

**THE INTERACTION OF HELIUM ATOMS WITH EDGE DISLOCATIONS IN  $\alpha$ -Fe**—H. L. Heinisch, F. Gao, and R. J. Kurtz (Pacific Northwest National Laboratory)

**OBJECTIVE**

The objective of this work is to quantitatively describe at the atomic level the fate of helium atoms produced in metals and alloys by the neutrons in a fusion reactor.

**SUMMARY**

Formation energies, binding energies, and the migration of interstitial He atoms at and near the center of an  $a/2\langle 111 \rangle\{110\}$  edge dislocation in  $\alpha$ -Fe are determined using molecular dynamics and conjugate gradient relaxation methods. Results are compared as a function of the distance of the interstitial He atoms from the center of the dislocation and the amount of excess volume around the dislocation. Interstitial He atoms have negative binding energy on the compression side of the dislocation and strong positive binding energy on the tension side. Even at low temperatures, interstitial He atoms in the vicinity of the dislocation easily migrate to positions near the center of the dislocation, where they form crowdion interstitials with binding energies in excess of 2 eV.

**PROGRESS AND STATUS**

**Introduction**

An important first step in mitigating helium effects in fusion reactor materials is to understand the fate of helium with respect to the microstructural features with which it can interact. Molecular statics, molecular dynamics and the dimer method of potential surface mapping are being used to study the fate of helium in the vicinity of dislocations in alpha-iron. We report here on results of conjugate gradient relaxation calculations of formation energies of He atoms in interstitial positions about the dislocation, which are used to map the locations of the most stable configurations of the He atom-dislocation interaction. In addition, some molecular dynamics simulations at 100 K have been performed to study the migration of interstitial He atoms within about 1 nm from the center of the dislocation. The correlation of this information with the spatial distribution of excess volume around the dislocation is also discussed. It is hoped that understanding the He disposition in these simple examples, including the response to excess volume and the effects of dislocation stress fields, will also provide insight and tools for analyzing He disposition in more complicated microstructural environments.

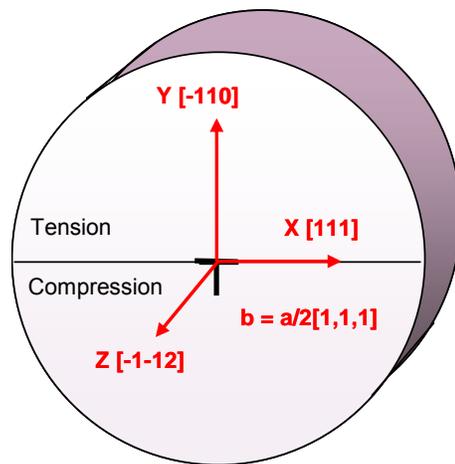
**Modeling**

An  $a/2\langle 111 \rangle\{110\}$  edge dislocation was created along the axis of a cylindrical cell of body-centered cubic Fe atoms by displacing the atoms according to the anisotropic elastic displacement field of the dislocation, then relaxing the entire model. The model is periodic along the dislocation line. One He atom was then placed within the cell, and the cell was again relaxed to determine the He interstitial formation energy and atomic configuration. In all cases the set of interatomic potentials due to Ackland[1], Wilson and Johnson[2], and Beck[3] were used for the Fe-Fe, Fe-He and He-He interactions, respectively. Interstitial formation energies were calculated for He atoms initially at both octahedral and tetrahedral sites at various locations about the dislocation. Relaxation calculations were also performed for an interstitial He atom near the corner of a jog on the dislocation.

Using the same computational cell, molecular dynamics (MD) simulations were performed at a lattice temperature of 100 K for individual interstitial He atoms starting from several different positions about the dislocation for simulated times as long as 8.4 ps. Excess volume in the vicinity of the dislocation was determined using a "Voronoi volume" approach to determine the volumes associated with various interstitial sites, where the volume is centered at the interstitial site.

## Results

Figure 1 shows the orientation of the computational cell and the relative positions of the compressive and tensile stress fields of the dislocation. Calculations were performed for He atoms placed at crystallographically equivalent interstitial positions along a line normal to the dislocation slip plane. This was done along a line running through the center of the dislocation (along the y-axis in Fig. 1) as well as along lines parallel to the y-axis at lateral distances from the center. Both octahedral and tetrahedral interstitial sites were examined. In these simulations a He atom in an octahedral interstitial position is slightly more stable than in the tetrahedral interstitial position both in the perfect Fe lattice and in the vicinity of the edge dislocation. However, octahedral interstitial He atoms placed within about 2 Burgers vectors of the dislocation center relax into crowdion interstitial sites along the direction of the Burgers vector,  $[111]$ , resulting in significant displacements of Fe atoms along the close-packed row.



**$a/2[111] [-1-12]$  Edge Dislocation**

Fig. 1. Cylindrical computational cell for an  $a/2 [111] [-1-12]$  dislocation in  $\alpha$ -Fe.

The binding energies of interstitial He atoms to the dislocation are shown in Fig. 2, plotted as a function of their initial unrelaxed positions. The binding energy is the difference between the formation energy of the interstitial He atom in the perfect lattice and in its relaxed position near the dislocation. As expected, the binding energy is negative (repulsive) in the compressive field of the edge dislocation and positive (attractive) in the tensile field. The He atoms that relax to the crowdion interstitial positions have binding energies in excess of about 1-2 eV, depending on their location, while the He atoms placed farther from the dislocation center relax to positions near their original octahedral interstitial sites and have significantly smaller binding energies.

The “reconstruction” of octahedral and tetrahedral interstitial configurations into crowdion configurations takes place as part of the relaxation process, thus no thermal energy is added to the system other than that arising from the artificial creation of the initial unrelaxed configuration. To investigate the role of crowdion formation further, MD simulations at a lattice temperature of 100 K were performed for individual octahedral interstitial He atoms starting at various distances from the dislocation. In Fig. 3 a composite of their individual trajectories is shown. In these cases, octahedral interstitial He atoms beginning well away from the dislocation center migrate to the layer of atoms nearest the slip plane, and become crowdion interstitial defects.

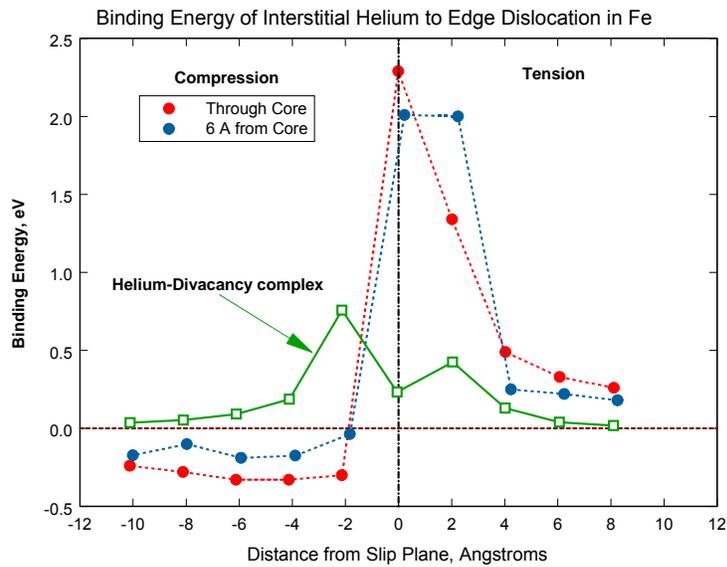


Fig. 2. Binding energies of interstitial He atoms at various positions near the edge dislocation. The green points (boxes) are binding energies for He-divacancy complexes.

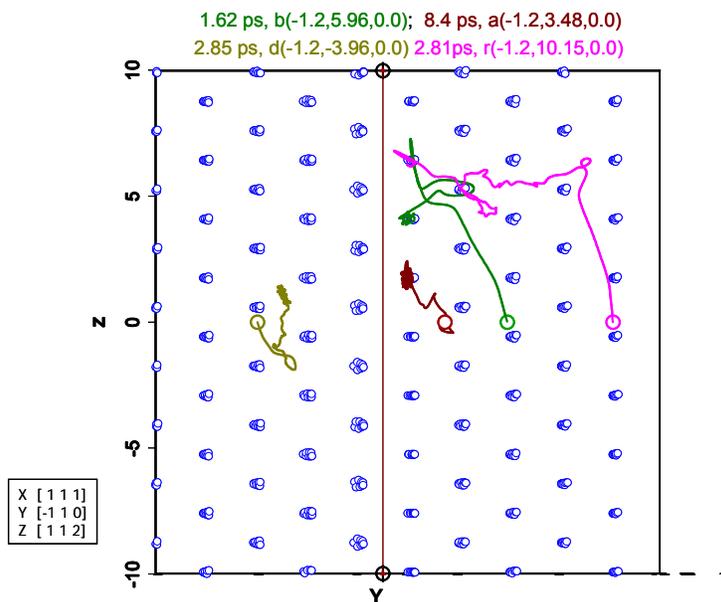


Fig. 3. Trajectories of interstitial He atoms in  $\alpha$ -Fe migrating at a temperature of 100 K. The figure is a composite of 4 individual migration simulations. The large circles are starting positions of He atoms and the small blue circles are initial positions of Fe atoms. The vertical line lies along the center of the dislocation. The compression region is to the left of the line. The simulated migration time for each He atom is at the top of the figure.

In each case in Fig. 3 the He interstitials were initially at non-equilibrium positions, so they quickly gained some initial kinetic energy that may have allowed them to more easily migrate short distances to their final positions. On the tension side of the dislocation the He interstitials migrated to crowdion positions in the row of atoms at the slip plane. On the compression side the He atom did not migrate far

before being trapped in an octahedral interstitial location. Simulated times ranged from 1.6 ps to 8.4 ps,, but in all cases the majority of that short time was spent in the final configuration. Quantitative diffusion information for these defects and others will be obtained from long time-high temperature MD simulations and Dimer saddle point energy determinations that are in progress.

Relaxation calculations have also been performed to determine formation and binding energies of He-divacancy complexes near the dislocation. This defect is essentially a divacancy with a He atom trapped in it. Although this complex can be represented in models initially as a substitutional He atom and a neighboring vacancy, when relaxed the He atom prefers to reside at a position that is somewhat off its initial position in the direction of the neighboring vacancy, and it can easily jump to the nearest neighbor vacancy. This complex migrates in a perfect crystal by a mechanism similar to that of single vacancy migration, and the He atom is dragged along, to be described in more detail elsewhere [4]. Figure 2 also contains the binding energies for He-divacancy complexes at various positions around the dislocation, similar to the locations used for the individual interstitial He atoms. Figure 2 shows that the binding energy of the He-divacancy complex to the dislocation is positive on both the compression and tension sides of the dislocation, and it is of significant magnitude only within about 7-8 Å from the center of the dislocation.

## Discussion and Conclusions

As expected, interstitial He atoms are attracted to the tension side of the dislocation and repelled from the compression side. He atoms initially in octahedral or tetrahedral interstitial positions within about 2 Burgers vectors of the center of the dislocation on the tension side of the dislocation relax to crowdion positions. Elsewhere around the dislocation and in a perfect Fe crystal He crowdions are not the most stable interstitial configuration.

The formation of stable He crowdions can be associated with excess volume, but the correlation appears to depend on more than just the excess volume in a single interstitial site. Figure 4 shows the He interstitial binding energy as a function of the excess octahedral interstitial volume, where the excess

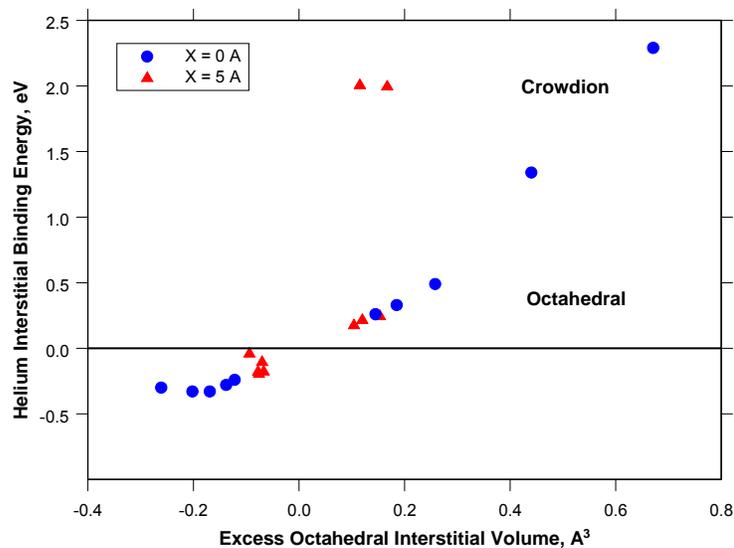


Fig. 4. Helium interstitial binding energy as a function of excess octahedral interstitial volume in  $\alpha$ -Fe.

volume is defined as the difference between the volume of the octahedral interstitial site near the dislocation and that at a similar location in the perfect crystal. There is a good correlation between the binding energy and the excess volume for octahedral interstitial positions along a line through the center of the dislocation and normal to the slip plane ( $x=0$ ). With increasing excess volume the binding energy increases, as does the tendency to form crowdion interstitials. However, along a parallel line not through the center ( $x=5$  Å) the correlation, if any, is more complicated. Perhaps the “softness” of the lattice configuration surrounding a given interstitial site beyond the nearest neighbor atoms plays a role in the ability to relax to a crowdion. Also, another factor may be that the line along  $x=5$  is not on an axis of symmetry of the stress field.

These results indicate that interstitial He atoms are either repelled from or trapped at edge dislocations in  $\alpha$ -Fe, depending on the direction of approach. He is trapped as a crowdion with 1-2 eV greater binding energy than as an octahedral interstitial. Thus, it is likely that interstitial He will be strongly trapped at edge dislocations, perhaps forming clusters and bubbles as the He concentration increases. Preliminary results for multiple He interstitials near a dislocation indicate that they can form clusters. Other preliminary results indicate that interstitial He is more strongly bound to jogs than to straight dislocations. Trapped as a crowdion, interstitial He is unlikely to migrate along the edge dislocation by “pipe diffusion.” However, the results in Fig. 2 indicate that the He-divacancy complex defects have much weaker binding to the dislocation than do interstitial He atoms, and they are evidently attracted near the center of the dislocation in both the tension and compression regions of the dislocation stress field. Work is in progress to determine the migration characteristics of He-divacancy complexes in the vicinity of dislocations.

### Future Activities

Work is in progress on He interactions with screw dislocations in  $\alpha$ -Fe, including He interstitials and He-divacancy complexes. Dimer calculations are in progress to determine He migration mechanisms and saddle point energies in the vicinity of edge and screw dislocations.

### References

- [1] G. J. Ackland, D. J. Bacon, A. F. Calder, and T. Harry, *Phil. Mag.* A75 (1997) 713.
- [2] W. D. Wilson and R. D. Johnson, *Interatomic Potential and Simulation of Lattice Defects*, Plenum (1972) 375.
- [3] D. E. Beck, *Mol. Phys.* 14 (1968) 311.
- [4] F. Gao, H. L. Heinisch, and R. J. Kurtz, to be presented at the Second International Conference on Multiscale Materials Modeling, UCLA, Los Angeles, October 11-15, 2004.