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Structural changes in elastically stressed crystallites under irradiation

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ABSTRACT

The response of elastically stressed iron and vanadium crystallites to atomic displacement cascades was investigated by molecular dynamics simulation. Interatomic interaction in vanadium was described by a many-body potential calculated in the Finnis–Sinclair approximation of the embedded atom method. Interatomic interaction in iron was described by a many-body potential constructed in the approximation of valence-electron gas. The crystallite temperature in the calculations was varied from 100 to 600 K. The elastically stressed state in the crystallites was formed through uniaxial tension by 4–8% such that their volume remained unchanged. The energy of a primary knock-on atom was varied from 0.5 to 50 keV. It is shown that the lower the temperature and the higher the strain degree of an initial crystallite, the lower the threshold primary knock-on atom energy for plastic deformation generation in the crystallite. The structural rearrangements induced in the crystallites by an atomic displacement cascade are similar to those induced by mechanical loading. It is found that the rearrangements are realized through twinning.

1. Introduction

The creation of advanced materials for nuclear power engineering requires detailed atomic scale research in the peculiarities of structural changes in materials exposed to mechanical loads, heat, and irradiation, because it is at the atomic level that the defect structure responsible for subsequent changes in the performance of materials nucleates [1]. Dynamic loads and requirements for high spatial resolution are a handicap to experimental study of nucleation and evolution of microscale structural transformations. The problem can be solved by using computer simulations. One of the most efficient ways to inquire into dynamics of microscale structural transformations in a material under high-energy actions is molecular dynamics (MD) simulations [2–5].

Structural materials used in nuclear power engineering experience, along with irradiation, thermal and mechanical loads [6]. So it is of interest to elucidate to what extent mechanical loads can affect their radiation-induced behavior. In view of polycrystalline structure of metal materials, part of their grains can be supposed to get stressed due to constrained boundary conditions. Atomic displacement cascades and formation of primary radiation defects in these stressed regions will differ from those in unstressed regions. In this context, it makes sense to define at what loads the radiation response of a metal becomes considerably different from the response of non-loaded material [7–9].

So, the molecular dynamics study of atomic displacement cascades in stressed iron crystallites [7] showed that the number of point defects survived in the crystallites under tension in the direction ⟨1 1 1⟩ was smaller than their number in unstressed crystallites. This effect was well pronounced at a strain of 0.1%. It was supposed that this was due to enhanced mobility of self-interstitial atoms (SIAs) and hence to their intense recombination with vacancies. The number of SIAs in clusters did not depend on applied load, whereas the number of interstitial dumbbells oriented parallel to the tension direction changed with increasing strain. The authors of [8] performed molecular dynamics simulation to study the effect of external stress on the defect production rate and defect cluster size distribution in copper crystallites under the action of atomic displacement cascades. The model crystallites were subjected to uniaxial and overall deformation in the range from −1% to 1%. The calculations showed that the defect production rate in an atomic displacement cascade increased both under uniaxial tension and compression. It was found that larger clusters were generated at higher defect production rates. In the molecular dynamics simulation of generation of atomic displacement cascades in stressed zirconium crystallites [9], the latter were

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deformed along the axes a ([$10\bar{1}0$]) and c ([0001]) of an elementary cell. The uniaxial strain was varied from −1% to 1%. It was shown that the external stress mostly affected the cluster size rather than the number of radiation defects. In particular, the size of SIA clusters increased under loading along the axes a and c, and the size of vacancy clusters increased under tension along the axis a and decreased under compression along the axes a and c. In the present work, computer simulation was performed to study the atomic-scale behavior of crystallites under complex loading: mechanical deformation and irradiation.

2. Materials and methods

The materials under study were iron and vanadium the alloys of which are widely used in nuclear power engineering. All calculations were performed by the molecular dynamics method using the LAMMPS package [10]. Atomic interaction in vanadium was described by the many-body potential [11] calculated in the Finnis–Sinclair approximation [12]. Interatomic interaction in iron was described by a many-body potential [13] constructed in the approximation of valence-electron gas. Repulsive part of these potentials was fitted to universal screened Coulomb potential [14]. The chosen potentials provide good accuracy in describing the elastic characteristics of material, formation and migration energies of point defects, lattice parameter, etc., and this is significant for correct simulation of nucleation and evolution of plastic deformation and atomic displacement cascades.

One of the most important characteristics for simulation of primary radiation damage in a material is the threshold displacement energy E_{TD} which defines the minimum energy necessary for an atom to displace from a lattice site with the formation of a stable Frenkel pair. This characteristic depends on the crystallographic direction of atomic displacement and crystallite temperature [15]. Calculated and experimental values of E_{TD} for iron and vanadium are presented in Table 1. Threshold displacement energy value for each direction was obtained on the base of 500 calculations.

Comparison of the calculated and experimental values of E_{TD} (Table 1) shows that the interatomic potentials used in our study provide quite correct description of the threshold displacement energy in iron and vanadium except for [100] direction in vanadium. Note that calculations with these potentials demonstrate a stable dumbbell configuration of interstitial atoms along

Table 1
Threshold displacement energy for iron and vanadium.

Material	Direction	Temperature (K)	E_{TD} (eV)	
			MD calculation (present paper)	Experiment
Fe	[100]	36	16	17 [16]
	[110]		30	30–35 [16]
	[111]		30	20 [16]
V	[100]	300	15	30 [17]
	[110]		37	39 [17]
	[111]		27	34 [17]

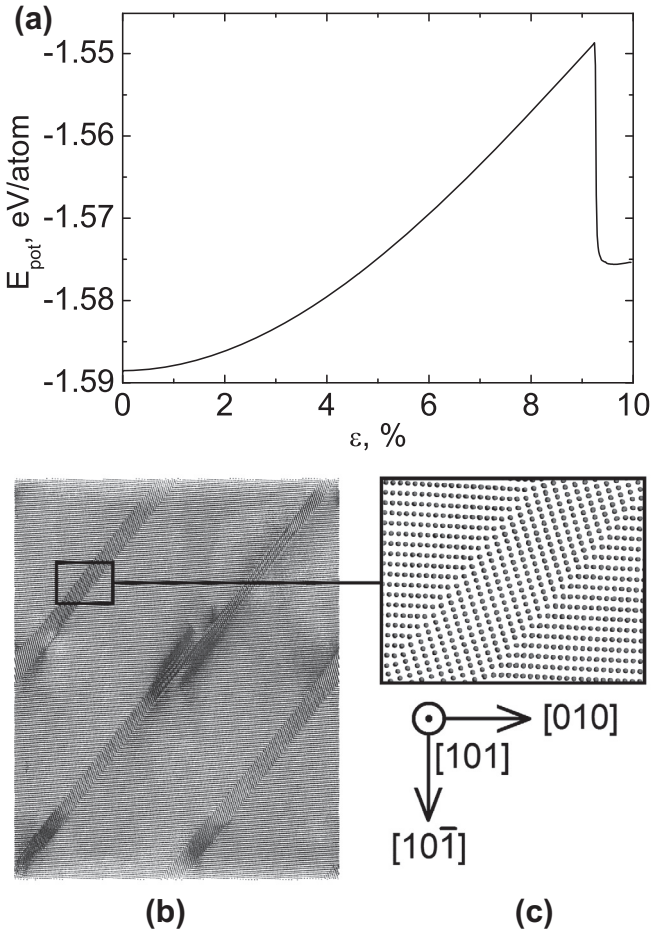

Fig. 1. Potential energy per atom vs. strain in the vanadium crystallite (a); crystallite projection onto the plane (101) at a strain of 9.65% (b); twin-containing structural fragment (c).

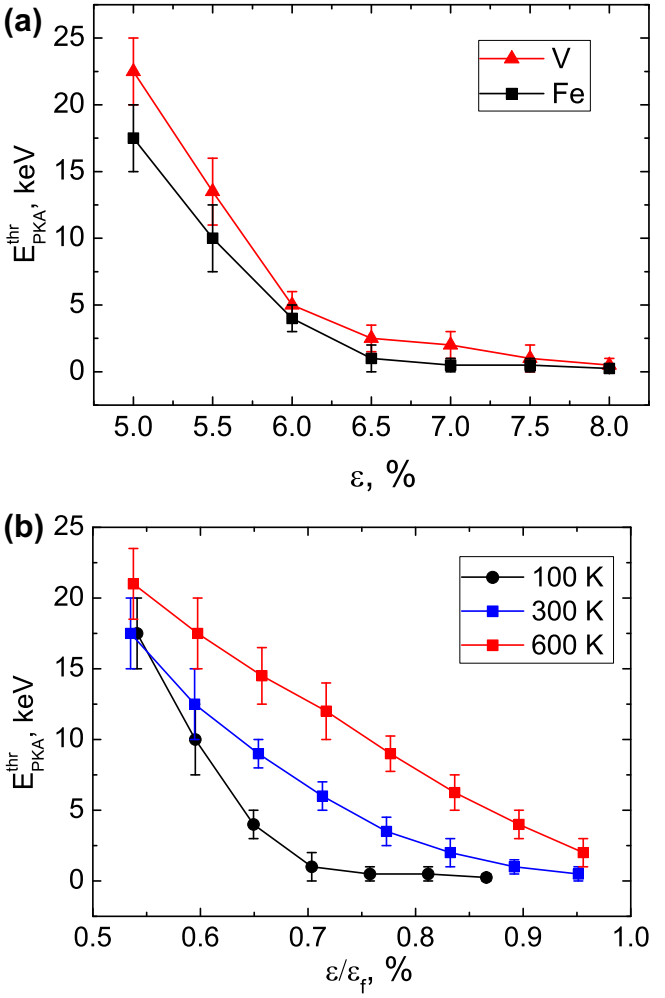

Fig. 2. Threshold PKA energy required for generation of structural rearrangements vs. strain in iron and vanadium (a) and in iron at different temperatures (b).