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Generation of shock waves in iron under irradiation

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ABSTRACT

Molecular dynamics simulation is employed to study peculiarities of the formation and propagation of shock waves generated by atomic displacement cascades in iron crystallites under irradiation. The interaction of shock waves with point defects and their clusters is investigated. Atomic interactions are described with the use of the pair central-symmetric potential. Parameters of shock waves generated by atomic displacement cascades are evaluated and their dependence of the crystallographic direction, energy of a primary knock-on atom, and crystallite temperature is determined. These waves are shown to cause point defect clusters to rearrange.

1. Introduction

It is common knowledge that primary radiation damage of materials is caused by atomic displacement cascades produced due to collisions of high energy neutrons with lattice atoms. This results in collective atomic displacements and formation of point defects and their clusters [1–4]. Besides, atomic displacement cascades heat locally the material and generate shock waves that propagate over large distances from the cascade core [5–8]. For example, the theoretical model based on experimental observations has been developed in [8], which gives estimates of the volume influenced by atomic displacement cascades through shock waves. In particular, it explains the formation of amorphous zones during Ni ion implantation into polycrystalline Al, their size and density. According to this model each displacement cascade produces "the volume of influence" in which temperature and point defect concentrations are such that enhanced diffusion leads to precipitation of Ni atoms in this volume and further amorphization. At a rather high primary knock-on atom (PKA) energy atomic displacement cascades are split into subcascades [9] that also generate their shock waves. The interaction of these waves can affect not only structural defects existing in the material, but also the evolution of the atomic displacement cascade. The effect of these waves on evolution of atomic displacement cascades has been studied elsewhere [6,7,10]. The authors of [6] relate the formation of large clusters of self-interstitial atoms (SIAs) at the cascade periphery to supersonic shock waves generated by an atomic displacement cascade. According to their calculations, for the time less than 0.1 ps after the initiation of PKA hypersonic recoils could appear in the cascade. These atoms pass ahead a shock wave from the main cascade and generate its own. When they meet, the wave from the main cascade injects atoms to low density regions formed by hypersonic recoils. At subsequent recovery of the crystallite structure injected atoms become interstitial and form a cluster. Atomic displacement cascades in copper and nickel thin films are simulated in [7]. The authors note collective atomic displacements resulting from the cascade generated well away from the crystallite surface. The analysis of the simulation data shows that the atomic displacement cascade heats the radiation-damaged area, which leads to high internal stresses in the vicinity of this area. These stresses induce the formation of an interstitial dislocation loop, which terminates at the surface and presents a well-ordered island of adsorbed atoms. The influence of atomic displacement cascades on pre-existing point defects in copper, aluminum, gold, platinum, and silicon is studied in [10]. The simulation results illustrate that cascades have little or no effect on the distribution of pre-existing point defects outside the liquid core of the cascade while in gold heating of the crystallite due to the cascade causes SIAs to migrate.

The crystal structure of real materials always contains various defects [11–13]. It is therefore interesting to study peculiarities

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of interaction of shock waves generated by atomic displacement cascades with structural defects of the irradiated material.

2. Material and method

The investigation is carried out on iron, whose alloys are widely used in nuclear power engineering. All calculations employ the molecular dynamics method using the LAMMPS package [14]. The atomic interaction is described using the pair central-symmetric potential [15] taking into account the contribution of many-body interactions in the approximation of valence-electron gas. The selected potential permits a highly accurate description of elastic properties of the material, energy of nucleation and migration of point defects, lattice parameter and threshold displacement energy, which is essential for the correct simulation of primary radiation damage. The simulated crystallites contain from 200 thousand to 84 million atoms and have a cubic form with ⟨1 1 0⟩ axes. Periodic boundary conditions are set in all directions. The PKA energy ranges from 15 eV to 40 keV. The temperature of specimens is set to 0, 10 and 300 K.

3. Generation of elastic waves at primary radiation damage

Note that shock waves are always generated at the atomic level due to an elementary act of radiation, i.e., generation and annihilation of a Frenkel pair. In the present paper the formation of such defect is simulated by specifying a momentum to an atom. The calculations are performed at 0 K for the three directions of the PKA momentum: [1 0 0], [1 1 0], and [1 1 1]. The PKA energy (15 eV) is so chosen as to be slightly less than the minimum threshold displacement energy for the considered directions of the PKA momentum (the minimum value for the [1 0 0] direction comprises 16 eV).

Fig. 1 illustrates the stress distribution in slices of the simulated iron crystallites after the generation of PKAs in them. The studied fragments contain PKAs and present layers composed of three atomic planes. In all cases the PKA momentum is directed along the *X* axis. The assigned PKA momentum results in shock waves. First propagates a compression shock wave (blue color, negative stress) and then follow a tension wave (red color, positive stress) and weaker disturbances. Note that the shock wave front propagates with different velocities along considered directions, which makes its shape different from a spherical one [16–20]. Thus, for PKA momentums along ⟨1 1 0⟩ and ⟨1 1 1⟩ the wave front is in the same direction while for those alone ⟨1 0 0⟩ the wave propagates with the highest velocity in the close-packed directions [1 ± 1±1]. Due to internal friction and expansion of the generated front the wave amplitude decreases with time (Fig. 2).

A wave initiated by a PKA has the highest amplitude and lowest attenuation if its momentum is applied in the close-packed direction ⟨1 1 1⟩. In this case within 0.3 ps a dynamic crowdion is formed in the direction in which the focused shock wave propagates with the supersonic velocity ~12500 m/s to a distance of about 5 nm. After the crowdion recombination the initiated shock wave propagates with the sound velocity of ~6200 m/s. At the PKA displacement along ⟨1 0 0⟩ the focused wave propagates through the atom chain along this direction for 0.15 ps at the supersonic velocity ~9500 m/s. As atoms in the chain regain their sites, the wave velocity reduces to the sound one. The material behaves differently in a ⟨1 1 0⟩ direction of the PKA momentum. In particular, there is no focused collisions. During the first 0.05 ps the PKA momentum is transmitted to atoms in the [1 1 0], [1 1 1] and [1 1 $\bar{1}$] directions with subsequent return of PKA to its site. As this takes place, the initiated wave propagates with the sound velocity at all time during the calculation. It should be noted that up to the temperature 300 K the curve form is similar to those for 0 K, except for the region of linear attenuation of the stress wave amplitude, where its values for higher temperatures are 2–5 GPa lower. First of all, this is due to thermal fluctuations affecting the generation and propagation of shock waves.

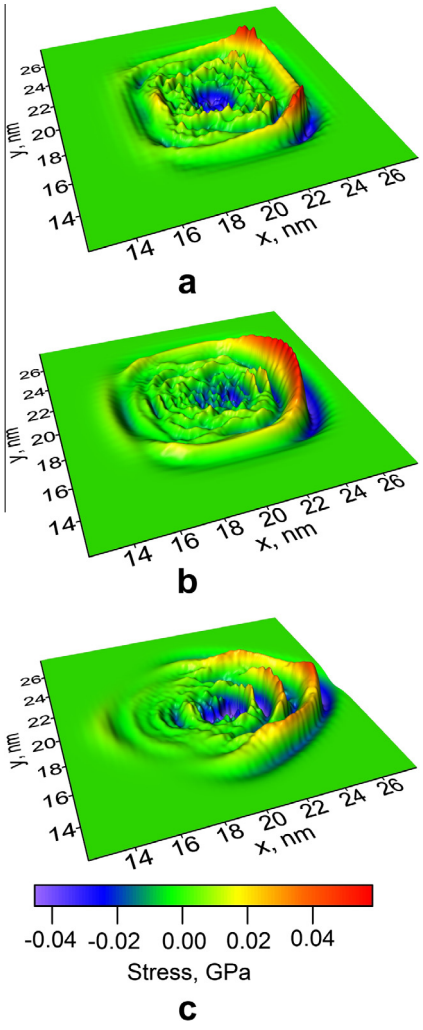

Fig. 1. Stress distribution at the time moment 0.9 ps in slices of the crystallites for different directions of the PKA momentum: (a) [1 0 0], (b) [1 1 0], and (c) [1 1 1]. The crystallite temperature is 0 K.

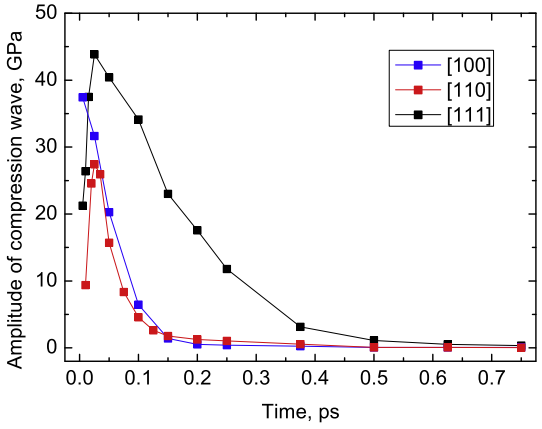

Fig. 2. Amplitude of compression waves after the generation and annihilation of a Frenkel pair versus time for different directions of the PKA momentum.