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Atomistic simulation of structural damage during ion irradiation of iron single crystals

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Abstract. The evolution of atomic displacement cascades initiated near free surfaces with different crystallographic orientations in bcc iron specimens was studied on the base of the molecular dynamics approach. The craters surrounded by adatom mounds were formed in the case of the (111) surface irradiation. The dislocation loops consisted of vacancies were generated after the (110) surface irradiation. The dislocation Burgers vector was a/2 <111> or a <100>. It was shown that the type of structural damage is determined by the anisotropy of propagation of shock waves generated by atomic displacement cascades. For energies of the atomic displacement cascade lower than 20 keV the number of adatoms and survived point defects was higher for specimen with the (110) free surface due to the different character of surface damage. The increase in the cascade energy up to 20 keV results in formation of almost the equal number of survived point defects for the (110) and (111) free surfaces as displacement cascades were developed on larger distance from the irradiated surfaces.

1. Introduction

Ion irradiation has a wide area of application from scientific research to industrial processes. One of the most important is the surface modification of material. Generally, the study of structural changes in the surface region of the irradiated material is conducted for ion energies from tens to hundreds of keV. For such energies ions penetrate in the material to a depth of few tens of nanometers. It is known that collision of ion with lattice atoms leads to generation of atomic displacement cascades near the surface of the material. The peculiarities of generation and evolution of atomic displacement cascades in the surface region during ion bombardment are actively investigated [1-6]. It was shown that the free surfaces have a significant impact on the evolution of atomic displacement cascades. In particular, the number of survived point defects in crystallites with the irradiated surface may be two orders of magnitude greater than the corresponding number in bulk samples [5,6]. If a cascade is generated in the volume of the material the fraction of self-interstitial atoms (SIAs) in the formed clusters is higher than the fraction of vacancies. In the case of the near-surface cascade the fraction of clustered vacancies is always higher than the fraction of SIAs. This is due to the fact that most of the SIAs compared to the vacancies escape to the free surface and form adatom islands on it. The free surfaces influence not only the number and position of survived point defects, but also the type of the formed damage near the surface. In particular, the formation of craters and dislocation loops in the surface region after the ion irradiation was found in the experimental [1-4] and theoretical studies [5,6]. Experiments on Xe^+ ion irradiation of In, Ag, Pb, Au showed that the number of craters per ion increases with an increase in the material density [1]. Dislocation loops in the irradiated metals are

observed in experiments [2-4] and computer simulations [5,6]. For example, a greater number of loops was indicated in the thick iron sample, as compared to the bulk material, irradiated with Fe+ ions of energy 500 keV [2]. Detected loops were identified as interstitial and mostly had the Burgers vector a <100>. Vacancy loops of two types a / 2 <111> and a <100> were formed near the free surface in molybdenum irradiated with ions Sb + [3]. Experimental data on the iron and Fe-Cr alloy irradiated with Fe+ and Xe+ ions of energies 100-150 keV also showed the presence of two dislocation types in samples: a / 2 <111> and a <100> [4]. Similar loops were observed in molecular dynamics simulations when atomic displacement cascades were generated in iron specimens near the (100) and (110) free surfaces [5,6]. Irradiation was carried out with an energy of iron atoms ranging from 25 to 100 keV.
It can be expected that the irradiation of the samples with lower energies will lead to larger structural changes in the surface region, as a cascade will develop closer to the surface. This should also increase the influence of the free surface orientation on the number and character of the distribution of the generated defects. In this connection, the molecular dynamics simulations were conducted to study the features of structural changes in the iron samples during Fe+ irradiation of free surfaces with different crystallographic orientations.

2. Methodology

Simulation of atomic displacement cascades formed under ion irradiation was performed using a software package LAMMPS [7]. Interatomic interaction was described by the many-body potential [8] constructed in the Finnis-Sinclair approximation. The objects of the study were cube-shaped iron crystallites with 20 nm edges. One of the crystallite faces with the indices (110) or (111) was subjected to irradiation. Similar to [9-11] in order to simulate the collision of an ion with the crystallite the momentum directed in the volume of the sample normal to the free surface was given to the one of surface atoms – the primary knocked atom (PKA). The PKA energy in various calculations was ranged from 1 to 20 keV. The temperature of the samples was 300 K. The face opposite to the irradiated surface was fixed in the direction of PKA momentum. Periodic boundary conditions were used in other directions. The determination of the position of point defects (vacancies and SIAs) in the irradiated sample was based on the calculation of the occupancy of the Wigner-Seitz cells. To identify the structure of extended defects and determine the type of generated dislocations Common Neighbor Analisys [12] and Dislocation Extraction Algorithm [13] were used.

3. Results and discussion

The simulation showed that the number of survived vacancies in the bulk is always exceeds the number of SIAs for both free surfaces. This is due to the higher mobility of SIAs, which escape to the free surface and form islands of adatoms on it. The dependence of the number of vacancies and SIAs in the bulk on the PKA energy for the considered free surfaces is presented in Fig.1. The figure shows that in the sample with the (110) surface the number of vacancies and SIAs is larger than in the sample with the (111) surface. This is due to different morphology of the damage caused by cascades on surfaces. The crater surrounded by adatom islands is formed when a PKA with energy of 5 keV or more is generated at the (111) surface (Fig. 3a). In the case of the (110) surface a crater is not formed, although adatom islands are present. They have a larger area and more ordered structure. In the volume of the crystallite near the surface a large cluster is formed, which is a vacancy-type dislocation loop with the Burgers vector a<100> or a/2<111> (Fig. 3b). It should be noted that the local increase of the atomic volume may lead to the formation of a new phase in the material [14, 15].

In the present work the size of the crater on the (111) surface and the vacancy cluster near the (110) surface was estimated and expressed in the number of vacancies. Calculations showed that the sizes of crater and vacancy loop coincide within statistical error. The average size of the crater and dislocation loop as a function of the PKA energy is shown in Fig. 2. Note that the generation of the PKA on the free surface leads to the sputtering of some atoms from the crystallite and escape of atoms to the

surface of the specimen. Their amount increases with increasing the PKA energy. The number of adatoms and sputtered atoms is always higher for the (111) surface. The formation of greater number of sputtered atoms and adatoms during irradiation of the (111) surface explains the lower amount of SIAs in samples with a given surface. For the considered surfaces the difference in the amount of adatoms and the sputtered atoms increases with the growth of the PKA energy and disappears at 20 keV. This is because the main part of the cascade develops at a greater distance from the surface. Therefore, the effect of the irradiated surface orientation on the number of formed defects is reduced.

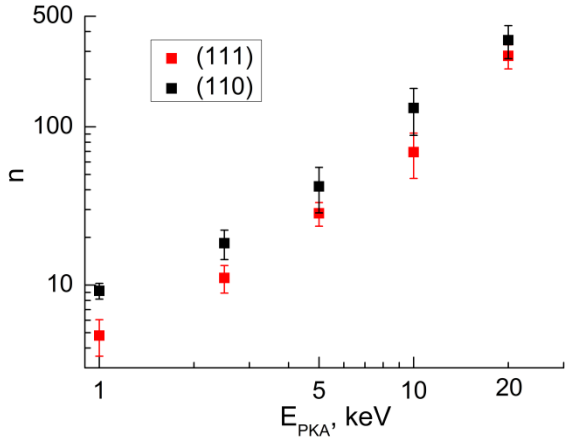


Figure 1. The number of survived point defects in the volume of the crystallite versus the PKA energy for cascades near the free surfaces (110) and (111).

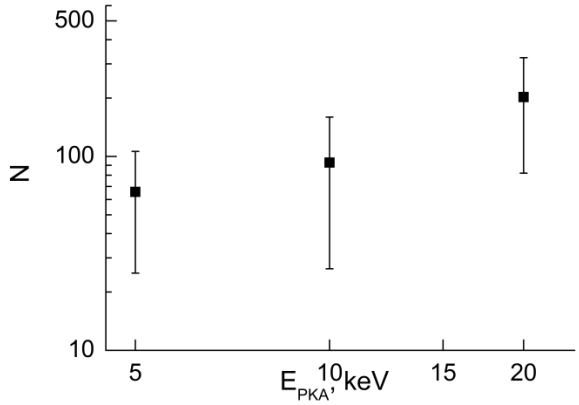
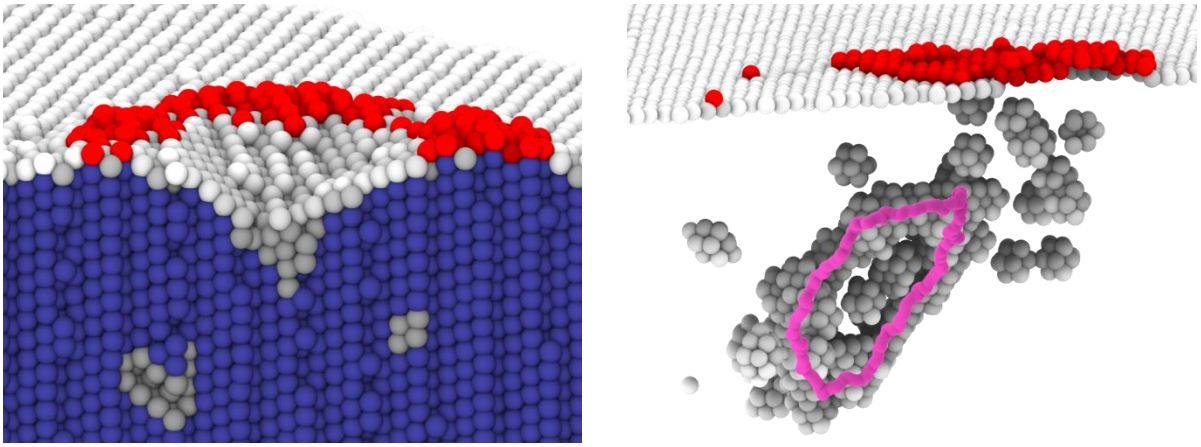


Figure 2. The average size of the crater on the (111) surface and vacancy loop in the sample with the (110) surface (in vacancy count) versus the PKA energy.



(a) (b)

Figure 3. Slices of crystallites containing the crater on the (111) surface (a) and the dislocation loop a<100> under the (110) surface (b). Red color marks adatoms, blue - atoms having the bcc local environment, grey - atoms with a distorted local environment. In figure b atoms with the bcc local environment are not shown, the dislocation with Burgers vector a<100> is highlighted in pink.

Different character of the damage caused by the generation of the PKA on free surfaces is connected with anisotropy of motion of shock waves formed by atomic displacement cascades in the volume of the crystallite [16]. The waves propagating along close-packed directions <111> have the highest amplitude [17]. Under the irradiation of the (111) surface one of these waves reaches the free surface with the amplitude sufficient to form a crater. When the PKA is generated on the (110) surface

the shock wave propagating in the direction normal to the free surface has the amplitude insufficient for the formation of the crater. However, the passage of this wave leads to the escape of large amount of SIAs to the (110) surface. As a result, a large vacancy cluster representing a dislocation loop is formed in the sample.

The formation of a crater on the (111) surface characterized by a denser packing of the atomic planes, compared with the (110) surface, is in good agreement with the experimental data [1]. Authors found that the irradiation of denser materials with ions results in more frequent formation of craters at the free surfaces. It was shown in [6] that the probability of a crater formation increases with decreasing a distance from the atomic displacement cascade to the free surface. This is because the amplitude of the shock waves generated by the atomic displacement cascade is quickly attenuates with the distance traveled.

Calculations have shown that atomic displacement cascades generate shock waves approximately at the same distance from the considered free surfaces. Therefore, the packing of atomic layers parallel to the free surface plays an important role in the formation of the crater or the dislocation loop.

4. Conclusion

The evolution of atomic displacement cascades initiated near the free surface differs significantly from the cascade behavior in the bulk. The type of resulting damage of the irradiated free surface largely depends on its crystallographic orientation. Craters are formed after generation of displacement cascade on the (111) free surface. Dislocation loops of vacancy type are nucleated near the irradiated (110) surface. As a result, the specimen with this surface contains the higher number of survived point defects than the specimen with the (111) surface. Difference in the number of survived point defects vanishes with increasing cascade energy. Formation of a crater or dislocation loop is connected with anisotropic character of motion of shock waves generated by atomic displacement cascades. This anisotropy is caused by different packing of atomic planes parallel to the irradiated free surfaces.

References

[1] Donnelly S E and Birtcher R C 1999 *Philos. Mag.* A **79** 133–45
[2] Prokhodtseva A, Décamps B and Schäublin R 2013 *J. Nucl. Mater.* **442** S786–9
[3] English C A and Jenkins M L 2010 *Philos. Mag.* **90** 821–43
[4] Jenkins M L, Yao Z, Hernández-Mayoral M and Kirk M A 2009 *J. Nucl. Mater.* **389** 197–202
[5] Aliaga M J, Schäublin R, Löffler J F and Caturla M J 2015 *Acta Mater.* **101** 22–30
[6] Osetsky Y N, Calder A F and Stoller R E 2015 *Curr. Opin. Solid State Mater. Sci.* **19**(5) 277–86
[7] Plimpton S 1995 *J. Comp. Phys.* **117** 1–19
[8] Mendelev M I, Han S, Srolovitz D J, Ackland G J, Sun D Y and Asta M 2003 *Philos. Mag.* A **83** 3977–94
[9] Zolnikov K P, Korchuganov A V, Kryzhevich D S, Chernov V M and Psakhie S G 2015 *Nucl. Instr. Meth.* B **352** 43–6
[10] Psakhie S G, Zolnikov K P, Kryzhevich D S, Zheleznyakov A V and Chernov V M 2009 *Phys. Mesomech.* **12**(1–2) 20–8
[11] Psakhie S G, Zolnikov K P, Kryzhevich D S, Zheleznyakov A V and Chernov V M 2009 *Crystallogr. Rep.* **54** 1002–10
[12] Honeycutt J D and Andersen H C 1987 *J. Phys. Chem.* **91** 4950–63
[13] Stukowski A and Albe K 2010 *Modelling Simul. Mater. Sci. Eng.* **18**(8) 085001
[14] Zolnikov K P, Psakhie S G and Panin V E 1986 *J. Phys. F: Met. Phys.* **16**(8) 1145–52
[15] Psakhie S G, Kryzhevich D S and Zolnikov K P 2012 *Tech. Phys. Lett.* **38** 634–7
[16] Zol'nikov K P, Uvarov T Y and Psakh'e S G 2001 *Tech. Phys. Lett.* **27** 263–5
[17] Korchuganov A V, Zolnikov K P, Kryzhevich D S, Chernov V M and Psakhie S G 2015 *Nucl. Instr. Meth.* B **352** 39–42

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