Journal of Nuclear Materials 386–388 (2009) 102–105

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Dislocation–void interaction in Fe: A comparison between molecular dynamics and dislocation dynamics

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A B S T R A C T

Multiscale modeling, including molecular dynamics (MD) and discrete dislocation dynamics (DDD) methods, appears as a significant tool for the description of plasticity and mechanical properties of materials. This research concerns the influence of irradiation on the plasticity of pure Fe and focuses on the interaction of a single dislocation with a spherical void at various geometries. MD simulation shows that the void strengthening is proportional to the interaction area. Stress field around the void influences also the dislocation passage. DDD calculation coupled to finite element method (FEM) is used to simulate the interaction of an edge dislocation with a void. DDD calculations present a good match to the MD simulation results at the near-atomic scale. They highlight the impact of image forces on the dislocation due to the free internal surface of the void and the one of its surrounding stress field.

1. Introduction

The materials for the plasma facing components of future fusion reactors are a key issue in the realization of fusion energy systems because of the high heat and irradiation fluxes that degrade their mechanical properties. Ferritic base steels are being extensively studied since these alloys are considered to be first candidate materials [1].

Multiscale modeling appears nowadays as a major tool for the description of the plasticity of materials [2–4]. The objective here is to predict the mechanical behavior after irradiation. More precisely, we model the dislocation–defect interaction by MD simulations at the atomic scale, which can be used by DDD and FEM simulations, which are based on elasticity of continuum for higher scale simulation.

In fusion reactors materials vacancies are created due to primary knocked on atoms (PKA) and subsequent displacement cascades, which tend to form nanometric voids. In addition helium is produced by (n-α) transmutation reaction, in larger amount than what is formed in classical fission reactors. Due to its low solubility in metals He tends to aggregate in the form of few atom clusters or nanometric bubbles [5,6]. Presence of He bubble may weaken or strengthen the material depending on the density of He. We have shown that in pure iron a low content He bubble is a weaker obstacle than a void, whereas a high density He bubble is a stronger obstacle than a void [7].

The present work is focused on the simulation of the interaction of an edge dislocation with a nanometric void, in pure α-iron, and is used as a benchmark to compare MD and DDD simulations at the near-atomic scale.

2. Simulation methods

The atomistic simulation of a dislocation interaction with a defect in Fe crystal under an applied constant strain rate includes two steps. First step is to create a sample containing a void and a dislocation according to the elasticity theory of dislocations [8]. Second step is to move the dislocation using MD simulation, which is based on the embedded atom method [9]. The first step is performed using the code DISLOC [10] and the second one using the code MOLDY [11].

MD sample consists of a $14 \times 25 \times 20\ \text{nm}^3$ box containing a $1/2a_0\langle 1\,1\,1\rangle$ edge dislocation in $\langle 1\,1\,2\rangle$ direction and a spherical void of 2 nm in diameter located at 7 nm away from the dislocation. Dislocation slip plane, $\{1\,1\,0\}$, is placed at various heights relative to the void center. The box is subdivided in several regions consisting of (1) the mobile region where the atoms follow Newton equation, (2) an upper frozen region whose atoms control the deformation of sample and are forming a free surface, (3) the bottom region containing the thermal bath and (4) static atoms located in the bottom region to fix the specimen. Periodic boundary conditions are applied both along the dislocation line and along the Burgers vector. A detailed description of the simulation method is given in Ref. [10]. The shear stress resulting from the applied imposed strain rate is calculated from the forces between atoms in

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doi:10.1016/j.jnucmat.2008.12.069

the central region at each time step of 1 fs. Dislocation speed is 60 ms^{-1}. Annealing of 5 ps at 100 K is performed prior to the straining to stabilize the temperature. The many-body empirical potential, derived by Ackland [12], is used for Fe–Fe interactions.

The DDD code used in this study is an adaptation of the code TRIDIS [13] devoted to FCC structure and further developed for BCC structure. The effective stress applied on the dislocation is obtained as the superposition of the applied stress field, the image force and the internal stress field generated by all dislocation segments within the box. The image stress field is computed by coupling the DDD code to the FEM software, CAST3M-v07 [14]. In the DDD–FEM simulation, a 2 nm void is located within a cylindrical volume that is 12.5 nm in radius and 10 nm in height (Fig. 1). It should be reminded that such model uses only elasticity theory and no core effect of dislocations is taken into account. The cylinder axis is in ⟨1 1 0⟩ direction and corresponds to the normal of the dislocation glide plane. The simulated volume is meshed with 2340 twenty-nodes elements implying 3168 nodes. The finite element calculation enforces the boundary conditions induced by the presence of the cavity for which the surfaces are traction free.

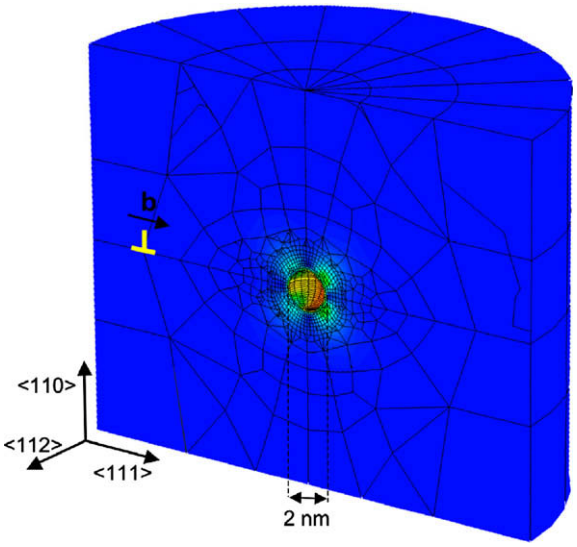

Fig. 1. Cross section of cylindrical sample meshing used to simulate the interaction of an edge dislocation with a 2 nm void located in the center of cylinder, for DDD–FEM calculation, and the stress filed due to the edge dislocation created in the void surrounding.

3. Results and discussion

MD modeling is used to evaluate the stress–strain response of the dislocation–void interaction. We record the obstacle strength as the maximum stress at which the dislocation escapes from the void. The height h of the dislocation glide plane relative to the void center is varied. Central interaction ($h = 0$) and also $h = 0.5$, 1 and 1.5 nm interaction heights have been investigated (Fig. 2(a)). For $h = 1$ nm and $h = 1.5$ nm the dislocation passes the 2 nm void tangentially and above it, respectively.

Fig. 2(a) shows a monotonous decrease in strength with increasing height of dislocation glide plane up to 1 nm. Increasing the distance h of dislocation glide plane reduces the release stress because the interaction area sheared by the dislocation line is decreased. Further increase in dislocation height, at $h = 1.5$ nm, gives a stronger drop in the critical stress. Although in the last case the dislocation moves above the void and there is no direct dislocation–void interaction, the stress–strain response is in the level of hundreds of MPa (Fig. 2(a)). Indeed there is a short-range stress field in the GPa range extending up to 0.5 nm in the bulk

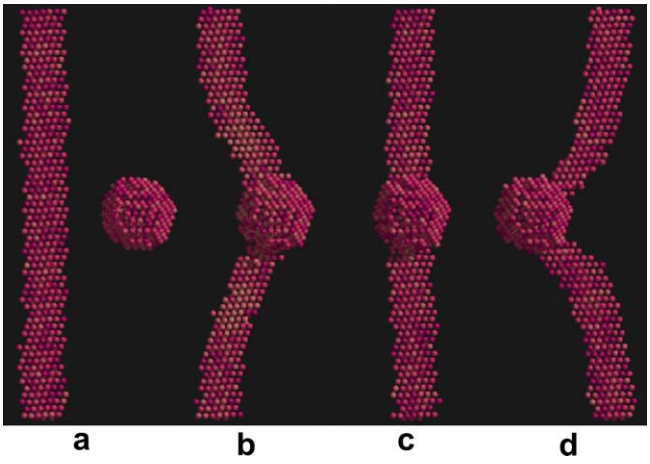

Fig. 3. Interaction stages of a gliding dislocation with a void for central interaction, obtained by MD. (a) Dislocation glide before interaction, (b) its attraction to the void, (c) its passage through the void and (d) its bowing just before the release.

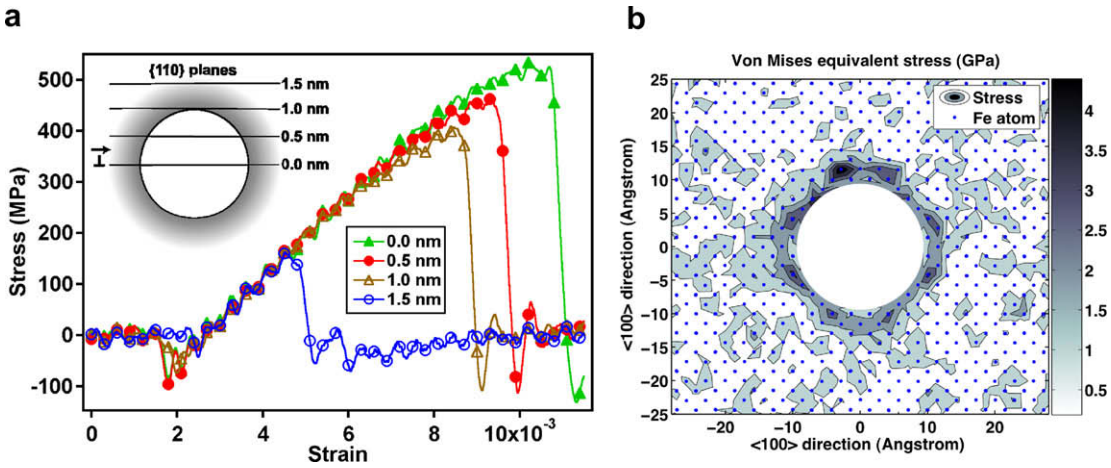

Fig. 2. (a) Stress–strain response of edge dislocation-2 nm void interaction at various dislocation heights, and (b) von Mises equivalent stress map of lattice surrounding the void after annealing for 5 ps at 100 K by MD.

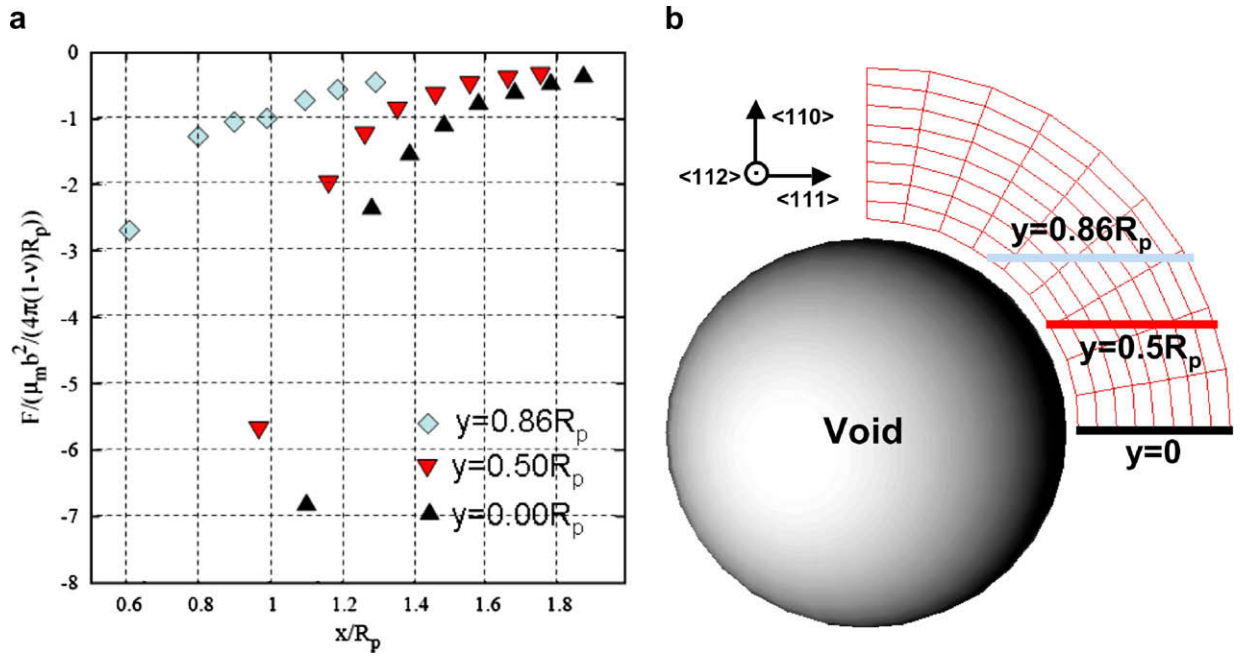

Fig. 4. (a) Normalized image force induced on an edge dislocation located at *x/Rp* from the void centre, where *Rp* is the void radius, obtained by DDD–FEM simulations, and (b) schematic of void and dislocation glide planes at various heights.

(Fig. 2(b)). The stress–strain response results thus, from the interaction of the stress field around the void with that of the dislocation bottom region.

In addition, MD results show that the edge dislocation is attracted by the void as indicated by the dislocation bowing towards the void just before touching it (Fig. 3(b)). This points at the effect of the image forces induced by the internal free surface, even though the void is nanometric. Image forces on a dislocation arise from the interaction of the dislocation strain field with an interface due to elastic constants mismatch between the two sides. It is called 'image' force as it increases inversely proportional to the distance of dislocation to the interface, as if it was interacting with a virtual dislocation in the other side of the interface. This force is attractive here due to zero elastic constants in the void and the dislocation tends thus to escape in the free surface.

The exact same geometry was reproduced in DDD–FEM simulation. It was observed that the presence of an edge dislocation in the vicinity of the void could generate a stress field in the void surrounding due to image forces (Fig. 1). Fig. 4(a) shows the results of a static simulation where the image forces are computed for different position of the dislocation. Each point corresponds to a DDD–FEM computation. Image forces induced by the presence of the void free surface are computed on an infinitely long edge dislocation located at a distance *x* from the void center taken along ⟨1 1 1⟩ direction and at a height *y* measured along ⟨1 1 0⟩ direction (Fig. 4(b)). As depicted in Fig. 4(a), image forces are always attractive and the highest for an edge dislocation located in the sphere mid plane and decreases with increasing dislocation glide plane height.

These results are in good agreement with the ones observed by MD simulation, e.g., in Fig. 3(b), showing the dislocation attraction by the void. Again, image forces push the edge dislocation towards the void. In addition image forces will force the dislocation to be perpendicular to the free surface (e.g. Fig. 3(d)). This seems to hinder the dislocation release from the void. It should be noted that the obstacle strength depends mainly on exit mechanisms, which relate to the mobility of the screw parts of the interacting dislocation [7].

4. Conclusion

Various simulation methods are capable to describe the nanoscale phenomena occurring after the irradiation in materials, which are difficult to observe and explore with experimental methods. In this paper, MD simulations were compared to DDD simulations in the case of the interaction of an edge dislocation with a void. It is found that the image forces induced by the void free surfaces push the dislocation toward the void. This effect decreases with increasing distance of the dislocation glide plane relative to the void center. In addition, increase in dislocation height weakens the dislocation–void interaction because of decrease in the void sheared area by the dislocation. It appears that the stress field surrounding the void also impacts the dislocation mobility, in that it hinders its passage in the vicinity of the void. The DDD simulation could successfully reproduce at the near-atomic scale the image forces due to the internal free surface of the void and its reduction with increasing the dislocation glide plane height.

Acknowledgments

This work, supported by European Communities under the contract of association between EURATOM and Confédération Suisse, was carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission. The Paul Scherrer Institute is acknowledged for the overall use of the facilities.

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