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Atomic level simulations of interaction between edge dislocations and irradiation induced ellipsoidal voids in alpha-iron

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ABSTRACT

High concentrations of vacancies tend to be formed inside the metal materials under irradiation, and then accumulate and cluster together gradually to promote the formation of nanovoids. Generally, these voids act as obstacles for dislocation glide and thereby change/degrade the mechanical behavior of irradiated materials. In this work, the interaction between ellipsoidal nanovoids with edge dislocations in alpha-iron has been studied by atomic simulations. The results illuminate that the ellipsoidal void's semi-major axis on the slip plane and parallel to the dislocation line is the dominant factor controlling the obstacle strength of ellipsoidal nanovoids. Two other semi-major axes, which are perpendicular to the glide plane and parallel to the Burgers vector, respectively, can also influence the critical resolved shear stress (CRSS) for dislocation shearing the ellipsoidal void. The intrinsic atomic mechanisms controlling above phenomena, such as nanovoid-geometry spatial constraint and nanovoid-surface curvature on dislocation evolution, have been discussed carefully. The classical continuum model has been amended to describe the dislocation-ellipsoidal nanovoid interaction base on current results. In addition, the influence of temperature on the CRSS of ellipsoidal nanovoids has also been investigated.

1. Introduction

Because of the collisions of highly energetic particles, the mechanical behavior of irradiated metals changes and degrades significantly. High concentrations of Frenkel pairs, *i.e.* vacancy-interstitial defect pairs, are formed due to the effects of primary knock-on atoms (PKA). These primary defects can further cluster together to form various irradiation induced defects such as nanovoids, precipitates, dislocation loops, stacking fault tetrahedrons and so on [1]. Generally, these defects can lead to irradiation hardening (*i.e.* yield strength increases and ductility decreases) by hindering the dislocation glide during deformation. It is very important to understand how the interactions between dislocations and these defects can influence the mechanical behavior of materials employed in nuclear power systems. To date, a large number of studies have been carried out to investigate the irradiation induced defects-dislocation interaction by different approaches, such as experimental observations [2–5], discrete dislocation dynamics (DDD) [6–8], and atomistic simulation methods [9–14]. Although these studies are very helpful to comprehend the irradiation induced defect-dislocation interaction and the further inducing degradation of mechanical behavior, there are still some underlying mechanisms to be fully understood. In addition, the geometric models suggested in previous researches are too idealistic. Studies on more realistic models may provide new insights into the mechanical behavior of irradiated metals.

Nanovoid is one kind of ubiquitous defect occurs in irradiated metals. Previous researches [15] suggested that large voids (>2 nm in diameter) in the alpha-iron generally act as strong obstacles to dislocations motion, *i.e.* when a dislocation intersect with a nanovoid, a high magnitude of shear stress is needed for the corresponding de-pinning process. Consequently, it was concluded that the nanovoids have a great contribution to the irradiation hardening effect. As a matter of fact, the obstacle strength of nanovoids or bubbles is actually controlled by the atomic scale mechanisms, which are hard to observe by experimental methods [1,16]. Fortunately, recent large-scale atomic-level simulation provides us an effective tool to investigate the details of the interactions between irradiation induced voids and moving dislocations. In the past decade, numerous atomic-level simulations have been carried out to investigate dislocation–nanovoids interactions in irradiated metals. A variety of influencing factors have been investigated, such

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as the loading rate [15,17], inter-atomic potentials [18,19], temperature [20,21], *etc.* However, all of these investigations assume the shape of voids in metals to be perfectly spherical, which is not always the case. In fact, the shape of voids in metals is generally irregular [22]. In a more realistic situation, the shape of nanovoids should be more close to the near-spherical (*i.e.* ellipsoidal), and the interaction between dislocations with spherical nanovoids should only be a specific case. To our best knowledge, only Kohler et al. [23] had briefly studied the hardening effects induced by the ellipsoidal shape of Cu-precipitates. In this work, the interaction between an edge dislocation and an ellipsoidal void in BCC α-Fe is studied by atomic simulations. A wide range of nanovoid geometries are taken into account to investigate the effects of three semi-major axes on the dislocations-nanovoids interaction.

This paper is organized as follows. The atomic simulation model is described in Section 2. In Section 3.1, the simulation results at $T = 0$ K are provided in detail. The relative atomic mechanisms for dislocation-void interactions are discussed in Section 3.2. In Section 3.3, the theoretical models are amended to describe the interactions between dislocations and ellipsoidal nanovoids. The influence of temperature (*i.e.* $T = 300$ K and 500 K) on the dislocation-nanovoid interaction is investigated in Section 3.4. Finally, Section 4 ends the paper with some main conclusions.

2. Model and method

The molecular statics (MS) and molecular dynamics (MD) simulations were carried out using the LAMMPS code [24]. The visualization tool, Ovito [25], was employed to analyze the atomic configuration. The method for building the atomic model of dislocation-nanovoid interaction is analogous to that by Osetsky and Bacon [26], which is briefly summarized as follows.

As shown in Fig. 1, the x, y, and z axes of the coordination system are aligned to $[1\,1\,1]$, $[\bar{1}\,\bar{1}\,2]$, and $[1\,\bar{1}\,0]$ directions, respectively. In addition, the corresponding edge lengths of the simulation cell in these directions are L_x, L_y, and H, respectively. A straight edge dislocation is introduced in the middle plane $z = H/2$ with a Burgers vector $b_{Burg} = 1/2[1\,1\,1]$. Periodic boundary conditions are imposed along x and y directions. To apply the shear loading, three $\{\bar{1}\,1\,0\}$ atomic layers at $\pm z$ surfaces are set to be rigid. Since the periodic boundary conditions are applied similar to Daw et al. [27], the model actually simulates an array of edge dislocations with a spacing of L_x encounter with a row of voids with interval L_y. The initial edge length L_x in the dislocation gliding direction varies within the range of 45—74 nm, while the other edges are kept fixed as $L_y = 41.4$ nm and $H = 24.1$ nm. The ellipsoidal nanovoid can be described by $\left(\frac{x-x_0}{a^2}\right)^2 + \left(\frac{y-y_0}{b^2}\right)^2 + \left(\frac{z-z_0}{c^2}\right)^2 = 1$, with (x_0, y_0, z_0) being the void center and (a, b, c) the three semi-major axis lengths as shown in Fig. 1(b). The distance between the nanovoid and dislocation core is set large enough to prevent the initial interaction between them.

Two Finnis–Sinclair type many-body potentials [28] derived by Ackland et al. [29] and Ackland et al. [30], are found to be appropriated [31] for modeling the pure $\alpha - Fe$ system. For the current problem about the dislocation-nanovoids interaction, Terentyev et al. [19] showed that the newer potential by Ackland et al. [30] may predict a curious difference between $T = 0$ K and $T = 1$ K. When the temperature is above 100 K, it has been proved that differences in the edge-dislocation void interaction with these two potential are not distinct [19,20]. Since both MS and MD simulations are intended to be performed in this study, the older potential developed by Ackland et al. [29] is adopted in the current work. The lattice parameter a_0 at $T = 0$ K is selected as 0.28665 nm [29], and it is changed to 0.2875 nm and 0.2880 nm at $T = 300$ K and 500 K, respectively, which are obtained by relaxing a perfect crystal with zero pressure condition at these two target temperatures. The purpose of adopting different lattice parameters at different temperatures is to avoid the thermal expansion effect [20]. For the MS simulations, ε_{xz} is applied with a fixed increment $\Delta\varepsilon = 10^{-4}$ at each step, and then the whole system is relaxed completely by the conjugate gradient method. The MD model was first annealed at the target temperature for 10 ps, then the shear loading was applied with a constant strain rate $\dot{\varepsilon} = 5 \times 10^6$ s^{-1}, and time steps are selected as 4 fs and 2 fs for $T = 300$ K and 500 K schemes, respectively. In addition, the temperature fluctuation ΔT was controlled to be less than 1.5 K during all MD simulations.

In both MS and MD studies, the shear stress can be calculated through the total net force **F** applied on all atoms in the upper rigid slabs by

$$\tau = \sigma_{xz} = F_x / A_{xy}, \tag{1}$$

where F_x is the x component of **F** and A_{xy} is the area of the xy cross section (with its normal being the z axis) of the simulation model. The configurations of dislocation cores can be determined by the atomic centro-symmetry parameter [32].

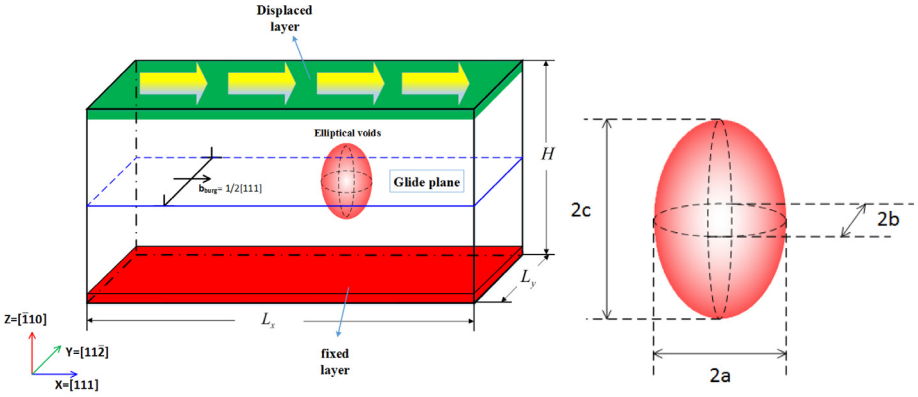

Fig. 1. Schematic of the (a) modeling system and (b) the geometry of ellipsoidal nanovoid.