

**THE INTERACTION OF HELIUM ATOMS WITH SCREW DISLOCATIONS IN  $\alpha$ -Fe**—H. L. Heinisch, F. Gao, and R. J. Kurtz (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 the migration energies, binding energies, and diffusion mechanisms of He atoms in and near screw dislocations in  $\alpha$ -Fe are studied using atomic-scale simulations.

**EXTENDED ABSTRACT**

This report is based on information presented at ICFRM-12, December 4–9, 2005, and a publication to be published in the Journal of Nuclear Materials.

**SUMMARY**

Formation energies, binding energies, and migration energies of interstitial He atoms in and near the core of an  $a/2\langle 111 \rangle$  screw dislocation in  $\alpha$ -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 binding energies to the screw dislocation that are about half the magnitude of binding energies to the  $a/2\langle 111 \rangle\{110\}$  edge dislocation in  $\alpha$ -Fe. Migration energies of interstitial He atoms for diffusion toward the dislocation and for pipe diffusion along the dislocation are about the same magnitude for the screw and edge dislocations, despite a significant difference in their migration mechanisms. Interstitial He atoms diffuse along the dislocation cores with a migration energy of 0.4–0.5 eV.

**PROGRESS AND STATUS**

**Introduction**

A detailed study of how He interacts with dislocations and other microstructural features is needed to develop improved kinetic Monte Carlo and rate theory models for prediction of long-time material behavior in the high helium environment of fusion reactor materials. 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 calculations of formation energies of He atoms in interstitial positions about a screw dislocation, as well as the migration energies for “pipe diffusion” of He atoms trapped within the dislocation core. A comparison of the interactions of interstitial He with screw and edge dislocations is discussed.

**Computer Simulations**

An  $a/2\langle 111 \rangle$  screw dislocation was created along the axis of a cylindrical cell of body-centered cubic Fe, oriented as in Fig. 1(a). The dislocation was introduced by displacing the atoms according to the anisotropic elastic displacement field of the dislocation, then relaxing the entire model with fixed boundary conditions. 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 in an array of positions at various distances from the dislocation line. 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

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Johnson [2] and Beck [3] were used for the Fe-Fe, Fe-He, and He-He interactions, respectively. Excess volumes associated with lattice sites in the vicinity of the dislocation were determined using the "Voronoi volume" atomic volume technique [4].

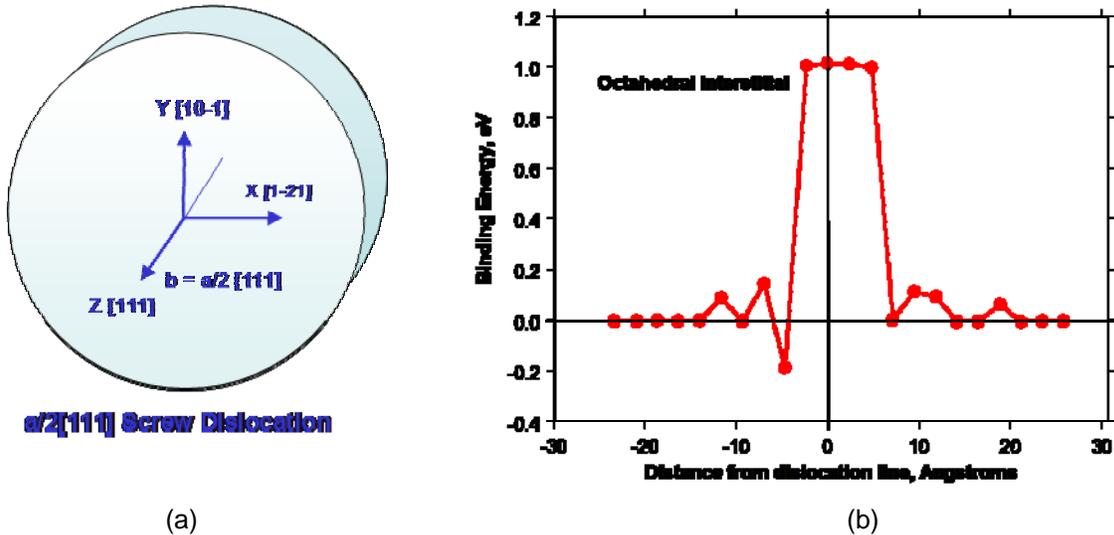


Fig. 1. a) The orientation of the computational cell for the  $a/2\langle 111 \rangle$  screw dislocation in  $\alpha$ -Fe. The dislocation line and Burgers vector lie along  $[111]$  (the  $z$ -direction, out of the page) and b) binding energies of relaxed interstitial He atoms as a function of their distance from the center of the screw dislocation along the  $[1 -2 1]$  direction ( $x$ -axis).

The Dimer method [5] was used to determine saddle point energies for possible transitions of interstitial He atoms to other locations, starting from a number of relaxed He atom positions about 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 screw dislocation are shown in Fig. 1b, plotted as a function of their initial unrelaxed positions at octahedral sites (somewhat distorted in the core region) along a line through the center of the dislocation. The Helium atoms relaxed within their octahedral interstitial positions, and they have maximum binding energies of about 1.0 eV, relative to octahedral He in the perfect Fe lattice. Helium atoms placed farther away from the dislocation core also relax to positions near their original octahedral interstitial sites, and they have significantly smaller binding energies that decrease with distance from the dislocation. The binding energy of interstitial He to the  $a/2\langle 111 \rangle$  screw dislocation is less than half the maximum binding energy of interstitial He to the  $a/2[111]$   $\{110\}$  edge dislocation [6]. Also, unlike octahedral interstitial He in and near the edge dislocation, there are no locations near or in the screw dislocation core where octahedral interstitial He atoms spontaneously assume a crowdion configuration. Undoubtedly, this is related to the much smaller excess volume associated with the screw dislocation.

The Dimer method was used to determine the migration pathways and migration energies for diffusion of a He interstitial initially placed at various octahedral interstitial positions about the screw dislocation, chosen with regard to the symmetry of the dislocation stress field and the core field, as shown in Fig. 2a. Interstitial He atoms within a radius of about 0.3 nm from the center of the dislocation migrate as octahedral interstitials along the screw dislocation with a migration energy of  $E_m \sim 0.4\text{--}0.5$  eV. See Fig. 2b. He atoms within a radius of up to 1.0 nm from the center of the dislocation migrate preferentially toward the center of the screw dislocation with a migration energy of  $E_m \sim 0.2\text{--}0.4$  eV. Thus, there is a cylindrical region about the screw dislocation within which interstitial He atoms are attracted to the dislocation. The interstitial He atoms become trapped near the dislocation, but they can easily migrate along the dislocation.

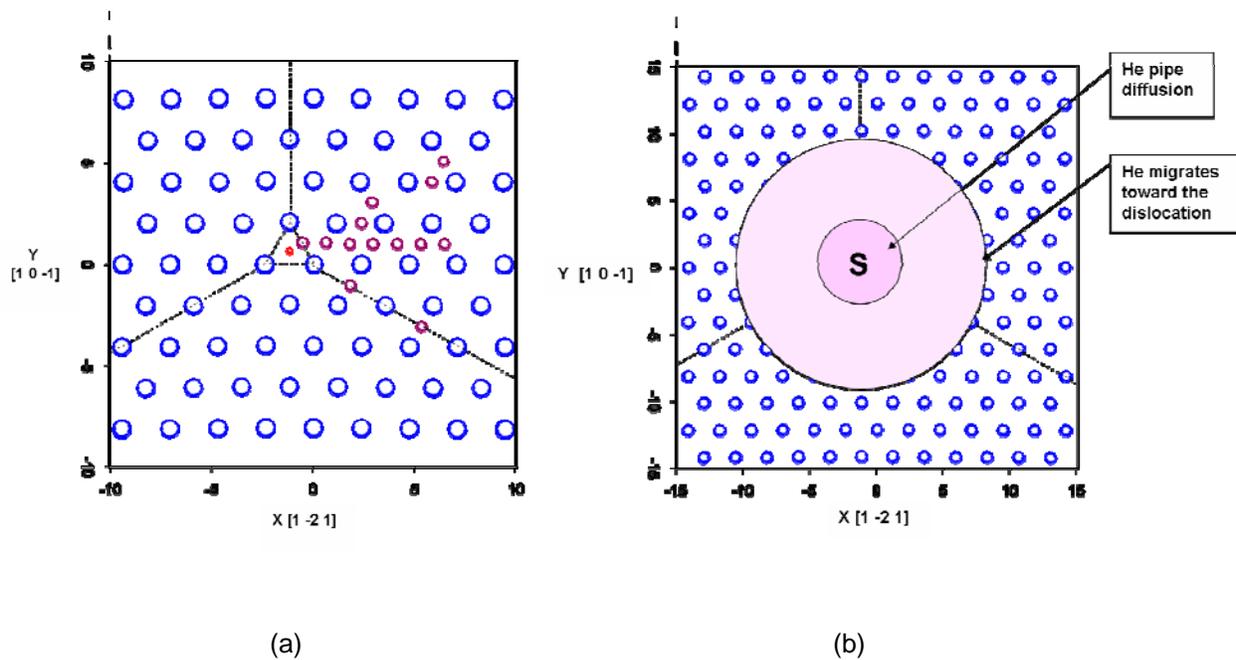


Fig. 2. a) Locations of the initial positions of a single interstitial He atom prior to relaxation. The large circles are Fe atom rows, and the small circles are the various initial He atom positions. The dislocation line is along the  $z$  axis (into the page) at the center of the dashed triangle. The  $z$ -components of all the He locations are approximately the same. Dimensions of the axes are in Angstrom units. b) The cylindrical volumes centered on the screw dislocation line (into the page) within which an interstitial He atom migrates preferentially toward the dislocation and migrates along the dislocation, i.e., pipe diffusion.

## Conclusions

The results of these simulations indicate that interstitial He atoms are attracted to and trapped at  $\langle 111 \rangle$  screw dislocations in  $\alpha$ -Fe. Within about 1 nm from the screw dislocation core He atoms migrate as octahedral interstitials preferentially toward the dislocation core, and in this form He atoms can migrate along the dislocation with a migration energy of 0.4–0.5 eV.

**References**

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