8.1 Nucleation of He Bubbles at Grain Boundaries of α-Fe — L. Yang, F. Gao, H. L. Heinisch and R. J. Kurtz (Pacific Northwest National Laboratory)*

This is the Extended Abstract for a paper in preparation for journal submission.

The formation of He bubbles in bulk or at grain boundaries (GBs) has major consequences for the structural integrity of first-wall materials. To gain insight into He effects, the accumulation of He atoms and nucleation of He bubbles in a Σ3<110>{112} GB of α-Fe is being studied using molecular dynamics with our newly developed Fe-He potential [1]. It is found that the accumulation of He atoms, the formation of He bubbles, and the evolution of the GB structure all depend on the He concentration and temperature. When a He concentration of 1% is introduced within the GB region at temperatures higher than 600 K, small He clusters are formed, and a few Fe self-interstitial atoms (SIAs) are emitted from the He clusters. The SIAs easily migrate to the nearby atomic planes and form <111> crowdions. At a He concentration of 5%, a few large He clusters are found, in platelet form, and dislocations are also formed at the peripheries of these large He clusters. At 10% He concentration the atomic structure of the GB is significantly changed due to the formation of large He clusters, and the large number of SIAs that are emitted can rearrange to form an extra atomic plane within the GB, resulting in the self-healing of the deformation induced by He accumulation and the GB climbing along the $[\bar{1}12]$ direction.

For this initial study, a Σ3<110>{112} GB has been employed to investigate the nucleation and growth of He clusters. He atoms are inserted randomly within 8 atomic layers near the GB at the He concentrations of 1%, 5% and 10%, which are the ratios of the number of He atoms to Fe atoms within the considered atomic layers. After He insertion, the cell was quenched to 0 K for 10 ps to achieve the minimum energy configuration, followed by a temperature rescaling to the required temperature. During the MD simulations at 300 K, almost all He atoms aggregate to the GB plane, and a few small He clusters are formed (He_n n=2-6). The emission of SIAs is not observed for these small clusters, but the displacements of the surrounding Fe atoms increase with the increasing size of the clusters.

The final distribution of He interstitials at 5% at 800 K is shown in Figure 1, from which it is clearly seen that some large He clusters are formed, and they exhibit platelet-like structures. Also a number of SIAs are emitted from the clusters, and they collect at the periphery of the large He clusters. It is of interest to note that the number of the collected SIAs is sufficiently large so as to lead to the formation of dislocation loops (see the insets in Figure 1). The population of these dislocation loops increases with increasing simulation time, and they are distributed at the periphery of the He clusters.

When the He concentration increases to 10%, many He clusters are formed after the simulation cell is quenched to 0 K, and some SIAs near the He clusters are spontaneously created due to the high He concentration. Similar to the simulations at lower concentrations, He atoms rapidly diffuse to the GB plane during the MD simulations at all the temperatures considered and form many larger He clusters with platelet-like structures. As a result, a large number of SIAs are

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created. It is of interest to see that these SIAs do not cause a large deformation of the GB, and the atomic arrangements of the GB are similar to those of the original structure without He atoms. To understand this, the evolution of the GB structure as a function of the simulation time is explored. Figure 2 shows several snapshots of the GB structure simulated at 300 K, but includes only Fe atoms for clarification. The atomic plot at 3 ps shows that the GB structure is largely deformed and highly disordered. Longer time MD simulations clearly indicate that these disordered Fe atoms within the GB start to reconstruct at 10 ps, forming an extra atomic layer which is above the original GB plane. It is also observed that some single He atoms and small He clusters migrate quickly within the GB plane and are absorbed by the large He clusters at 300 K. At 1 ns, it can be clearly seen that a perfect GB plane forms, and the crystal heals itself by SIA accumulation and atomic reconstruction. It is of great interest to note that the GB plane climbs up one atomic plane along the $[\bar{1}12]$ direction, as shown at 1 ns in Figure 2.

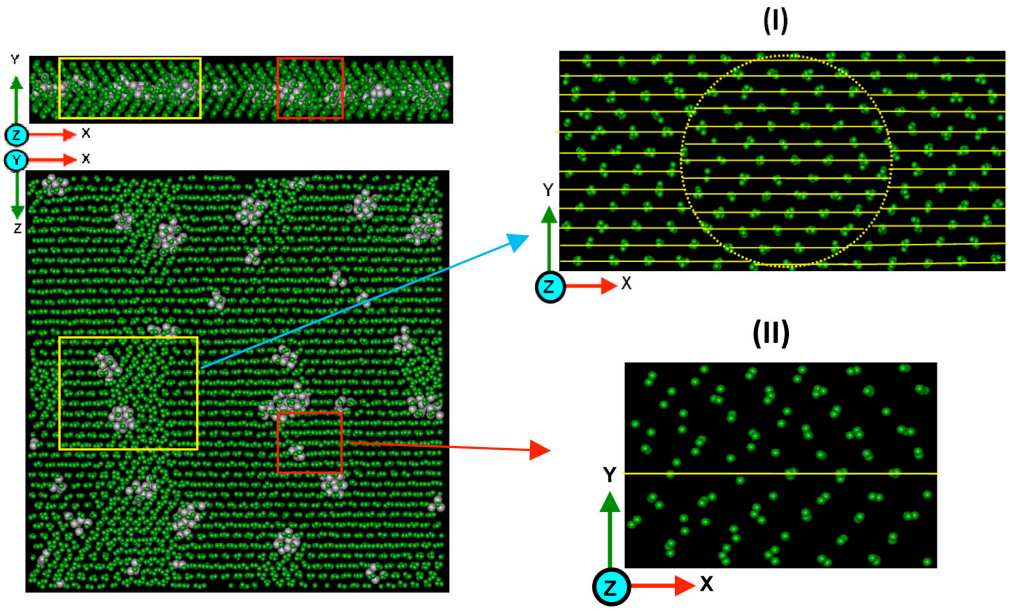

Figure 1. Final atomic configurations of Σ3 GB with a 5 % He concentration at 300 K in α-Fe. The He atoms are omitted from the inset figures I and II.

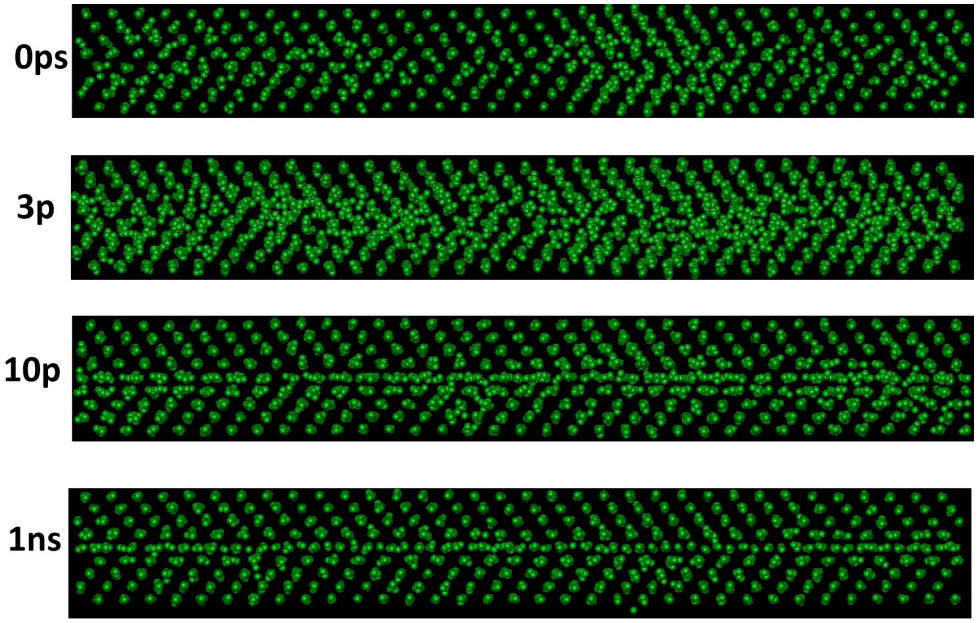

Figure 2. Four snapshots showing the structural evolution of the S3 GB with a 10% He concentration in a-Fe at 300 K, where the simulation time is indicated in each plot.

REFERENCE

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