

INTERACTION OF VACANCIES AND HELIUM ATOMS WITH $a/2$ $\langle 111 \rangle$ SCREW DISLOCATIONS IN α -Fe - H. L. Heinisch, F. Gao, R. J. Kurtz (Pacific Northwest National Laboratory)¹

OBJECTIVE

The objective of this research is to understand the fate of lattice defects and He atoms produced in metals and alloys by fusion neutron-induced transmutation reactions. In the present work the migration energies and diffusion mechanisms of vacancies and He atoms in and near screw dislocations in α -Fe are studied using atomic-scale simulations.

SUMMARY

Migration energies of vacancies and He atoms in and near the core of an $a/2\langle 111 \rangle$ screw dislocation in α -Fe were determined in atomistic simulations using conjugate gradient relaxation and the Dimer method for determining saddle point energies. Results for defects in initial positions in and near the screw dislocation core were obtained for migration toward and away from the dislocation line, as well as along the dislocation line direction. For both vacancies and individual interstitial helium atoms migration is favored toward and along the screw dislocation. Vacancies trapped in the dislocation core migrate along the dislocation with a migration energy of about 0.4 eV, which is about half the migration energy of vacancies in the perfect crystal.

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. A key element of He effects is the role that vacancies play in these interactions. In the present work molecular statics, molecular dynamics and the dimer method of potential surface mapping are being used to study vacancy-dislocation interactions within the core and 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 migration energies of vacancies in the vicinity of a screw dislocation, including migration of vacancies within the dislocation core.

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. In previous studies [1] conjugate gradient relaxations were performed to determine binding energies for single He atoms placed at various substitutional and interstitial positions in the dislocation-distorted lattice and at various distances from the dislocation line. Also in those studies the Dimer method [2] 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. Within about 1 nm from the dislocation core center, single He atoms were found to be attracted to the screw dislocation and to preferentially migrate along it, Fig. 1(b).

The Dimer results give the migration energies and saddle point atom configurations for defects 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 having the lowest energy. Thus, it is useful for locating unexpected and competing transitions, which can be especially

¹ Pacific Northwest National Laboratory (PNNL) is operated for the U.S. Department of Energy by Battelle Memorial Institute under contract DE-AC06-76RLO-1830.

important in exploring a complicated potential energy landscape such as near a dislocation or a grain boundary.

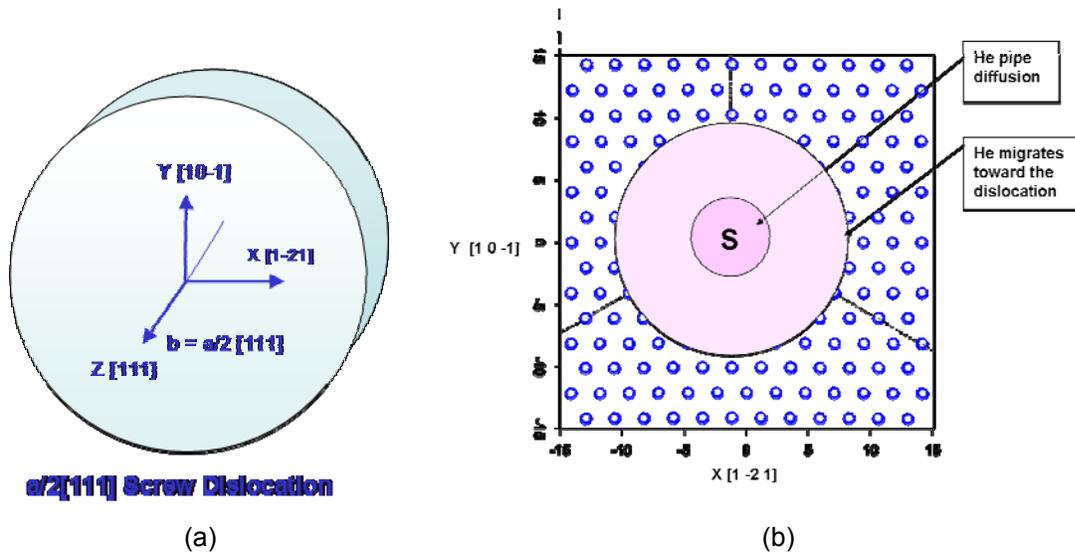


Figure 1. a) The orientation of the computational cell for the $a/2\langle 111 \rangle$ screw dislocation in α -Fe. The dislocation line and Burgers vector lie along $[111]$ (the z-direction, out of the page), b) Regions of attraction of interstitial He atoms toward the center of the screw dislocation and migration along it.

In the present study Dimer calculations were performed to determine saddle point energies for the migration of single vacancies in and near the screw dislocation. In these calculations a single vacancy was introduced at various locations within the regions near the dislocation illustrated in Fig. 1(b), and at each location saddle point energies for transitions corresponding to migration toward, away from or along the dislocation line were identified. In addition, at many of the same locations, similar calculations were also performed for divacancies of various orientations relative to the dislocation line. Initial studies of He-divacancy stability within the screw dislocation were also performed.

In all cases the set of interatomic potentials due to Ackland [3], Wilson and Johnson [4], and Beck [5] were used for the Fe-Fe, Fe-He and He-He interactions, respectively. These potentials were used primarily because they have been used extensively by us and others investigating He disposition in α -Fe. We have tested other potentials, especially the more recently developed Fe-Fe potential by Mendelev et al. [6], in similar calculations, and we find it gives somewhat smaller values for the formation and migration energies. However, the energies calculated using the Mendelev potential tend to scale with those determined using the Ackland potential. Thus, we expect that the phenomena observed in these simulations will be the same with either potential, but the energies will be somewhat smaller proportionally using the Mendelev potential.

Results

In the earlier work [1] single interstitial He atoms placed at various locations in the vicinity of a $\langle 111 \rangle$ screw dislocation were found to migrate preferentially toward the dislocation core with a migration energy of $E_m = 0.2 - 0.4$ eV within a region of about 1 nm radius. He atoms are trapped in the core region with a binding energy of $E_b \sim 1$ eV relative to their energy in a perfect Fe lattice. He atoms trapped within the core region were found to migrate along the dislocation core with a migration energy of $E_m \sim 0.4$ eV. Migration energies of He and vacancy defects in the perfect crystal and along the dislocation are summarized in Table 1.

Vacancies. In the present simulations vacancy migration trajectories were determined starting well outside the core of the screw dislocation and continuing until the “trapped” vacancy migrates along the dislocation line. Two views of such a trajectory are displayed in Fig. 2. The differences in the energies for hopping forward and back between the same atom locations are shown in Fig 2a, illustrating that the vacancy’s path is “downhill” (i.e. the vacancy in the matrix is attracted to the dislocation) until it approaches the region in the dislocation at which it is most strongly trapped. Once trapped in the core region, the vacancy migrates back and forth along the dislocation with migration energy of 0.43 eV, which is about half the migration energy required for vacancy migration in the perfect crystal.

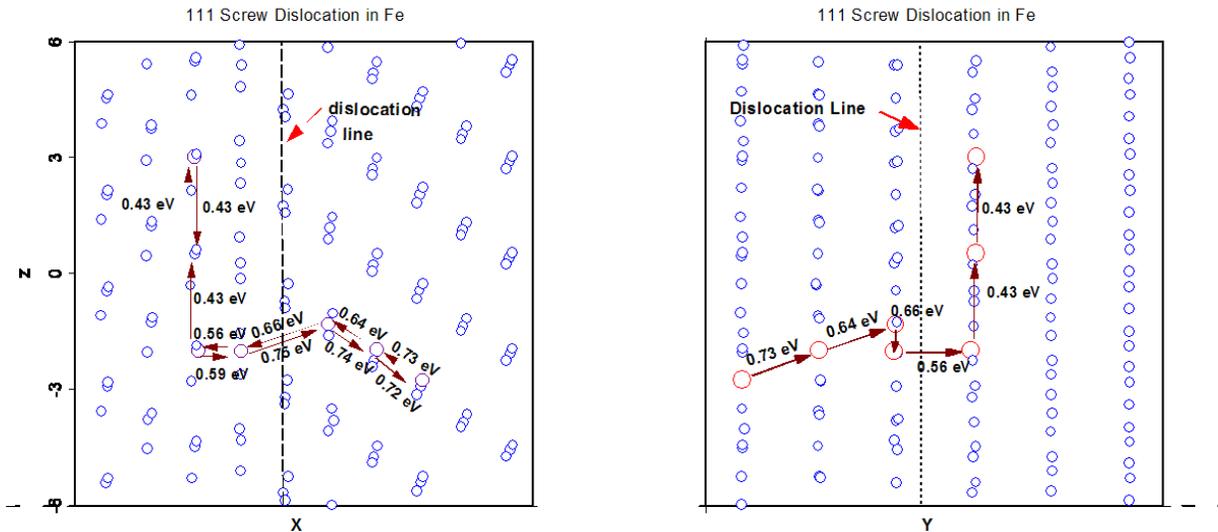


Figure 2 Two views of one possible path for a single vacancy migrating from nearly perfect crystal to become trapped in a $\langle 111 \rangle$ screw dislocation and subsequently migrating along the dislocation line. (a) The X-Z plot on the left shows the transition energies for hopping from one atomic location to another in both directions. (b) The Y-Z plot on the right shows the same path rotated by 90 degrees about the dislocation line.

Divacancies. In the perfect Fe crystal divacancies that consist of second nearest neighbor (2nn) sites are slightly more stable (by ~ 0.05 eV) than first nearest neighbor (1nn) divacancies. Divacancies migrate in the perfect crystal by hopping alternately between 2nn and 1nn configurations with an overall migration energy of $E_m = 0.89$ eV.

For divacancy migration near and within the screw dislocation there are a number of possible transition state pathways, including intermediate metastable states, for divacancy migration and dissociation, depending on location and orientation of the divacancy relative to the dislocation. The following conclusions are based on a sampling of the possibilities: Within the screw dislocation the 2nn divacancy is overall more stable than the 1nn divacancy by up to 0.21 eV. However, the 1nn divacancy stability depends on the orientation of the two vacancies relative to the dislocation line. Overall, the most stable divacancy configuration within the dislocation is as 1nn along the direction of the dislocation line. Based on limited initial investigations, it appears that the probability of dissociation of the divacancy is greater within the screw dislocation than in the perfect crystal. Migration of a divacancy within a screw dislocation is similar to migration in the perfect crystal, i.e. hopping alternately between 1nn and 2nn configurations, but with a slightly smaller migration energy of $E_m = 0.82$ eV in the dislocation.

Helium-Divacancy Complex. In the perfect crystal the He-divacancy complex is much more stable (by 0.27 eV) in the 1nn configuration where the vacancies are first nearest neighbors and the He atom sits in a stable position between the lattice site and the midpoint of the two 1nn sites, compared to the 2nn configuration, where the He becomes a substitutional He in one of the vacancies. In the perfect crystal the migration energy of the He-divacancy, from the initial 1nn configuration via an intermediate 2nn configuration to another 1nn configuration, is $E_m = 1.13$ eV.

Near the core of a screw dislocation the He-divacancy complex is also more stable in the 1nn configuration, and the migration energy of the complex is about the same as in the perfect crystal, $E_m = 1.11$ eV, for hopping from the 1nn configuration into a 2nn configuration. However, for at least one case within the dislocation, a He-divacancy complex in the higher energy 2nn configuration can more easily decompose to an immobile substitutional He plus a migrating vacancy (activation energy = 0.56 eV) than to continue (or return) to a stable 1nn He-divacancy complex (activation energy = 0.69 eV).

Defect Type	Migration Energy in Perfect Crystal, eV	Migration Energy in Screw Dislocation, eV
Interstitial He atom	0.08	0.40*
Vacancy	0.78	0.43
Divacancy	0.89	0.82
He-Divacancy	1.13	1.11

*Minimum, along dislocation line.

Table 1. Defect migration energies in α -Fe for migration in the perfect crystal as well as within $\langle 111 \rangle$ screw dislocations calculated using the Dimer method for determining transition state saddle point energies.

Conclusions

The results of these simulations indicate that single vacancies are attracted to and trapped at $\langle 111 \rangle$ screw dislocations in α -Fe. Within the dislocation core, vacancies migrate along the core with $E_m = 0.43$ eV, about half the migration energy within the perfect crystal. Single He atoms, migrating as octahedral interstitials, are also attracted to the screw dislocation and can migrate along the dislocation with a migration energy of 0.4 – 0.5 eV. Thus, with both single vacancies and interstitial He atoms easily trapped at the screw dislocation and highly mobile along it, the probability of forming substitutional He in the dislocation is high. Understanding how or whether these trapped He atoms are involved in He bubble formation may be more clearly revealed by our continuing studies of the stability, mobility and interaction of small He and vacancy clusters.

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