulk or the stressed region around the GB plane of α-Fe, mimicking the He accumulation at different concentrations. In the present work the nucleation and growth of small He bubbles and the formation and evolution of SIAs and dislocation loops are investigated at both the ∑3 and ∑73b GBs in α-Fe as He atoms are inserted one by one into each GB.

Simulation Methods

Two symmetric tilt GBs with a common <101> tilt axis (Σ3 and Σ73b) were created to investigate the nucleation and growth of small He bubbles in the GBs. The block sizes of the Σ3 and Σ73b GBs are 84.07Å × 79.00Å × 80.69Å and 103.50 Å × 70.00 Å × 80.76 Å, consisting of 45,560 and 48,000 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 the [1 12 -1], [-616] and [101] directions in the Σ73b GB model.

The NVT (constant number of atoms, volume and temperature) ensemble is chosen in the present simulations with a time step of 1 fs. He atoms are inserted one by one into the simulation boxes. After each helium atom insertion, the configuration is quenched to 0 K, followed by a temperature rescaling to 300 K and an additional 100 ps to anneal at the same temperature. For the insertion of the next He atom, the configuration is quenched back to 0 K, the temperature is rescaled to 300 K, and the simulation block is equilibrated for 100 ps. A similar procedure is repeated during the simulations.

Results and Discussion

The first He atom is inserted into a most favorable interstitial site in the GB plane. After inserting 4 He atoms in the ∑3 GB, the He cluster moves slightly away from the GB plane and a <111> crowdion SIA is created within the GB plane. The emitted SIA quickly migrates along the <111> direction within the GB plane during the annealing process because of its small migration energy (0.01 eV). After the ninth He is inserted, the displacements of the Fe atoms around the He cluster increase, leading to a few Fe atoms near the He cluster being displaced from their original sites along the <111> and <112> directions, which releases the pressure accumulated

during the insertion of He atoms. However, the maximal displacement of the Fe atoms around the He cluster is less than 1 Å. The insertion of the 11th He atom results in forming the second <111>crowdion SIA. The addition of the 13th He atom leads to the formation of the third <111> crowdion SIA, and most of the displaced Fe atoms around the He cluster return to their original positions. With further insertion of He atoms, more SIAs are formed, but all the SIAs are collected at the periphery of the He cluster.

It is of interest to note that after inserting 45 He atoms, a dislocation loop with a Burgers vector of b = 1/2<111> is clearly formed. Fig. 1 shows the structures and atomic configurations of the ∑3 GB in α-Fe before and after annealing for the 45 He atoms inserted.

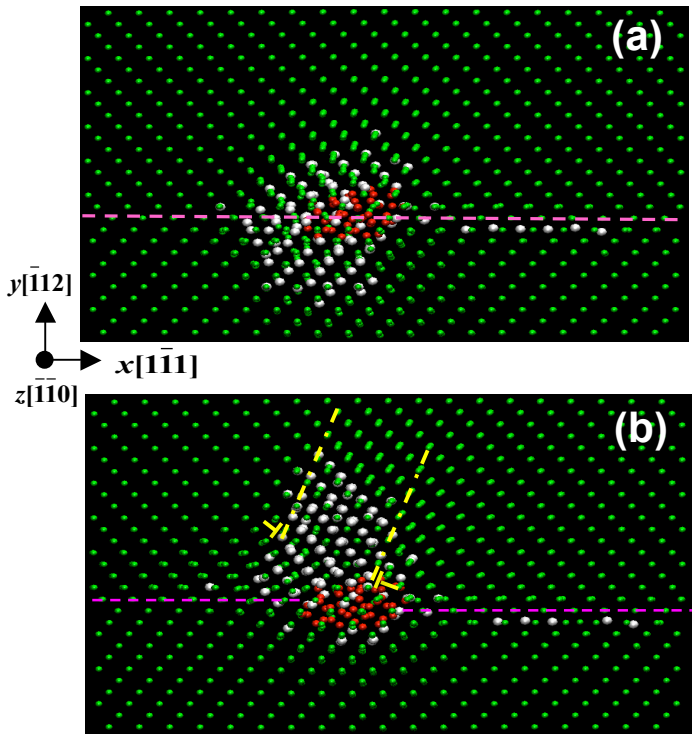

Fig. 1. Atomic configurations of the Σ3 GB together with the cluster of 45 He atoms in α-Fe: (a) before annealing and (b) after annealing 0.1ns at 300 K, where red spheres are He atoms, white spheres represent the Fe atoms with the stress of 8 GPa and larger, green spheres represent the Fe atoms with the stress of less than 8 GPa, purple dashed lines indicate the grain boundary plane.

It is clearly seen that the large number of SIAs formed at the periphery of the He cluster are distributed on both sides of the GB plane. However, during the annealing process, most SIAs move along the [-112] direction from the bottom of the GB plane to the top of GB plane after 27,000 MD steps. Within a short time (about 17 ps), a ***b*** = 1/2<111> dislocation loop is formed and attached to the He cluster on one side of the GB plane. Also, it can be seen that the GB plane on the right of the He cluster remains the same after the formation of the dislocation loop, but that on the left of the He cluster the GB climbs up one atomic layer along the [-112] direction.

This might be attributed to the interaction of the GB plane with the SIAs as they migrate through the GB plane. With further insertion of He atoms, the dislocation loop is observed to grow larger by collecting more SIAs. Finally, the dislocation loop with a total of 45 SIAs is emitted from the He bubble after inserting 97 He atoms.

In order to more generally understand the effects of GB structure on the growth of He bubbles and the formation of SIAs in α-Fe, the same approach is applied to study the nucleation and growth of He clusters or bubbles in a $\sum$73b<110>{661} GB. The nucleation and formation of He clusters and SIAs in the $\sum$73b GB is significantly different from that observed in the $\sum$3 GB, primarily because the $\sum$73b GB is a low angle GB containing intrinsic dislocations distributed along the [-1 -1 12] direction. The first He in the $\sum$73b GB is inserted in a most favorable interstitial site near the dislocation core, such that an Fe atom is pushed away from its lattice site and the He shares the lattice vacancy with the Fe atom, forming a Fe-He dumbbell along the <111> direction within the dislocation core. When the second, third and fourth He atoms are inserted, the Fe atoms near the He atoms are displaced slightly, but they are still associated with their sites. After the insertion of the 5th He atom, a second Fe is emitted from the He_5 cluster. It is of interest to note that the two SIAs prefer to distribute along the [-1 -1 12] direction within the dislocation core, evidently being attracted by the excess volume within the dislocation core. During further insertion of He atoms, more Fe atoms around the He cluster are pushed out from their lattice sites and aggregate at the dislocation core. Fig. 2 shows the configurations of the Σ73b GB projected on different planes, along with the cluster of 83 He atoms. It is clear that many SIAs are formed within the dislocation core, and they prefer staying within the core due to the strong interaction of the SIAs and the core.

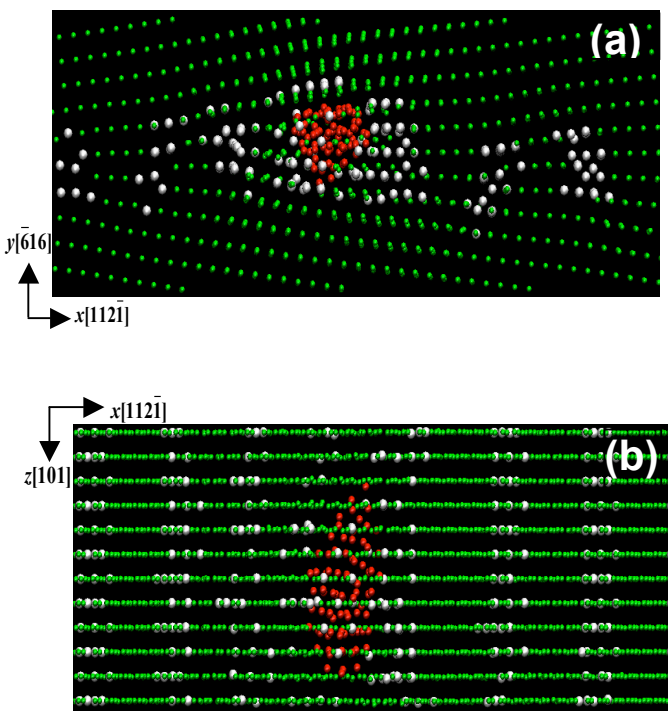

Fig. 2. Atomic configurations of the Σ73b GB together with the cluster of 83 He atoms projected on: (a) the (101) plane and (b) the (-616) plane, where the representation of spheres are the same as those in Fig. 1.

The He atoms are distributed along the dislocation line in the ∑73b GB, forming a longitudinal platelet-like shape that is often observed in experiments. Most of the SIAs at the periphery of the He cluster are reconstructed along the [-1 -1 12] direction, leading to the migration of the dislocation along the [-1 -1 12] direction.

CONCLUSION

The nucleation and growth of He bubbles in the S3 and S73b GBs in α-Fe are studied using molecular dynamics, and the evolution of the material structures due to the He accumulation and the growth of He bubbles is analyzed in detail. It was found that the nucleation and growth of He bubbles, as well as the formation of SIAs, at the different GBs is significantly different. In the S3 GB a 1/2 <111> dislocation loop is formed and emitted by the increasing size of the He bubble. However, in the S73b GB the insertion of He atoms induces the intrinsic dislocation to migrate along the [-1 -1 12] direction. Also, it is observed that in the S3 GB the He bubble is almost spherical, but in the S73b GB it has a longitudinal shape along the dislocation line.

REFERENCES

[1] L. Yang, F. Gao, H. L. Heinisch, and R. J. Kurtz, In *DOE/ER-0313/50-Volume 51 Semiannual Progress Report December 31, 2011*.
[2] L. Yang, H. Q. Deng, F. Gao, H. L. Heinisch, R. J. Kurtz, S. Y. Hu, Y. L. Li, and X. T. Zu, to be published in *Nucl. Instr. Meth. B*.
[3] N. Gao, H. Van Swygenhoven, M. Victoria, and J. Chen, *J. Phys.: Condensed Matter* **23** (2011) 442201.
[4] F. Gao, H. Q. Deng, H. L. Heinisch, and R. J. Kurtz, *J. Nucl. Mater.* **418** (2011) 115.
[5] G. J. Ackland, M. I. Mendelev, D. J. Srlolovitz, S. Han, and A. V. Barashev, *J. Phys.: Condensed Matter* **16** (2004) s2629.
[6] R. A. Aziz, A. R. Janzen, and M .R. Moldover, *Phys. Rev. Lett.* **74** (1995) 1586.