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Effect of interatomic potential on the behavior of dislocation-defect interaction simulation in α-Fe

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ABSTRACT

Molecular dynamics simulation is one of the most useful methods to model defect generation and subsequent change in mechanical properties in material that will suffer irradiation in the future fusion reactors. This work is aimed at showing the influence of the empirical interatomic potential for the Fe–Fe interaction on the simulated shearing of α-Fe containing one edge dislocation interacting with one nanometric void sitting on its glide plane. The recent potentials derived by Ackland et al. [G.J. Ackland, D.J. Bacon, A.F. Calder, T. Harry, Philosophical magazine a-physics of condensed matter structure defects and mechanical properties 75 (1997) 713], Mendelev et al. [M.I. Mendelev, S. Han, D.J. Srolovitz, G.J. Ackland, D.Y. Sun, M. Asta, Philos. Mag. 83 (2003) 3977] and Dudarev–Derlet [S.L. Dudarev, P.M. Derlet, J. Phys. Condens. Matter 17 (2005) 7097] are used to identify critical parameters. The stress–strain responses are obtained under imposed strain rate and at temperatures ranging from 10 to 700 K at constant volume. It appears that different potentials give different strengths and rates of decrease of obstacle strength with increasing temperature. Results are analyzed in terms of dislocation core structure and thermal expansion. Implications for the choice of the potential are given.

1. Introduction

Low activation ferritic-martensitic steels are being extensively studied since these alloys are considered to be candidate materials for the blanket and first wall of fusion reactors [1–9]. Although the ferrite-based steels are relatively resistant to swelling and maintain good fracture toughness at irradiation temperatures above about 700 K, they are prone to loss of ductility at lower irradiation temperatures [10]. This limits the mechanical performance and lifetime of these alloys under fusion irradiation conditions. However, the complexity of the microstructure of these alloys hinders a detailed analysis of the underlying microscopic mechanisms, and studies are presently focused on model alloys, starting with pure Fe and Fe–Cr alloys [11]. Hence, in this research, pure α-Fe and molecular dynamics (MD) simulation are utilized to investigate the irradiation-induced effects, in particular the void, on the mechanical properties of this material.

Multiscale modeling appears as a major tool for the description of plasticity of materials, which includes MD simulations. They are used extensively nowadays in the study of the interaction of a dislocation with an obstacle, for example, in the case of voids and Cu precipitates in Fe (bcc) [12–17] and stacking fault tetrahedron in Cu (fcc) [18–20]. Although different works dealt with strengthening of irradiation induced fcc and bcc materials by dislocation-obstacle interaction, there is still a lack of understanding about its temperature dependence, the effect of size and type of obstacle. Moreover, the impact of the chosen empirical potential on these phenomena is generally overlooked.

In this work we consider the strengthening of bcc Fe due to the interaction of a perfect edge dislocation and a nanometric void using different interatomic potentials, as a function of void size and temperature. Three different empirical interatomic Fe–Fe potentials, namely the ones by Ackland et al. [21], Mendelev et al. [22] and Dudarev and Derlet [23], were used, which in the following are called 'Ackland', 'Mendelev' and 'Dudarev–Derlet', respectively. The atomic structure of edge dislocation core for various interatomic potentials was evaluated. Simulations are conducted at constant volume under imposed strain rate and the stress–strain response is recorded. To investigate the effect of thermal expansion at elevated temperatures the simulation box size was adjusted to be stress free.

2. Simulation method

The simulation method, detailed in [24], is briefly described here. The first step in MD simulation is to create a sample with an edge dislocation and a cavity with specific size in a perfect bcc crystal. The dislocation was described using anisotropic elasticity of the continuum, which is implemented in code Disloc. The second step allows

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the dislocation to relax by conjugated gradient to form appropriate dislocation core structure. In the last step MD simulation allows the edge dislocation to glide toward the void under imposed strain rate, which is achieved by Moldy code. The dislocation glides under shear strain applied to upper part of sample crystal whereas the lower part is fixed. Fig. 1 illustrates the MD sample consisting of a box including one edge dislocation in [1 1 2] direction and a void centered on the dislocation slip plane, (1 1 0). The box is built up of several regions. In region denoted M atoms are mobile and follow Newton's equation. Periodic boundary conditions are applied along x and y. The upper region D is a layer of atoms, which control the deformation of the sample and it is constrained to remain static. Each atom in D is displaced in the y direction (arrow) by a fixed increment at each time step corresponding to the imposed strain rate. Region T is a thermal bath used to control the temperature of the sample by rescaling the velocity of atoms every 100 steps. It was shown that the temperature increase in the core of the gliding dislocation, is not important for the specimen when only one passage of the dislocation is considered [24]. Region S contains atoms that are static and anchor the sample and thus avoids its drift in the direction of the applied stress or strain.

In present work the simulation time step is set to 1 fs and total simulation time is around 500 ps. A 5 ps annealing prior to straining is performed to equilibrate temperature. The resulting dislocation speed is 60 m s^{-1}, following the selected imposed strain rate of $3 \cdot 10^{-8}$ fs^{-1}, and the simulation box contains about half a million Fe atoms. The simulations are performed at six temperatures (10, 100, 200, 300, 400, 500 and 700 K) and five different void diameters (1, 2, 3, 4 and 5 nm). Box size is fixed to 25 nm and 20 nm in y and z directions, respectively, but the size in x dimension varied with void size (13, 14, 15, 16 and 17 nm) to keep interspacing of the voids in the direction of the dislocation line constant due to periodic boundary condition.

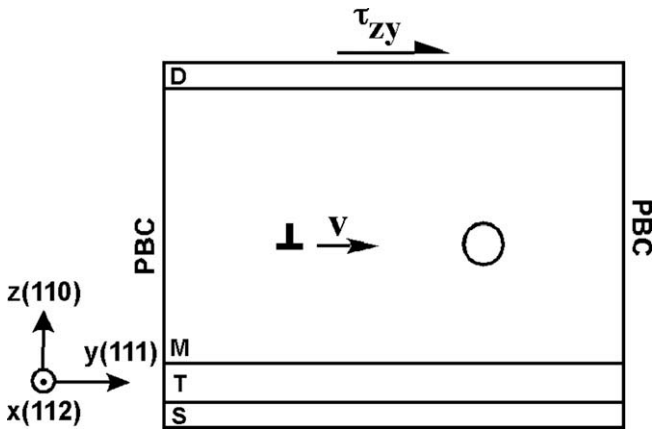

Fig. 1. Schematic view of simulation box containing an edge dislocation and a cavity. Imposed shearing, dislocation movement and different regions of the box are shown in this image. Periodic boundary condition are set in x and y directions.

The selected Fe–Fe potentials are the ones of Ackland et al. [21], Mendelev et al. [22] and Dudarev and Derlet [23], which are all using the embedded atom method [25], which implies a pair potential part and an 'embedding' part that depends on electronic density. Relative to Ackland potential, Mendelev provides better point defect properties, such as the correct relative formation energies between the <1 1 0> and the <1 1 1> self-interstitials, a critical topic in α-Fe and radiation damage. The Dudarev–Derlet potential provides the same improvement, relative to Ackland, and the inclusion of magnetic effects, such as the ferromagnetic transition upon lattice straining. Mendelev potential has the longest range, of 5th nearest neighbor, while the other two, Ackland and Dudarev, have range of 2nd and 3rd nearest neighbor. The nominal lattice parameter is 2.8665, 2.8553 and 2.8665 Å for the Ackland, Mendelev and Dudarev–Derlet potential, respectively. It should be noted that these empirical potentials are usually fitted at zero temperature, to an arbitrary selection of properties, which for those potentials include point defect properties and elastic constants. Simulation performed at finite temperatures should thus be taken with caution, in addition to the fact that MD simulations are approximate at temperatures below Debye temperature because of the inequality between the kinetic and potential energies. Our MD simulations are performed within these approximations.

3. Results and discussion

3.1. Temperature and size effect

Three stages of interaction of an edge dislocation with a 4 nm void at 200 K using Dudarev–Derlet Fe potential are illustrated in Fig. 2, which shows (Fig. 2(a)) the glide of dislocation towards the defect, prior to interaction, (Fig. 2(b)) attraction of the edge dislocation to defect in the vicinity of void and (Fig. 2(c)) release of dislocation after bowing out from void. Fig. 2(c) shows that the dislocation in bowing pulls two dislocation segments, pinned at the void, that have a near-screw character. Note that in these images only atoms having potential energy higher than chosen threshold energy are displayed. In Fig. 2(c) the shearing of the void by the edge dislocation is nearly complete. To have a clearer view of the shearing phenomenon cross cuts of the sheared void with different sizes are displayed (Fig. 3). These images show the way a cavity is sheared by passage of an edge dislocation, as it has been shown for void [13] and He bubble [24] using Ackland Fe interatomic potential. The shearing introduces a step in the void at the entry location where the dislocation first touches the void and at the exit location where the dislocation escapes from the void. Interestingly, the exit step occurs at a different height relative to the entry step. This event is evidenced by the horizontal line drawn in Fig. 3(d) showing the lower height of the exit step. This has been shown by Osetsky et al. [13] and explained as the result of the formation of a jog on the edge dislocation.

Fig. 4 shows the stress–strain curve of edge dislocation interaction with a 1 and 3 nm void at various temperatures obtained with

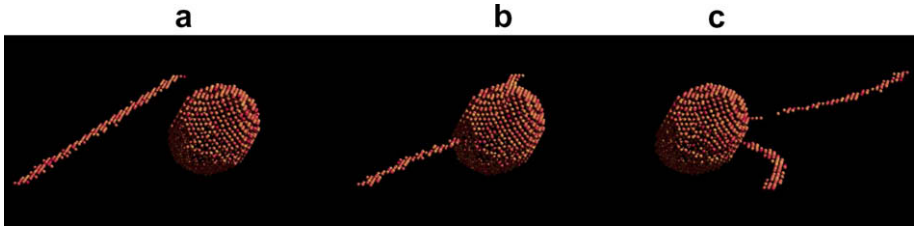

Fig. 2. Interaction of an edge dislocation and 4 nm void in bcc iron simulated by MD method at 200 K; (a) dislocation glide under imposed strain rate, (b) dislocation attraction in the vicinity of void and (c) dislocation bowing and shearing of the void.