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Features of Structural Response of Mechanically Loaded Crystallites to Irradiation

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Abstract. A molecular dynamics method is employed to investigate the origin and evolution of plastic deformation in elastically deformed iron and vanadium crystallites due to atomic displacement cascades. Elastic stress states of crystallites result from different degrees of specimen deformation. Crystallites are deformed under constant-volume conditions. Atomic displacement cascades with the primary knock-on atom energy up to 50 keV are generated in loaded specimens. It is shown that irradiation may cause not only the Frenkel pair formation but also large-scale structural rearrangements outside the irradiated area, which prove to be similar to rearrangements proceeding by the twinning mechanism in mechanically loaded specimens.

Keywords: atomic displacement cascades, plastic deformation, molecular dynamics

INTRODUCTION

The scientific basis for producing advanced materials for nuclear power engineering requires a detailed investigation of the nature and features of structural changes in materials at the atomic level under mechanical, thermal and irradiation action. This is due to the fact that the defect structure affecting operational characteristics nucleates at the atomic level. Dynamic loads and high demands on spatial resolution give no way of experimental observation of the origin and evolution of structural changes at the microlevel. These difficulties might be resolved by using computer simulation methods. One of the most effective approaches to investigate the dynamics of structural rearrangements in the material at the microlevel under high energy action is the molecular dynamics method [1–6].

Structural materials used in nuclear power engineering are subjected, along with irradiation, to thermal and mechanical action [7–9]. Our interest therefore is in determining how significant could be the influence of mechanical load on the radiation-induced behavior. Taking into account the polycrystalline structure of metal materials, it can be supposed that its separate grains are in constrained conditions which affect the development of atomic displacement cascades. Of interest is to determine levels of mechanical load under which the metal response to irradiation differs sufficiently from that of the unloaded material. The present paper carries out the computer simulation of the atomic behavior of crystallites under complex loading, namely, mechanical deformation and irradiation.

MATERIALS AND METHODS

Simulated materials are iron and vanadium, which are widely used as the base in alloys for nuclear power engineering. All calculations are performed within the molecular dynamics method. The interatomic interaction in iron is described using the potential [10], which takes into account the contribution of many-body interactions in the approximation of valence electron gas. Interatomic interactions in vanadium are described by the Finnis-Sinclair many-body potential [11]. The chosen potentials enable an accurate description of elastic characteristics of the material, energy of nucleation and migration of point defects, threshold displacement energies, lattice parameter, etc., which is essential for the correct simulation of origin and evolution of plastic deformation as well as generation and development of atomic displacement cascades (Table 1).

Advanced Materials with Hierarchical Structure for New Technologies and Reliable Structures
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TABLE 1. Computed and experimental values of studied material characteristics at 0 K temperature. a_0—lattice parameter, C_{ij}—elastic constants.

Material characteristic	Fe		V	
	Simulation	Experiment	Simulation	Experiment
a_0, Å	2.8665	2.8600 [12]	0.30200	0.30204 [14]
C_{11}, GPa	243.0	243.1 [13]	238.2	238.2 [14]
C_{12}, GPa	138.0	138.1 [13]	122.0	122.0 [14]
C_{44}, GPa	122.0	121.9 [13]	46.8	46.8 [14]

Crystallites are simulated as parallelepipeds with edges oriented along cubic directions ⟨100⟩. Periodic boundary conditions are set in the calculations. The initial temperature of the simulated specimens is 100 K. Point defects are identified in the investigated crystallites by the following algorithm. Let us build spheres in sites of the initial lattice with the radius 0.3 of the lattice parameter. If a sphere contains no atoms when analyzing the loaded crystallite, the lattice site is assumed to be vacant. The case of more than one atom in a sphere corresponds to interstitial atomic configuration. A local type of the crystal lattice in the vicinity of each atom is determined by the common neighbor analysis.

RESULTS AND DISCUSSION

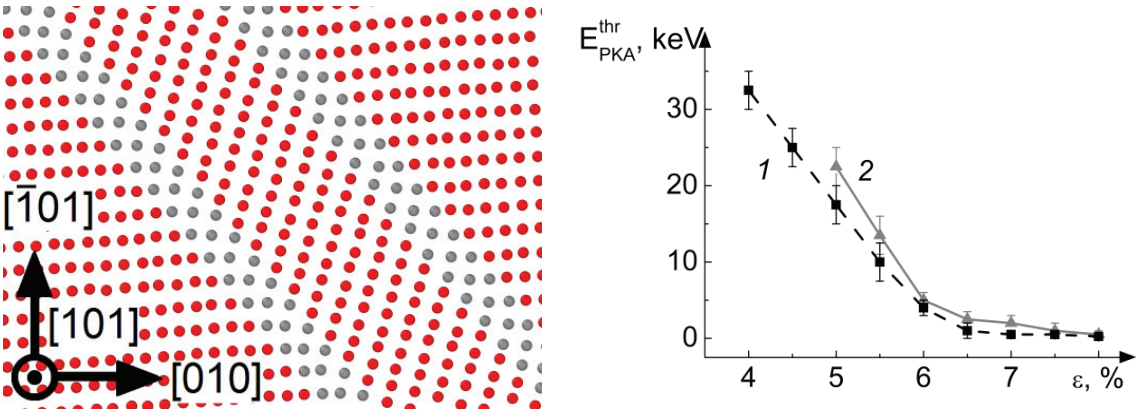
Mechanical Loading

Before simulating the behavior of a mechanically loaded material under irradiation, it is essential to study how plastic deformation originates and develops in the material under mechanical loading. Specimens undergo constant-volume deformation, which corresponds to the grain behavior in the material bulk in constrained conditions under mechanical loading [15]. Crystallites are deformed in the following way: a specimen is extended in the [010] direction with the rate 0.01 m/s and compressed in the other two [100] and [001] directions. The calculations show that a sudden stress decrease in the crystallite occurs at a certain threshold strain. The crystallite behavior in the threshold strain region is associated with the nucleation and development of the defect structure. Defects point to the fact that further accommodation of the structure under mechanical loading is possible only by plastic deformation. It should be noted that the threshold strain obtained in the above results far exceeds an elastic value characteristic of macro-sized specimens. Such behavior is typical of microscopic grains whose elastic region can reach ten and more percent of strain.

The analysis of structural rearrangements shows that twins start to emerge and evolve in vanadium and iron crystallites after reaching the threshold strain. A twin formed in the vanadium crystallite is shown in Fig. 1a. Note that the twin generation in the simulated crystallites is a thermal fluctuation process [16–20]. A similar response with the formation of twin structures is observed in iron crystallites which is in agreement with experiments [21].

Irradiation of Elastically Deformed Crystallites

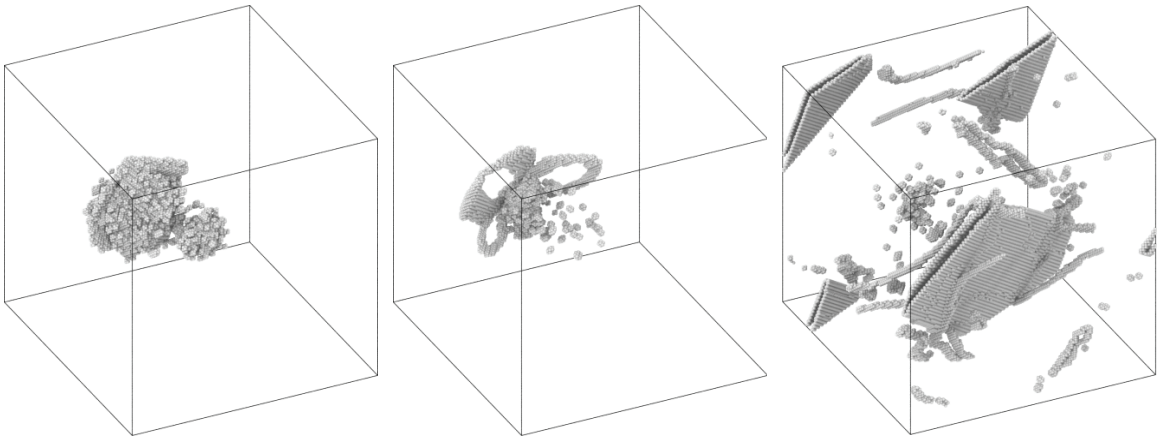
The effect of mechanical loading on the response to irradiation of crystallites is studied according to stress-strain curves. Before generating an atomic displacement cascade, the simulated crystallite is deformed to a certain strain held constant until structural relaxation. For each degree of crystallite deformation we found the minimum value of the atomic displacement cascade energy responsible for both the Frenkel pair formation and large-scale (relative to the simulated crystallite size) structural rearrangements. According to the calculations, the higher the degree of deformation, the lower the threshold energy $E_{\mathrm{PKA}}^{\mathrm{thr}}$ of a primary knock-on atom (PKA) that causes structural changes in the crystal (Fig. 1b). Note that at $\varepsilon > 5\%$ the $E_{\mathrm{PKA}}^{\mathrm{thr}}$ –ε dependences coincide for iron and vanadium specimens within the statistical error. At lower strain $E_{\mathrm{PKA}}^{\mathrm{thr}}$ of the vanadium crystallite increases faster than that of iron, in particular at $\varepsilon = 4.5\%$ it exceeds 50 keV. At the strain 6.5% the curves in Fig. 1b exhibit saturation and the PKA energy inducing plastic deformation is less than 1 keV. It should be noted that for such conditions the strain in the simulated specimens approaches the yield point.



(a) (b)

FIGURE 1. Projection of a slab of the vanadium crystallite onto plane (101) at the strain 9.65 %. Pink circles indicate atoms with the nearest neighbors corresponding to the bcc lattice; gray circles, to the disordered structure (a); the threshold PKA energy at which a cascade causes large-scale structural rearrangements versus the crystallite strain for iron (curve *1*) and vanadium (curve *2*) (b)

Structural rearrangements in the crystallites due to atomic displacement cascades are found to be similar to structural rearrangements induced by mechanical loading of the material. This is exemplified by the iron crystallite structure at different moments of evolution of an atomic displacement cascade (Fig. 2). At the ballistic stage of the cascade only Frenkel pairs form in the specimen (Fig. 2a) and thereafter twinning dislocation loops nucleate in the irradiated area (Fig. 2b). The structural analysis reveals that these dislocations have the Burgers vector 1/2 ⟨111⟩ and are located in planes {112}. Subsequent to accommodation of the material, a twin forms in the crystallite (twin boundaries are shown in Fig. 2c as large plates). Additionally, dislocation loops and point defects are observed in the material.



(a) (b) (c)

FIGURE 2. Defect structure of the iron crystallite extended to 5% at different time moments after generation of atomic displacement cascade: 1 (a), 5 (b), and 40 ps (c). Only atoms corresponding to the disordered structure are represented. The PKA energy is 25 keV

CONCLUSION

We have studied the onset and evolution of plastic deformation in elastically deformed iron and vanadium crystallites due to generation of atomic displacement cascades. If PKA energy is equal or greater than threshold energy irradiation induces not only the Frenkel pair formation but also large-scale structural rearrangements outside the irradiated area. As this takes place, the higher the degree of deformation of a simulated specimen, the lower the cascade threshold energy responsible for the formation and development of plastic deformation. Structural rearrangements in crystallites due to atomic displacement cascades are found to be similar to rearrangements proceeding by the twinning mechanism under mechanical loading of specimens.

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