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Atomistic simulations of the interactions of helium with dislocations in nickel

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ABSTRACT

The interactions of He with four dislocation types in face-centered-cubic (fcc) Ni are investigated by molecular dynamics simulations using an embedded-atom method (EAM) model. The binding energies of He in and near the cores of different dislocation types were calculated. Interstitial He has the strongest interaction with edge dislocations among the four investigated dislocations. Moreover, He has a negative binding energy on the compression side of the edge dislocation and positive on the tension side. Further calculations suggest that the attractive or repulsive natures of the He-dislocation interactions depend on both the direction of approach (compression versus tension side) and the positions of He relative to the strongest binding energy sites of the extended edge dislocation. The dependence may result in dislocation pinning via the character of the short-range interactions between interstitial He and neighboring Ni atoms.

1. Introduction

Structural material embrittlement by He is crucial in advanced nuclear fission reactors. These reactors operate at higher temperatures and higher irradiation doses [1], leading to the production of larger amounts of He. In addition, almost all structural materials can produce He by (n, α) transmutation reactions in the reactor conditions. He can accumulate both in the matrix and at defects such as dislocations and grain boundaries, because of the extremely low solubility of He in metallic materials. Accumulation can cause the formation of He bubbles and the further coarsening of these bubbles. Sufficient concentrations of He can significantly degrade the mechanical properties of materials, thus resulting in the embrittlement of the materials [2,3]. Embrittlement can decrease the strength and ductility [2,4], increase low-temperature irradiation hardening [5], and degrade the lifetime of the material [6].

Previous experimental studies have attributed He embrittlement to the clustering of vacancies and He atoms and the subsequent coarsening of bubbles and voids [7–9]. He was shown to promote cavity and dislocation loop growth [10–13], and to induce void swelling. In addition to these microstructural changes, interactions between He and defects also increased the hardness and decreased the ductility of materials [14,15]. More recent studies showed that He implantation increased the ultimate tensile strength of pure Ni [16,17] and decreased the yield stress and tensile strength of pure Fe (99.995%, Johnson-Matthey) [18]. At 750 °C, He ion irradiation greatly increased intragranular corrosion of Ni-based alloys in LiF–NaF–KF molten salts [19]. Although the issue of He embrittlement has attracted much experimental attention in recent decades, the basic mechanisms underlying these effects remain unclear. Experimental and theoretical studies demonstrate that dislocations are universal in metal structures and carry plastically deformed material. The mechanical behavior of a metal depends on the nature of dislocations and the interactions between dislocations and other defects within the metal. Therefore, microscopic mechanisms on the atomic scale regarding interactions between dislocations and He atoms are worth investigating to understand the mechanisms of He embrittlement.

Computer simulations provide important insight into the fundamental understanding of complex atomic-level processes of defects that affect the microstructural evolution of materials. Recently, particular attention has been focused on the interactions between He and various defects in α-Fe. Such interactions have been

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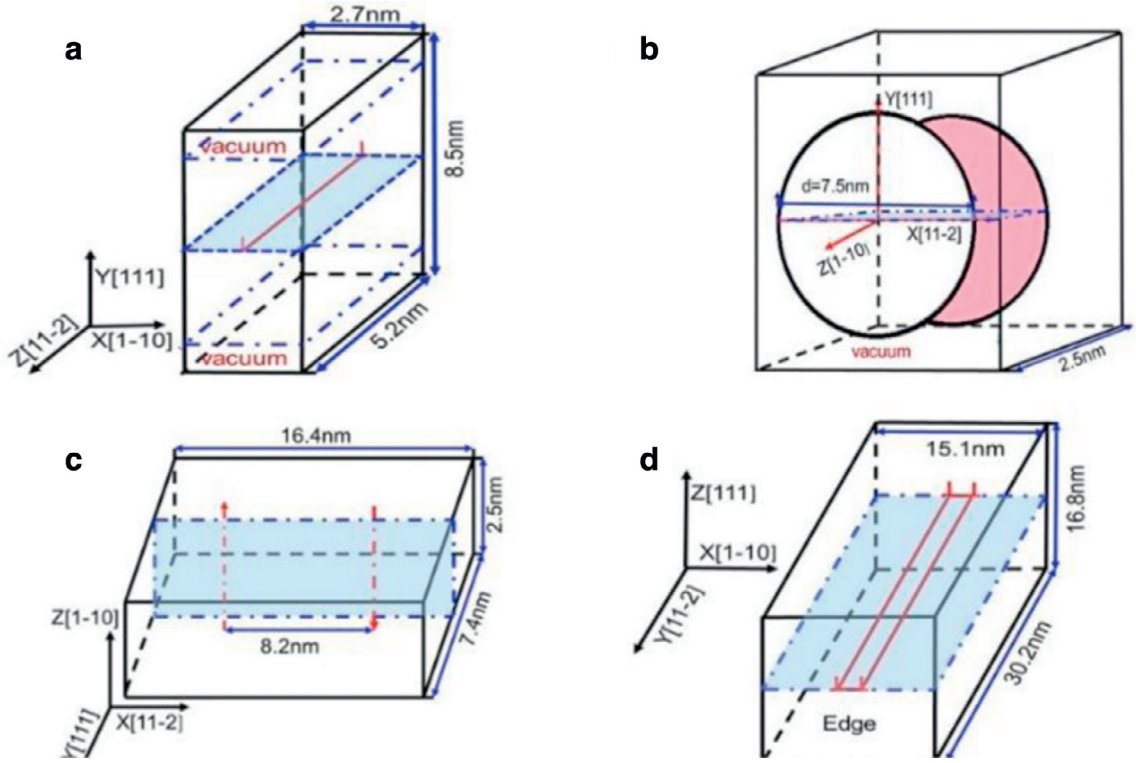

Fig. 1. Simulation system geometries. (a) Edge dislocation. (b) Screw dislocation where the dislocation line is the axis line (i.e., *z* direction). (c) Screw dislocation dipoles: the system has two screw dislocations; red arrows denote the sites of the two dislocations. (d) Extended edge dislocation obtained by dissociation of full edge dislocation. Shockley partials are denoted by inverse T; regions enclosed by red rectangular border represent stacking faults (SFs). All shaded areas represent slip planes.

systematically investigated using molecular dynamics, molecular statics, and kinetic Monte Carlo methods [20–25]. The results have shown that interstitial He is strongly trapped in dislocation cores; interstitial He is either repelled from or trapped by the same cores depending on the direction of approach by individual atoms [24], and the dislocations can provide migration paths for the diffusion of He [25]. Previous works have attained much knowledge on the issue, however, some mechanisms remain unclear, and many remaining problems are worth further study. The type of dislocation that eases the formation of He bubbles has not yet been determined. Moreover, the understanding of He atomic behavior in Ni is very limited, despite Ni being the main component of structural materials in molten salt reactors. Detailed interactions between He and different Ni dislocations remain poorly characterized.

This work investigates the behaviors of He in the presence of various dislocations in pure Ni and advances the understanding of the effects of He on the mechanical properties of metallic materials.

2. Simulation method

All molecular statics simulations in this work were performed using the three-dimensional molecular dynamics (MD) code LAMMPS developed at the Sandia National Laboratory [26]. Interatomic potentials employed here are the H. W. Sheng [27], Aziz [28], and Wei Zhang [29] to describe the interactions of Ni–Ni, He–He, Ni–He, respectively. For the Ni–He potentials employed embedded-atom method (EAM) model was fitted to formation energies of different defects, migration barrier and the behavior of small He clusters using the Potfit [30]. The lattice parameter a_0 and cohesive energy for fcc Ni is 0.35 nm and −4.44 eV/atom, respectively. During the energy minimization, the conjugate gradient (CG) method, with a time step of 0.5 fs and an energy tolerance equal to 10^{-12}, determined the relaxed configurations of the He and surrounding Ni atoms, as well as the energy of the relaxed configuration. The common neighbor analysis (CNA) [31] with a cutoff of 0.30 (nm) was used to recognize crystalline defects (i.e., non-fcc atoms) [32], and visualizations of the atomic configurations were obtained using the OVITO software package [33].

Four simulation systems were introduced for the four different crystal defects investigated in this study. First, we considered isolated edge dislocations; the simulations were performed on a rectangular box having *x*-, *y*-, and *z*-axes oriented along the $[1\bar{1}0]$, $[1\,1\,1]$, and $[1\,1\bar{2}]$ directions, respectively. The four atomic layers normal to the $[1\,1\,1]$ direction were removed to create two free surfaces, with two vacuum regions along the *y* direction. In addition, periodic boundary conditions (PBCs) were employed along the *z* (i.e. dislocation line direction) to mimic an infinitely long dislocation. PBCs were also introduced in the *x* or dislocation slip direction, to avoid dislocation-surface interactions. The dimensions of the simulation cells were $2.7 \times 8.5 \times 5.2$ nm, containing 9,072 atoms, as shown schematically in Fig. 1(a). Second, simulation cells containing a single isolated screw dislocation and screw dislocation dipoles were investigated, with *x*-, *y*-, and *z*-axes oriented along the $[1\,1\bar{2}]$, $[1\,1\,1]$, and $[1\bar{1}0]$ directions, respectively. The former model, containing the isolated screw dislocation, employed cylindrical cells with 10,340 atoms. The cylinder diameter and axis lengths were 7.5 nm and 2.5 nm, respectively, as shown schematically in Fig. 1(b). PBCs were employed along the *z*-axis. A vacuum region was created along the radial direction by removing atoms outside the cylindrical cell within a rectangular box. The latter model, containing screw dislocation dipoles, was composed of rectangular cells. The dimensions of these simulation cells were $16.4 \times 7.4 \times 2.5$ nm with 27,360 atoms, as shown in Fig. 1(c). PBCs were employed along all three directions. Finally, for simulation cells containing extended edge dislocations, simulations were