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Micromechanics mechanism of α-Fe with different types of edge dislocations under radiation damage

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ABSTRACT

Micromechanics mechanism of two α-Fe models with and without a/2⟨1 1 1⟩{1 1 0} edge dislocations is investigated under a constant strain rate of 10^9 s^{-1} at 800 K with 0.1 at.% He by molecular dynamics simulations. The results show that micromechanics behaviors are tailored by pressure release of He clusters and subsequent He bubbles coalescence. Furthermore, it is interested to notice that yield stress and strain of the model with dislocations is 0.06 and 10.52 GPa, which is lower than that of the model without dislocations (0.105 and 11.77 GPa), respectively. The reason for the acceleration is attributed to the consolidation of positive and negative edge dislocations, which induces the nucleation and growth of larger He bubbles.

1. Introduction

Reduced activation ferritic/martensitic steels, considered as first wall candidate materials in future nuclear fusion applications, have been widely investigated [1]. As we all know, radiation-induced phenomena mainly focus on a high flux of He formation and displacement damage. Extensive quantum mechanics and atomistic simulations have been used to examine physical properties of α-Fe under irradiation and the synergistic interaction of He atoms with the existing and radiation-induced defects, especially dislocations [2–7]. For example, it was found that interstitial He is strongly trapped to form He clusters in the core of dislocation [2], and diffusion of He clusters in the dislocation is faster than in the defect-free iron [3]. Furthermore, binding energies and mobility of He clusters to an a/2⟨1 1 1⟩{1 1 0} edge dislocations are investigated to mainly depend on He/V ratio and cluster size [4,5]. In addition, fracture behavior of He clusters impeding dislocation motion has been carried out [6,7]. Recently, Caro et al. [8] focus on He segregation to an edge dislocation and study the yield strength at different temperatures. They observed temperature determines the bubble diameters and spacing distribution on dislocations, thus altering the yield strength. Unfortunately, the combined study of different types of dislocations interacting with He segregation, and how this segregation modifies the yield strength is not available. Therefore, in this work, molecular dynamic (MD) simulations are carried out to explore the tensile behavior of α-Fe models with and without different types of edge dislocations under irradiation. The corresponding stress-strain responses are analyzed and how ultimately this affect fracture characteristics are discussed.

2. Modeling and methods

MD simulation was performed using LAMMPS code [9]. The Fe-He Potential is given by Caro et al. [8]. Fig. 1 shows the computational models used in the present study. The crystallographic orientation was x [1 1 1], y [$\bar{1}$ 0 1], z [1 −2 1], respectively. Two a/2⟨1 1 1⟩{1 1 0} edge dislocations, one positive edge and the other negative edge dislocation, were created in the matrix, as illustrated in Fig. 1(b). The distance d between two edge dislocations, is 3.5 nm. Geometrical dimensions of these two models are indicated in Table 1. The model A, used as a reference model, is α-Fe model without dislocations and B is α-Fe model with dislocations, respectively.

For these two models, periodic boundary conditions for x and z directions, and a rigid boundary condition for y direction were used. Initially, 0.1 at.% He atoms were randomly distributed in these two models. Then, they were relaxed using the conjugate gradient method to a minimum energy state, followed by temperature rescaling to 800 K and held there for 4 ns, when there was equilibrium state of He segregation. Afterwards, a uniaxial tension

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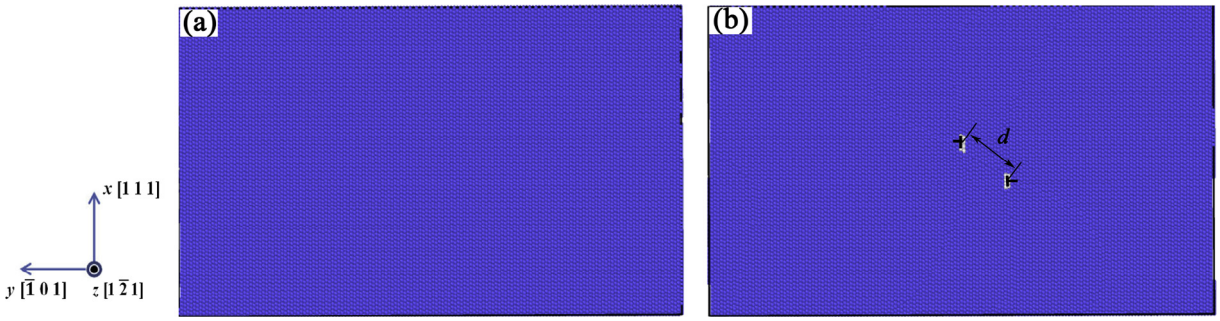

Fig. 1. Cross section of two models: (a) A model, (b) B model. Atoms were colored according to common neighbor analysis. The bcc atoms were colored in blue, and the distorted structure atoms (for example dislocations) were colored in white. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Geometrical dimensions of two models.

Models	*x*/nm	*y*/nm	*z*/nm	Number of dislocations	Number of atoms
A	20	32	4.6	–	256,000
B	20	32	4.6	2	255,720

with a strain rate of 1×10^9 s^{-1} was applied along the *x* direction. The system was simulated with adopting the canonical ensemble (NVT) with a time step of 1 fs. All the simulations were run at 800 K.

For the purpose of visualizing defects, colors were assigned to the atoms by using common neighbor analysis (CNA), which is implemented by the Open Visualization Tool (OVITO) [10]. The dislocations were analyzed using dislocation extraction algorithm (DXA) [11]. In this study, the body-centered cubic (bcc) atoms were colored in blue, the distorted structure atoms or He atoms were colored in white and the dislocation was in green line.

3. Results and discussions

3.1. He evolution in process of relaxation

In order to understand the migration and segregation of He atoms in detail, Fig. 2 shows several snapshots of He clusters distributions as a function of time (t = 0, 1.5 and 4 ns) in A and B models. The He atoms and dislocations were only extracted.

From Fig. 2(a) and (d), initial He atoms are randomly distributed in the matrix. Then, single He atoms migrate in process of relaxation due to their low migration energy [12], thus leading to the formation of small He clusters [13]. Yang et al. [14] had found that a He cluster with four He atoms is able to push out an iron interstitial, creating a He-V cluster at 800 K. In this study, as the size of He clusters increases, more self-interstitial atoms attached to He clusters, can be emitted, leading to the formation of 1/2 ⟨1 1 1⟩ dislocation loops [14,15]. As clearly shown in Fig. 2(b) and (c), for A model, when t is 1.5 ns, four 1/2 ⟨1 1 1⟩ dislocation loops are attached to He clusters and these loops length is 6.86 nm. When t is 4 ns, the loops number keeps increasing to 6 meanwhile the length expands to 15.33 nm. Analogous He bubble-loop complexes were also found in the experiments by Chen et al. [16]. For B model (Fig. 2(e) and (f)), when t is 1.5 ns, the number of new dislocation loops is 2 and whereafter there is

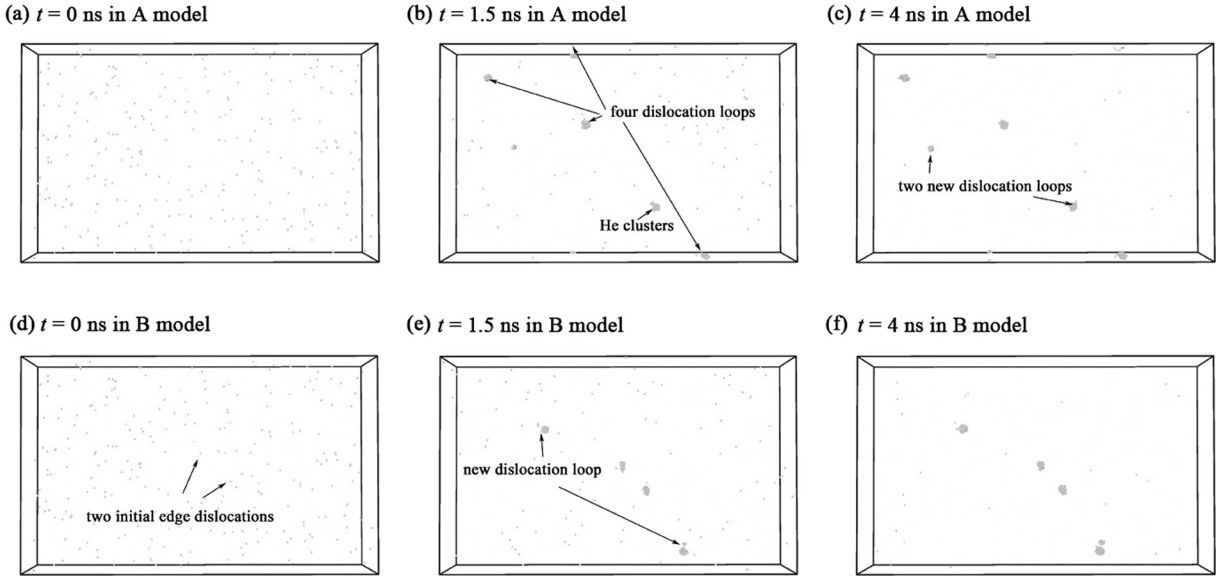

Fig. 2. (a–c) and (d–f) are distributions of He clusters as a function of time in A and B model, respectively.