Nuclear Instruments and Methods in Physics Research B 272 (2012) 33–36

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

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

Molecular dynamics simulation of ion focusing and crowdion formation in self-ion-irradiated Fe

Di Chen, Lin Shao *

Department of Nuclear Engineering, Texas A&M University, College Station, Texas 77843, United States

ARTICLE INFO

Article history:
Available online 2 February 2011

Keywords:
Molecular dynamics
Ion radiation
Iron
Interstitials
Vacancies

ABSTRACT

We have used molecular dynamics (MD) simulation to investigate damage and defect development in a ⟨1 0 0⟩ Fe substrate upon 2 keV Fe ion bombardment. The damage cascade formation is accompanied by atomic shifting over a limited distance along the direction of one atomic row, which leads to formation of crowdions aligned with ⟨1 1 1⟩ direction. At the end of structural relaxation and defect recombination, crowdions lead to formation of dumbbell defects – a type of vacancy–interstitial complexes having one vacancy between a pair of slightly displaced interstitials. The dumbbell defects are initially oriented along ⟨1 1 1⟩ direction. After a typical period of 0.2 ps, some dumbbell defects rotate towards ⟨1 1 0⟩ direction. Crowdion and dumbbell defect formation influence the time dependent damage buildups.

1. Introduction

Radiation damage resulting from ion solid interactions has been a subject of intensive research efforts during the past decades [1]. While studies on semiconductors and insulators are primarily driven by the need for ion beam modification [2], studies on radiation damage in metals has been driven greatly by the needs for materials applications in harsh environments, i.e. fission and fusion reactors [1,3]. Progress towards fundamental understanding of defect developments has been aided by emerging atomic scale characterization and quantum mechanics many-body simulations. Among them, molecular dynamics (MD) simulation is an important modeling tool to reveal the damage development at early stage of a few picoseconds. This time scale corresponds to damage cascade formation, a phenomenon involves damage deposition and subsequent quenching process in a period so short that materials behaviors cannot be predicted by knowledge obtained under equilibrium conditions [3].

Early MD simulation showed that damage cascade is featured by a vacancy rich core surround by an interstitial shell [3]. Damage cascade forms when the mean flying distance of projectile becomes comparable to the mean atomic distance of a target solid, thus they are created when projectiles or recoiled target atoms have a typical energy of a few keVs [3]. Later MD simulations show additional features of damage cascades [1]. A chain-like atomic displacements, so called crowdion [4], is formed along certain atomic row directions. Crowdion is initialized from the damage cascade core, and is a consequence of subsequent displacements along an atomic row. In literature, such displacements are described as ion focusing–atomic shifting over a limited distance along the direction of one atomic row. Displacements end when the last displaced atom does not have enough kinetic energy to displace the next atom.

At the end of damage cascade formation, most point defects disappear due to kinetic defect recombination. Surviving defects begin to take stable configurations after structure relaxation [5]. These defects are precursors to extended defects, which are the source of series of materials degradation phenomenon [5–7]. In this study, crowdion formation in self ion irradiated iron (Fe) is investigated by using MD simulation to obtain further atomic scale details.

2. Molecular dynamics simulation

MD simulation was performed by using LAMMPS (Large-scale Atomic Molecular Massively Parallel Simulator), an open source code maintained by Sandia National Laboratory [8]. The details about the parallel spatial-decomposition, neighbor-finding and communication algorithms can be found in Ref. [8]. The Fe–Fe interatomic potential was described by embedded-atom method (EAM) [9]. EAM is based on fitting to both experimental results and first principle calculations, and predicts thermal and mechanical properties with high accuracy. The EAM potential is generally superior to the second-moment approximation of the tight-binding method for simulation of metals [10]. In MD simulations, one 2 keV Fe atom bombarded a bcc Fe at room temperature, with an incident angle of 9° to avoid channeling effect. Random thermal oscillation of atoms, which is crucial to simulate defect reactions,

* Corresponding author.
E-mail address: lshao@mailaps.org (L. Shao).

0168-583X/$ - see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.nimb.2011.01.027

has been considered by following the standard procedure in MD simulation of damage creation [11]. The inelastic energy loss is not considered since electronic stopping is negligible for such low energy ion irradiation. The Fe target has a cell size of 14 $\times$ 14 $\times$ 14 nm which contains about 250,000 atoms. Periodical boundary conditions, except for the surface, were used but the cell size was large enough to contain a single damage cascade completely without damage overlapping. Damage developments up to 30 ps were simulated at a time step of 0.25 fs. An atom became an interstitial when it was located away from the lattice site with displacements at least 0.3 of lattice parameter [12]. A vacancy was created if there was no atom within the radius of 0.3 of lattice parameter [12]. The above criteria have been used generally in MD simulation of iron, with good sensitivity to identify dumbbell defects.

3. Results and discussion

Fig. 1 shows damage cascade evolution at 0.1 ps, 0.3 ps, 1 ps, and 30 ps after ion bombardment. For best imaging, the cell size is much smaller than the super cell used in MD simulation. The red circles refer to vacancies and the green circles refer to interstitials. From 0.1 ps to 0.3 ps, damage cascade volume is increasing. Also at 0.3 ps, chain-like crowdion defects form with a length ranging from 2 nm to 5 nm. The crowdion defect formation is realized by a series of substituting collisions, with a typical knock-on energy close to 30 eV (Fe displacement energy). At 1 ps, significant defect recombination leads to shrinkage of the damage cascade volume. Defect recombination also restores displacements along crowdions, but leave dumbbell defects at the end of crowdions. One dumbbell defect is featured by two interstitials sitting at each side of an empty lattice site. MD simulations show that the two interstitials are oriented along original crowdion direction. At 30 ps, most defects disappear. It is worthy to note that at this time scale dumbbell defects resulting from crowdion formation represent a considerable fraction of surviving defects.

Fig. 2 plots interstitial and vacancy numbers as a function of times. Displacements first increases, then decrease at a time longer than 0.3 ps. Interstitial and vacancy numbers are roughly the same at the beginning but vacancies begin to be slightly richer at about 0.3 ps, which corresponds to the time reaching a maximum cascade volume. Our analysis further suggests that the defect imbalance is caused by sputtering of atoms from the surface, which occurs when the damage cascade begins to touch the surface significantly.

One important feature observed in Fig. 2 is that beyond 0.3 ps, defect numbers show a second peak at about 0.45 ps. The time dependent damage buildups can be described by a small Gaussian peak superimposed on a big one. The second peak is attributed to delayed defect creation due to crowdion formation. While the damage cascade core begins to have defect recombination, crowdions are being formed. The time difference between 0.3 ps and 0.45 ps represents an effective lifetime of crowdion defects. The defects survived from crowdion relaxation play a role in determining the tail region of the curve. From 0 ps to 0.3 ps, the displacement buildups have a smooth curve which means the total number of defects is large enough that two peaks observed cannot be explained by statistic fluctuations. This has been further confirmed by repeating ion bombardment with different bombardment conditions, i.e. by changing incident angles (See Fig. 3).

Fig. 4 shows the relaxation of a typical crowdion defect as a function of times. At beginning, the crowdion is aligned along ⟨1 1 1⟩ direction. With increasing times, crowdion shrinks and, at times beyond 0.6 ps, the survived dumbbell defects begin to rotate

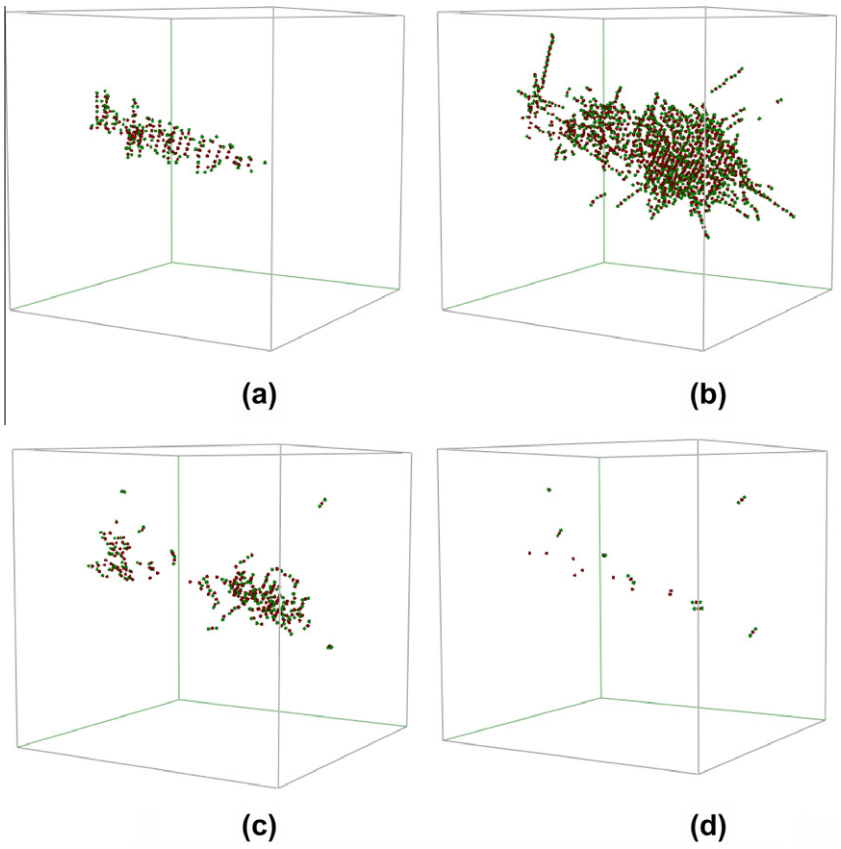

Fig. 1. Damage cascade evolution from MD simulation of a bcc ⟨1 0 0⟩ Fe crystal irradiated by one 1 keV Fe ion at 0.1 ps, 0.3 ps 1 ps, and 30 ps.