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Atomistic study on mixed-mode fracture mechanisms of ferrite iron interacting with coherent copper and nickel nanoclusters

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ABSTRACT

The effect of copper and/or nickel nanoclusters, generally formed by neutron irradiation, on fracture mechanisms of ferrite iron was investigated by using molecular statics simulation. The equilibrium configuration of nanoclusters was obtained by using a combination of an on-lattice annealing based on Metropolis Monte Carlo method and an off-lattice relaxation by molecular dynamics simulation. Residual stress distributions near the nanoclusters were also calculated, since compressive or tensile residual stresses may retard or accelerate, respectively, the propagation of a crack running into a nanocluster. One of the nanoclusters was located in front of a straight crack in ferrite iron with a body-centered cubic crystal structure. Two crystallographic directions, of which the crack plane and crack front direction are (010)[001] and (111)[$\bar{1}$10], were considered, representing cleavage and non-cleavage orientations in ferrite iron, respectively. Displacements corresponding to pure opening-mode and mixed-mode loadings were imposed on the boundary region and the energy minimization was performed. It was observed that the fracture mechanisms of ferrite iron under the pure opening-mode loading are strongly influenced by the presence of nanoclusters, while under the mixed-mode loading the nanoclusters have no significant effect on the crack propagation behavior of ferrite iron.

1. Introduction

Reactor pressure vessels (RPVs) of light-water nuclear reactors are generally made of low-alloy ferritic steels, and neutron irradiation is known to cause the hardening and embrittlement of the RPV steels, which is mainly attributed to the formation of solute nanoclusters such as Cu, Ni, and other alloying elements [1–5]. The presence of these nanometric features in irradiated RPVs is experimentally revealed by atom-probe tomography and small-angle neutron-scattering technique and indirectly confirmed by positron annihilation spectroscopy [6–12]. The copper rich precipitates obstruct the movement of dislocations resulting in the hardening of low-alloy ferritic steels. Ni is added to RPV steels to increase its hardenability, however it is found that Ni increases the sensitivity of its neutron embrittlement [13]. A number of possibilities has been proposed to explain how Ni increases the hardening, for example by increasing the obstacle strength of copper rich precipitates or by decorating a dislocation and then hindering its movement, however the mechanism is still not well-known [14].

The microstructural evolution of low-alloy ferritic steels induced by neutron irradiation also creates nano and micro voids by vacancy formation and growth in generally solute depleted regions [6,10,11,14]. Micro voids with high aspect ratio can be considered as micro cracks under tensile stresses, which may interact in a very complicated way with the other microstructural features such as grain boundaries, precipitates, voids, dislocations, stacking faults, and deformation twins. Specially, the formation of solute nanoclusters in low-alloy ferritic steels causes the hardening and embrittlement, that is, the fracture toughness may decrease, since dislocation activities near a crack tip are obstructed by the solute nanoclusters, and thus, energy dissipation through plastic deformation is restricted. Gordon et al. [15] investigated the effect of Ni and Cr solute atoms, as ordered substitutional elements, on the fracture mechanism of ferrite iron, also known as α-iron, by molecular statics (MS) simulation. They found that Ni and Cr atoms qualitatively modify the α-iron crack-tip response in several

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orientations. However, the fracture mechanisms of ferrite iron under the presence of nanoclusters have not been studied yet. Generally, a crack and dislocations emitted from the crack may interact with many solute nanoclusters distributed in iron matrix, which determines the dominant fracture mechanisms and the fracture toughness of the low-alloy ferritic steels. However, the collective behavior of interactions cannot be easily simulated with MS or molecular dynamics (MD) due to the limitation of simulation size. On the other hand, the atomistic study on the interaction between a crack and a nanocluster may provide an insight into the fracture mechanisms in the early stage of crack growth and the intrinsic fracture toughness of ferrite iron.

In the present study, MS simulations are performed to investigate a crack propagation behavior in ferrite iron with a body-centered cubic (BCC) crystal structure containing a solute nanocluster under pure and mixed-mode loadings. In the MS simulations, coherent Cu and/or Ni nanoclusters are considered to be the solute nanoclusters formed in ferrite iron during neutron irradiation. In Section 2, the equilibrium configurations of the coherent Cu and/or Ni nanoclusters are obtained by using a combination of an on-lattice annealing based on Metropolis Monte Carlo simulation and an off-lattice relaxation by MD simulation. MS simulations on the interaction between a crack and a nanocluster in BCC iron are performed in Section 3. The fracture mechanisms along two crystallographic directions, (010)[001] and $(111)[\bar{1}10]$, interacting with a nanocluster in ferrite iron are investigated in Sections 4 and 5, respectively. Finally, Section 6 concludes this study.

2. Construction of coherent nanoclusters

2.1. Construction of coherent Cu and Ni nanoclusters in ferrite iron

In order to find the equilibrium configuration of a coherent Cu and Ni nanocluster embedded in ferrite iron, the on-lattice annealing based on Metropolis Monte Carlo (MMC) simulations followed by the off-lattice relaxation based on MD is performed. This procedure was successfully utilized by Al-Motasem et al. [16,17] to find the optimum structure and energetics of coherent vacancy, copper, and nickel nanoclusters in BCC iron, and the same procedure is adopted here. A cubic periodic simulation cell containing 2000 atoms arranged in ferrite iron lattice is used. The atomic interactions between different species are described by the ternary Fe–Cu–Ni interatomic potential [18], referred to as BM potential. The BM potential was specially designed and tailored for investigations of radiation-induced damage in Fe alloys. The atomic interactions between the same species are described by the Mendelev potential for α-iron [19], copper potential from Mishin et al. [20], and nickel potential from Voter and Chen [21].

Twenty impurity atoms (twenty Cu atoms, twenty Ni atoms, or ten Cu atoms and ten Ni atoms) are randomly distributed on the atomic positions of BCC lattice in the periodic simulation cell, and the other atomic positions are filled with Fe atoms. In the MMC simulations, the positions of Cu, Ni, and Fe atoms are randomly exchanged and the total energy of the system is evaluated. If the atomic exchange decreases the total energy, the new configuration is accepted. Otherwise the new configuration is rejected unless a randomly generated number in the interval [0, 1] is less than $exp(-\Delta E/k_BT)$, where T, k_B, and ΔE are the temperature, the Boltzmann constant, and the energy difference between the new and old configurations, respectively. The simulation starts at 600 K and after 100 MMC steps the temperature decreases gradually by 60 K and 100 MMC steps are performed at each temperature. This procedure is repeated until 0 K is reached. Then, the off-lattice relaxation is performed with MD simulation, at which the atomic positions fixed at the α-iron lattice are relaxed. A single nanocluster is obtained in all cases considered as shown in Fig. 1. In the case of mixed $Cu_{10}Ni_{10}$ nanocluster, a core-shell structure where Ni atoms cover the surface of copper nanocluster is obtained. The details of nanoclusters such as number of atoms, their constituent elements and their binding energy are summarized in Table 1.

2.2. Residual stress around solute nanoclusters embedded in α-iron

Experimental measurements showed that both BCC Fe–Cu and Fe–Ni alloys have larger atomic volume in comparison to BCC Fe [22,23]. The change in atomic volume can be considered to be an eigen strain, giving rise to residual stresses around the embedded nanoclusters. Fig. 2 depicts the contour plots of normal stresses, σ_{11} and σ_{22}, and von Mises stress, σ_v, around three different nanoclusters (Cu_{20}, Ni_{20}, and $Cu_{10}Ni_{10}$), in which the atomic stresses are calculated from the Virial theorem [24]. As shown in Fig. 2, the normal stress distributions around the nanoclusters have strong directional dependence. In particular, the Nickel nanocluster produces the tensile residual stress in x_1 direction and compressive residual stress in x_2 direction. The distribution area of residual stresses is the largest near the nickel nanocluster. It is worth noting that normal stress σ_{22} is the dominant stress component affecting crack propagation, that is, positive (negative) residual stress σ_{22} would accelerate (retard) crack propagation. On the other hand, the presence of the nanoclusters also makes a material to have different atomic bond strengths depending on the constituent atomic species: Fe–Fe, Fe–Cu, Fe–Ni, and Cu–Ni. Consequently, the residual stress distributions and bond strength fluctuation around the nanoclusters could make the crack propagation near or through the nanoclusters complicated. In the subsequent sections, the effect of the nanoclusters on the fracture behavior of ferrite iron is investigated.

3. Molecular statics simulation of crack-nanocluster interaction

Several previous atomistic studies on fracture of ferrite iron have shown that the fracture behavior is strongly dependent on its interatomic potential [15,25,26]. It was found that the Mendelev-2 [19] and the Chiesa potentials [27] show generally the best agreement with the fracture experiments. Hence, the BM potential developed from Mendelev-2 potential is used in this study. The geometrical model to study the crack-nanocluster interaction in ferrite iron is illustrated in Fig. 3. The simulation cell consists of a cylindrical domain, about 12 nm in radius and contains approximately 100,000 atoms arranged in a BCC lattice. The thickness of the cylindrical domain is chosen to be three times larger than the cut-off radius of the interatomic potential ($\approx$1.6 nm), and in the thickness direction periodic boundary condition is applied. It is well known that fracture toughness does not only depend on the crack plane but also on the propagation direction [28,29]. In this study, two crystallographic orientations of the ferrite iron are considered. In the first configuration, a crack propagates along [100] direction in a typical cleavage plane of ferrite iron, namely the (010) plane, while in the second configuration, a crack tip lies on (111) plane and propagates along $[\bar{1}\bar{1}2]$ direction. The summary of crack configurations is given in Table 2.

One of the nanoclusters prepared in Section 2 is placed at a distance from the crack tip of about $3a_0$, where $a_0 = 0.2855323$ nm is the lattice constant of BCC iron. An initial edge crack is generated by imposing the displacement field corresponding to a mixed-mode K-field of linear elastic fracture mechanics [[30], Chapter 2] given as: