THE INTERACTION OF HELIUM ATOMS WITH EDGE DISLOCATIONS IN α-Fe—H. L. Heinisch, F. Gao, R. J. Kurtz, and E. A. Le (Pacific Northwest National Laboratory)

OBJECTIVE

The objective of this research is to understand the fate of He atoms produced in metals and alloys by fusion neutron induced transmutation reactions. In the present work we study the migration and diffusion mechanisms of He atoms in dislocations in α-Fe using atomic-scale methods of molecular dynamics and statics.

SUMMARY

Formation energies, binding energies, and migration energies of interstitial He atoms in and near the core of an a/2<111>{110} edge dislocation in α-Fe are determined in atomistic simulations using conjugate gradient relaxation and the Dimer method for determining saddle point energies. Results are compared as a function of the proximity of the He to the dislocation core and the excess interstitial volume in regions 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 the dislocation core, where they form crowdion interstitials oriented along the close-packed slip direction, with binding energies in excess of 2 eV. Crowdion interstitial He atoms diffuse along the core, transverse to the crowdion direction, with a migration energy of 0.4–0.5 eV.

PROGRESS AND STATUS

Introduction

Over time He atoms will partition among various sinks in the microstructure such as dislocations, grain boundaries and particle/matrix interfaces. Detailed knowledge of how He interacts with these microstructural features is needed to develop improved kinetic Monte Carlo and rate theory models for prediction of long-time material behavior. Molecular statics, molecular dynamics and the dimer method of potential surface mapping are being used to study the fate of He atoms in the vicinity of dislocations in alpha-iron, which we consider to be a first-order model for ferritic steels. We report here on the calculation 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. Also, the Dimer method was used to determine migration energies of He atoms trapped within the dislocation core. The correlation of this information with the spatial distribution of excess volume around the dislocation is discussed.

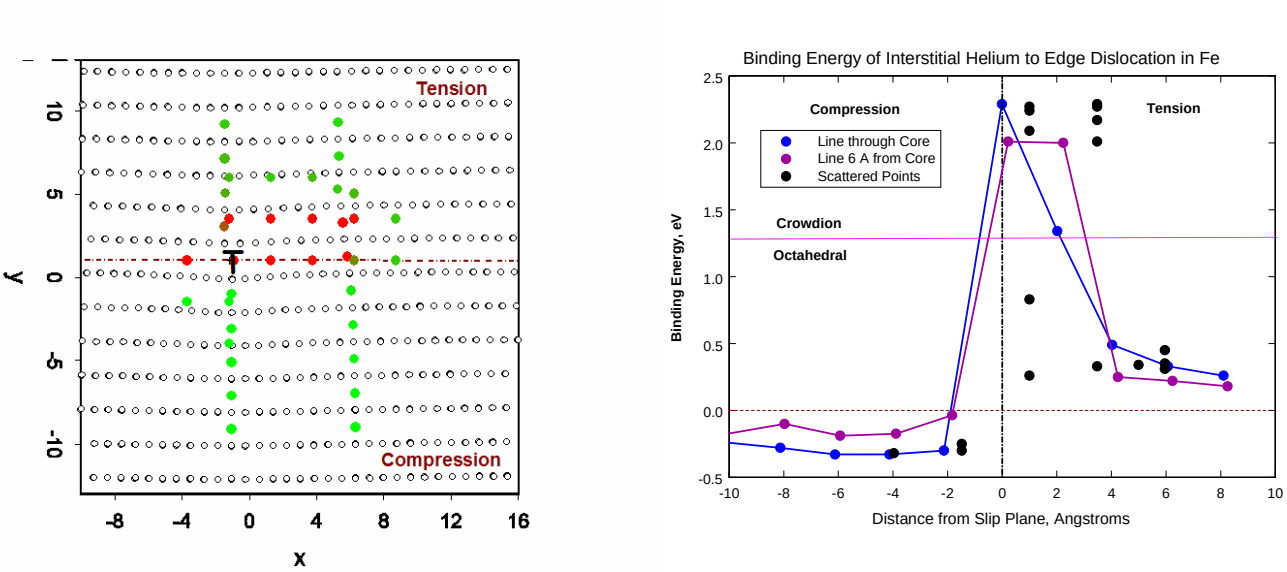
Modeling

An a/2<111>{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. Binding energy calculations were performed for He atoms placed at substitutional and interstitial positions in the dislocation-distorted lattice on both the tension and compression sides of the dislocation slip plane. Conjugate gradient relaxations were performed to determine the relaxed configurations of the He and surrounding Fe atoms, as well as the energy of the relaxed 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. Excess interstitial volumes associated with interstitial sites in the vicinity of the dislocation were determined using a variation of the Voronoi volume technique, where the volume is located at the center of an interstitial site.

The Dimer method [4] was used to determine saddle point energies for possible transitions of interstitial He atoms to other locations, starting from several positions near the dislocation. The Dimer results give the migration energies and saddle point atom configurations for He interstitials as they migrate from one equilibrium position to another. In a single run the Dimer method can find saddle points for more than one transition from a given starting configuration, not just the transition of lowest energy. Thus, it is useful for locating unexpected and competing transitions, which can be especially important in exploring a complicated potential energy landscape such as near a dislocation or grain boundary.

Results

The binding energies of interstitial He atoms to the dislocation are shown in Fig. 1b, plotted as a function of their initial unrelaxed positions as shown in Fig. 1a. Helium atoms initially within the dislocation core region relax to crowdion interstitial positions and have binding energies in excess of about 1–2 eV, depending on their location, with a maximum binding energy of 2.3 eV for (crowdion) interstitial He atoms in the core of the dislocation. Helium atoms placed farther away from the dislocation core relax to positions near their original octahedral interstitial sites, and they have significantly smaller binding energies that decrease with distance from the dislocation. However, MD simulations at a lattice temperature of 100 K show that interstitial He atoms beginning well away from the dislocation core migrate to the layer of atoms nearest the slip plane, and become crowdion interstitial defects [5]. Near the core the binding energies decrease more rapidly perpendicular to the slip plane than along the slip plane.



(a) (b)

Fig. 1. a) Locations of the initial position of a single interstitial He atom prior to relaxation. The open circles are Fe atom rows, and the filled, colored circles are the initial He atom positions. The dislocation line (T) is along the z-direction (into the page), and the z-components of all the He locations are approximately the same. b) Binding energies of relaxed interstitial He atoms as a function of their distance from the dislocation slip plane (dashed line in 1a) at the locations in 1a. The points connected by lines are those lying along the two vertical lines of atom positions through the dislocation core and 0.5–0.6 nm from the core, respectively.

The binding energies of relaxed interstitial He atoms to the dislocation can be associated with the excess interstitial volume at the various initial interstitial locations. In Fig. 2 the He binding energy is plotted as a function of excess interstitial volume for locations lying on the line through the dislocation core and along the line about 0.5–0.6 nm from the core, as depicted in Fig. 1a. There is apparently a strong correlation

between excess volume and binding energy for nearly all of the interstitial locations tested. However, in two of the tested locations with excess volume less than 0.0002 nm^3 the binding energy is greater than 2 eV, much higher than the correlation implied by the other data points would predict. These two outlying data points correspond to initial interstitial locations on and near the slip plane at 0.5–0.6 nm from the dislocation core.

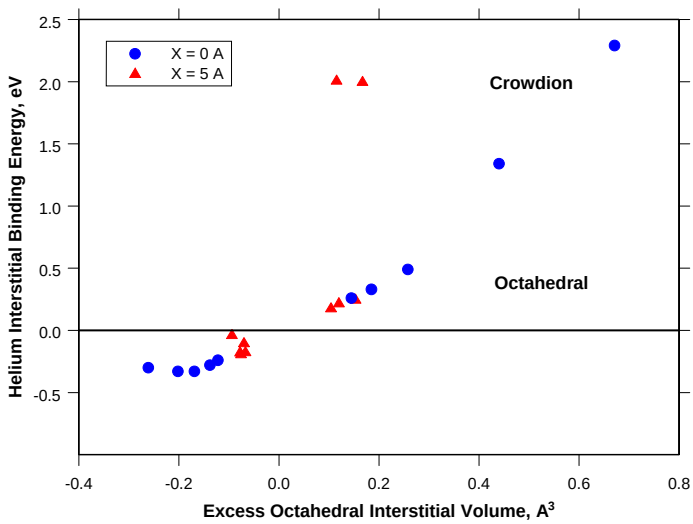


Fig. 2. Binding energy in eV of an interstitial He atom to an edge dislocation in α-Fe as a function of excess interstitial volume in $Å^3$. Values are shown for He atoms at positions along a line through the core (X=0) and at 5–6 A from the core (X=5) as depicted in Fig. 1a.

It is clear that He interstitials are strongly trapped on the tension side of edge dislocations, so it is unlikely they can easily migrate away from the dislocation except at very high temperatures. However, it may be possible for interstitial He atoms to migrate along the dislocation core. The Dimer method was applied to trapped He interstitials to determine the migration pathways and migration energies for diffusion near the edge dislocation. An interstitial He, initially in the crowdion configuration very near or in the dislocation core, is found to migrate along the dislocation line by jumping to a crowdion position in an adjacent close-packed row with a migration energy of about 0.4–0.5 eV, depending on its initial position and the jump direction.

Table 1 contains a summary of interaction energies of He-related point defects with <112> edge dislocations in α-Fe. Binding energies of substitutional He atoms near the edge dislocation were also calculated, and the maximum binding to the dislocation is 0.5 eV relative to substitutional He in the perfect Fe lattice. The migration energy of substitutional He bound to a dislocation has not been determined. In the perfect Fe lattice the migration energy of substitutional He is quite high, but our Dimer simulations show that a nearby Fe crowdion interstitial can easily “kick out” a substitutional He atom from its lattice site to become an interstitial He having high mobility with a migration energy of 0.08 eV. On the other hand, near the core of the edge dislocation the reverse of this reaction (an interstitial He atom “kicks out” an Fe lattice atom into a crowdion position) is energetically favorable. Thus, substitutional He atoms in or near an edge dislocation are likely to be relatively immobile, facilitating the formation of He clusters. Crowdion interstitial He atoms are strongly bound to the dislocation with a maximum binding energy of 2.3 eV in these simulations. Thus, for some of the highly mobile He interstitials produced under irradiation, once they are created, they will be quickly trapped at edge dislocations where they can migrate along the dislocations at fairly low temperatures in so-called “pipe diffusion.” It is interesting to note that their migration energy of 0.4–0.5 eV is in the same range as the migration energy for interstitial He atoms

within Σ3 and Σ11 grain boundaries (0.3–0.4 eV) determined from results of long-time molecular dynamics simulations [6]. Such grain boundaries also have significant regions of excess volume.

Table 1. Helium interaction energies with edge dislocations in α-iron

Binding Energy, eV Defect	Migration Energy, eV to Edge Dislocation	Perfect Fe	Dislocation
Substitutional He	0.50	--	--
Interstitial He	2.3	0.08	0.4–0.5
He_1V_2	1.2	> 1.1	--

Conclusions

The results of these simulations indicate that interstitial He atoms are either repelled from or trapped at edge dislocations in α-Fe, depending on the direction of approach. Near the dislocation core on the tension side He is strongly trapped as a crowdion with 1–2 eV greater binding energy than as an octahedral interstitial, and in this form He atoms can migrate along the dislocation with a migration energy of 0.4–0.5 eV. Helium binding to dislocations and He migration along dislocations can be at least qualitatively correlated with excess interstitial volume in the dislocation core.

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