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Citation: AIP Conference Proceedings **1683**, 020095 (2015); doi: 10.1063/1.4932785
View online: http://dx.doi.org/10.1063/1.4932785
View Table of Contents: http://aip.scitation.org/toc/apc/1683/1
Published by the American Institute of Physics

Mobility of Edge Dislocations in Stressed Iron Crystals During Irradiation

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Abstract. The behavior of $a/2\langle 111\rangle\{110\}$ edge dislocations in iron in shear loading and irradiation conditions was studied by means of molecular dynamics simulation. Edge dislocations were exposed to shock waves formed by atomic displacement cascades of different energies. It was shown that starting from a certain threshold amplitude shock waves cause displacement of edge dislocations in the loaded samples. Calculations showed that the larger the shear load and the amplitude of the shock wave, the greater the displacement of dislocations in the crystallite.

Keywords: edge dislocation mobility, shock waves, shear loading, atomic displacement cascades, molecular dynamics

INTRODUCTION

Irradiation creep of structural materials is largely determined by the mobility of dislocations in them. It also depends on the presence of other defects as well as internal stresses in the irradiated material. We note that the primary radiation damage is accompanied by the formation of shock waves [1–5] generated by atomic displacement cascades [6–9]. These waves can cover a sufficiently large distances from the core of cascades. They are responsible for the manifestation of such phenomena as “radiation shaking” [10], long-range effect [11], etc.

For example, it was shown by Kirsanov and Zhetbaeva [10] that radiation exposure can increase the mobility of point defects in the material. The authors proposed a mechanism of radiation-enhanced diffusion (“radiation shaking”), by which the generation and annihilation of unstable Frenkel pairs lead to the migration of interstitial atoms. Its essence lies in the fact that the generation and annihilation of Frenkel pairs in the material cause formation of the elastic waves associated with a local change of the atomic volume. The interaction of these waves with defects allows them to overcome migration barriers and facilitates their movement. This mechanism of radiation-enhanced diffusion was confirmed by the molecular dynamics simulations of generation and annihilation of Frenkel pairs in iron [5, 10].

Note that the shock wave interaction with dislocations may cause them to displace and thus contributes to irradiation creep of materials. Besides, preliminary mechanical loading influences not only the generation of shock waves and their parameters, but also the features of their interaction with the structural defects, particularly dislocations. Currently, irradiation creep of mechanically loaded materials (most parts of constructional details are subjected to a mechanical load) is insufficiently understood.

Due to this, the aim of this work is to study the elementary acts of irradiation creep in mechanically loaded crystal of iron. Within the framework of the molecular dynamics method [12–17] the features of $a/2\langle 111\rangle\{110\}$ edge dislocation motion caused by their interaction with the shock waves of varying amplitude in the loaded iron crystallite were studied.

Advanced Materials with Hierarchical Structure for New Technologies and Reliable Structures
AIP Conf. Proc. 1683, 020095-1–020095-4; doi: 10.1063/1.4932785

COMPUTATIONAL DETAILS

The calculations were performed using the software package LAMMPS [18]. Many-body potential calculated in Finnis-Sinclair approximation was used for a description of the interatomic interactions in iron [19]. The selected potential describes with good accuracy the lattice parameter, the elastic moduli of the material, energetic parameters of point defects, and the threshold displacement energy, etc., which is necessary for correct simulation of plastic deformation, as well as the generation and development of atomic displacement cascades.

The simulated specimen had the form of a parallelepiped with dimensions 40×20×30 nm along the directions $\langle 111\rangle$, $\langle 112\rangle$ and $\langle 110\rangle$, respectively. Its temperature was set at 300 K. Periodic boundary conditions were used in the $\langle 111\rangle$ and $\langle 112\rangle$ directions. For the formation of $a/2\langle 111\rangle\{110\}$ edge dislocation half of one (111) atomic plane in the simulated specimen was removed. The specimen was relaxed at zero pressure and a temperature of 300 K. The loading scheme of the crystallite is shown in Fig. 1. "Hard" and "soft" boundary conditions were used for simulation of shear loading in direction perpendicular to the plane of the dislocation glide. Several atomic layers at the bottom of the sample (block *F*) were rigidly fixed, while constant force in antitwinning direction (indicated by an arrow on Fig. 1) acted on the atoms of the few upper atomic layers (block *S*).

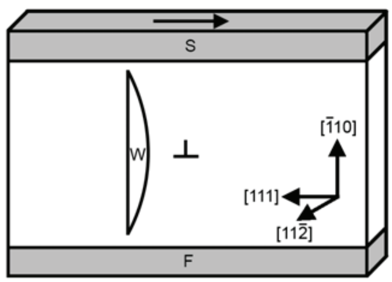

FIGURE 1. Loading scheme of simulated specimen

Shock waves were generated at a distance of 5 nm from the dislocation line. For this a certain velocity was added to atoms in block W whose direction coincides with the direction of the applied shear loading. The defining of a local type of crystal lattice in the neighborhood of each atom was based on the common neighbor analysis [20]. According to this analysis, the position of the dislocation was determined, which corresponds to the position of atoms with symmetry of nearest neighbors different from bcc lattice. The magnitude of the shear stress τ was calculated as follows: the force acting on the block S in the [111] direction from the other atoms of the specimen was divided by the area of the base unit, parallel to $(\bar{1}10)$ plane.

RESULTS AND DISCUSSION

A series of calculations for different values of shear stress and the amplitude of the shock waves were carried out in order to study the features of the irradiation creep in iron. Calculations showed that applying force to the upper block of specimen causes the dislocation displacement on a finite distance. In different series of calculations the force varied from 1.0×10^{-4} to 5.0×10^{-4} eV/A. After that, the shock wave was generated in the specimen, simulating perturbations connected with the formation of atomic displacement cascade.

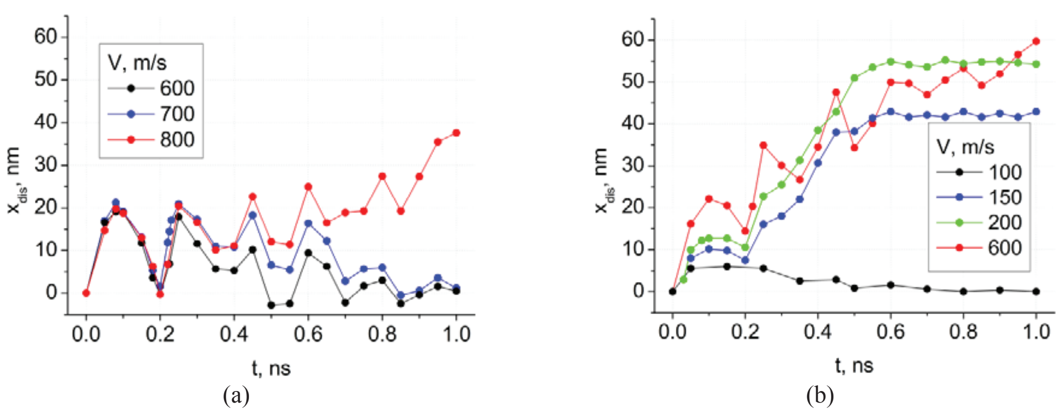

FIGURE 2. The dislocation position versus time for different amplitudes of the shock waves (V) and shear stresses of 7 (a) and 60 MPa (b)

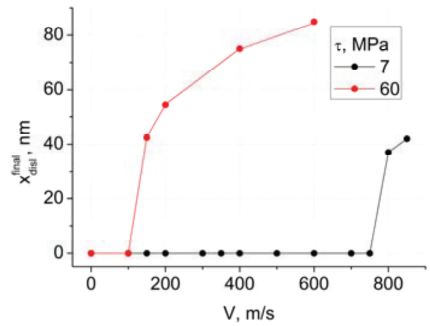

FIGURE 3. The final dislocation displacement versus amplitude of shock waves for different shear stresses

A shock wave propagation in the loaded crystallites leads to a displacement of dislocation if the amplitude of the wave is above a certain threshold. The dislocation position versus time for different amplitudes of the waves is presented in Fig. 2. It is seen that the greater the amplitude of the wave the larger displacement of dislocation in the crystallite. Simulation results showed that increasing shear stress leads to an increase in the dislocation mobility. This is manifested in the fact that shock waves of smaller amplitude at higher stresses displace dislocation on the larger distances. It should be noted that the velocity of the dislocations is approximately constant for each level of shear stress if the wave amplitude is equal or greater than the threshold value. Thus, for $\tau = 7$ MPa, it was 20–25 m/s, and for $\tau = 60$ MPa—100–125 m/s.

The results of comparing the final displacements of dislocations by shock waves in crystallites with varying degrees of shear stresses are shown in Fig. 3. It can be seen that the dislocation displacement in a crystal with $\tau = 7$ MPa requires a shock wave with an amplitude of more than 750 m/s, and for the specimen with $\tau = 60$ MPa is enough to generate a wave with an amplitude of less than 150 m/s.

Propagation of a shock wave in the crystallite leads to oscillations of the upper block of specimen, during which a constant force was applied. The amplitude of oscillation of the upper block increases with growth of the shear stress magnitude and the shock wave amplitude. The decrease of the oscillation amplitude of the upper block over time is due to the decay of the shock wave amplitude as a result of its interaction with the fixed bottom layers. We note that the displacement of dislocations (Fig. 2) correlates fairly well with the corresponding peaks of the curves in Fig. 4.

SUMMARY

On the basis of the calculations we can conclude that the shock waves generated by cascades of atomic displacements may influence on characteristics of dislocation displacements in mechanically loaded materials. The higher the mechanical loading of the material, the less energy of atomic displacement cascade is required to displace a dislocation.

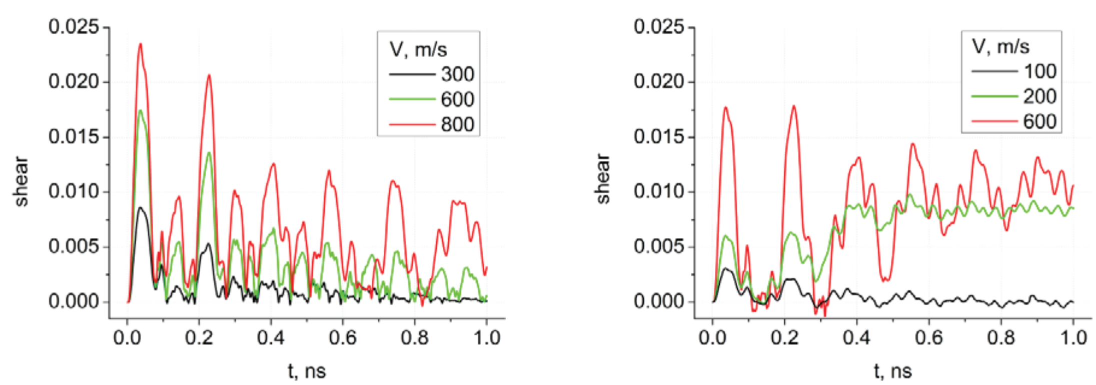

FIGURE 4. Shear versus time for different amplitudes of the shock waves at the shear stresses: 7 (a) and 60 MPa (b)

Distance covered by $a/2\langle 111\rangle\{110\}$ edge dislocation in α-iron after passage of the shock wave through the crystallite can reach tens of nanometers. A shock wave propagation in the loaded crystallites leads to a displacement of dislocation only if the amplitude of the wave is above a certain threshold. For stresses of order of 60 MPa threshold value of wave amplitude is higher than 100 m/s, while for 10 MPa it exceeds 750 m/s. Waves with higher amplitudes cause larger dislocation displacements (up to 85 nm).

ACKNOWLEDGMENTS

The work was performed under the agreement with JSC Bochvar VNIINM and with partial financial support of the Tomsk State University Competitiveness Improvement Program.

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