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Formation of iron hydride in α-Fe under dislocation strain field and its effect on dislocation interaction

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ABSTRACT

Atomistic simulation of hydride formation under dislocation strain field piled up at inclusions in α-Fe was performed using a new Finnis–Sinclair-type embedded atom method potential. Two 1/2 [1 1 1] $(1\,0\,\bar{1})$ edge dislocations were introduced in BCC α-Fe to study the effects of dislocation interaction on the formation of hydride. Our simulation demonstrated that the interaction of dislocation-inclusion could produce ultrahigh stress that resulted in the formation of iron hydride. In addition, the dissociation of one of the two 1/2 [1 1 1] edge dislocations into [0 0 1] + 1/2 $[1\,1\,\bar{1}]$ two perfect dislocations can occur under a large applied shear (5%) or smaller shear (0.5%) when a hydride plate forms, despite the dissociation not satisfying the energy condition of dislocation reaction. The [0 0 1] perfect dislocation is usually considered the origin of cleavage on {1 0 0} planes, which is not stable without large applied load or hydrogen. In our model, the densities of both dislocation and inclusion on the glide plane could be changed to correspond to the dislocation density and inclusion (carbide) density in real martensitic steels. The results indicated that low dislocation density and small size of inclusions could prevent the formation of hydride. From these findings, tempering was suggested as a measure of preventing hydrogen embrittlement because proper tempering can effectively reduce the residual stress caused by quenching, precipitate dispersive and fine carbides (inclusion) and, in addition, decrease dislocation density in quenching and tempering martensitic steels.

1. Introduction

Hydrogen embrittlement (HE), which usually results in a catastrophic failure of various metals, has received considerable attention for over a century [1]. In particular, in steels, the HE sensitivity increases with the increase in strength [2,3]. Therefore, the growing market for high-strength steels strongly demands techniques for preventing HE in steels. Understanding the HE mechanism is a prerequisite for this goal. So far, several HE mechanisms have been proposed and are categorized as follows: (1) hydride formation and cleavage [4,5], (2) hydrogen-enhanced decohesion [6], and (3) hydrogen-enhanced local plasticity (HELP) [7,8]. Hydride formation is seldom considered the leading mechanism of HE in steels because iron hydride is unstable at normal pressure, and thus, no hydride was experimentally detected in their fracture microstructure [9]. HELP is usually considered the most important mechanism of HE in steels because the fracture surface of hydrogen-embrittled specimen is plastic in nature [10], and dislocation multiplication is always observed in grains of subfracture surface [11]. Sofronis proposed the hydrogen shielding effect on the basis of hydrogen-induced volume and elastic moduli changes [12]. In-situ observation of dislocations in the environment by using a transmission electron microscope revealed that higher dislocation piling-up density and mobility in the presence of hydrogen support Sofronis' theory and HELP mechanism. However, the results of atomistic simulation conflicted with both hydrogen-enhanced dislocation mobility and hydrogen shielding effect [13].

Hirth calculated the Fermi-Dirac atmosphere of hydrogen at a stressed crack tip in Fe and showed that the saturation occurs at room temperature [14,15], indicating the probability of formation of iron hydride. As is well known, the high strength of steels results from the high densities of dislocations and carbides in the iron matrix. It can be assumed that the saturation of hydrogen or even the formation of hydride may occur within the strain field in the surrounding of dislocations and carbides in high-strength steels, and such a phenomenon may lead to the catastrophic performance of the material. However, little attention has been focused on this issue. It remains a great challenge to resolve the site occupation of

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H atom within an iron matrix experimentally because hydrogen is the lightest element and has extremely weak scattering cross-sections. As an alternative approach, atomistic simulation has been used to study hydrogen behavior and HE phenomenon in metals at atomistic scale for decades [16]. In this work, we investigated the possibility of hydride formation in dislocation strain field piled up at inclusions in α-Fe. We used the Monte Carlo (MC) method instead of the molecular dynamic (MD) method in grand canonical ensemble (GVT) to treat H charging during the structural relaxation for saving the computation time. The simulation accuracy of confined H in α-Fe relies on atomistic potentials, specifically speaking, on the accuracy of H-H interactions in α-Fe. Wen developed a new Finnis–Sinclair-type embedded atom method (denoted as the Wen16 potential) potential [17], and we applied it to the energy calculation in MC in the present work. In comparison with the Fe-H potential developed by Ramasubramaniam, Itakura, and Carter in 2009 (denoted as the RIC09 potential) [18], the Wen16 potential reliably describes the repulse interaction of H-H in the bulk of iron, which is in accordance with the density functional theory (DFT) calculations. With the Wen16 potential, the unrealistic clustering of H in the bulk of Fe is prevented; otherwise, the simulation will be inaccurate if H atoms are considered the forms of clustering in some high-content areas, such as dislocation cores or severely deformed regions.

The model in this work covers the essential identities, including high dislocation density and carbide density, of high-strength martensitic steels with BCC matrix. Carbide precipitates act only as obstacles on the glide plane of dislocations, and the effects of alloying elements and carbon in carbide on H were not considered. In this work, we intended to investigate the possibility of hydride formation because of the interaction of dislocation and inclusion (carbide) and reveal the relationship between hydride and the conventional HE mechanisms in steels.

2. Computational methods

The Wen16 potential for the Fe/H system developed by Wen [17] was used for atomic interactions in the present work. The simulation box is orthogonal with X, Y, and Z axes parallel to [1 1 1], $[1\,0\,\bar{1}]$, and $[1\,\bar{2}\,1]$, respectively, which contains approximately 100,000 Fe atoms. Lengths of the box along the X, Y, and Z axes were denoted as L_a, L_b, and L_c, respectively. Periodic boundary condition was assigned to X and Z directions, allowing unconstrained movement of dislocations along the X direction and fixed or free boundary along the Y direction. One $1/2[1\,1\,1]\,(1\,0\,\bar{1})$ edge dislocation was introduced by deleting one layer of the upper half $(1\,1\,1)$ plane followed by molecular static (MS) relaxation, and the direction of the dislocation line was $[1\,\bar{2}\,1]$, that is, parallel to the Z axis. Inclusions were created by assigning spherical area of different diameters (φ) with 2, 3 and 4 nm, and the atoms within the spherical area were kept at a fixed position. L_a was 9.89 nm and L_b 13.29 was nm. L_c was adjusted according to the diameter of inclusion to get an equalized distance between the inclusion and its duplicates along the periodical Z axis. Applied load was produced by reshaping the computational box to relative strain value. Typical structure under a mild load after MS relaxation is shown in Fig. 1. The conjugate gradient method was used for MS relaxation with the convergence criteria set as the change in force on each atom should be smaller than 10^{-6} eV/Å. Dislocation configurations were always relaxed with respect to the applied load by MS before H charging.

As HE is a phenomenon that relies on the diffusion of hydrogen atoms, the MC method was used for H charging and structure relaxation in GVT at 300 K, in which H was inserted atom-by-atom randomly into the matrix. Trial perturbations were performed atom-by-atom in one MC cycle, including displacement

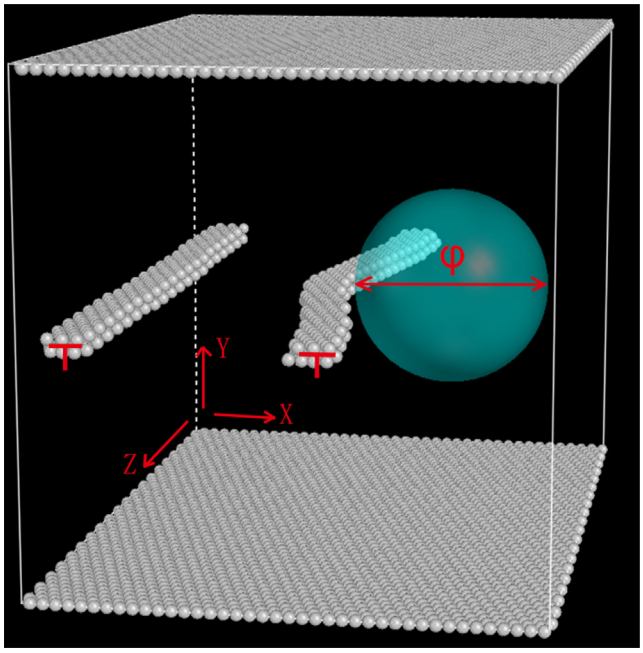

Fig. 1. Illustration of the initial structure of dislocation pileup model, with X, Y, and Z axes parallel to [1 1 1], $[1\,0\,\bar{1}]$, and $[1\,\bar{2}\,1]$ crystallographic axes, respectively. Two edge dislocations of $1/2[1\,1\,1]\,(1\,0\,\bar{1})$ Burgers vector were inserted and piled against a spherical inclusion whose diameter was denoted as φ. Boundary of inclusion is denoted by a translucent blue sphere. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

of atom, insertion of one H atom to a random position of simulation box, and deletion of an existing H atom. Total energy change determines whether one trial perturbation is accepted to adapt configuration according to Boltzmann distribution, so that at state of minimum total energy H atoms almost occupy the interstitial sites. This manipulation of H atoms actually enables them with infinite diffusion capability, allowing H atoms to achieve equilibrium concentration and distribution in a more efficient way, regardless of barriers. Details of the algorithm are well described in earlier works on the MC simulation of GVT [19]. The dependence of bulk concentration of H on chemical potential was determined in advance by the MC simulation at 300 K in perfect α-Fe lattice. A chemical potential of −2.4044 eV for H was applied throughout this work, and the corresponding bulk H concentration was 0.455 ppm (at.%), the concentration in pure Fe at a H_2 pressure of 55 MPa and 300 K [15].

Fe atom configurations were visualized by coloring each Fe atom according to the common neighbor analysis [20], which is used to identify atoms in a particular environment, such as FCC, HCP, or BCC structure, and also to identify dislocation core or other types of defects.

3. Results

3.1. Pileup of double dislocations

By setting a pileup group of double edge dislocations against rigid inclusions, we intended to study the effects of hydrogen on dislocation–dislocation interaction and dislocation–inclusion interaction.

In comparison with a cylindrical inclusion [13], more dislocations can pile up at the surrounding of a spherical inclusion at the same applied load. The minimum distance between two pileup dislocations can be determined by MS relaxation using different values of the applied load, inclusion size(φ), in-plane density of