

THE INTERACTION OF HELIUM ATOMS WITH EDGE DISLOCATIONS IN α -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 α -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.

