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MOLECULAR DYNAMICS SIMULATION OF NUCLEATION AND GROWTH OF DEFECTS IN THE ALLOY FE-CR IN THE CONDITIONS OF HIGH-ENERGY LOADING

KONSTANTIN P. ZOLNIKOV, ALEKSANDR V. KORCHUGANOV AND DMITRIJ S. KRYZHEVICH

Institute of Strength Physics and Materials Science of Siberian Branch of Russian Academy of Sciences (ISPMS SB RAS)
Akadenicheskii 2/4, 634055 Tomsk, Russia
e-mail: root@ispms.tomsk.ru, web page: http://ispms.ru/en

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Abstract. Features of primary radiation damages in the near-surface layers of the Fe-Cr crystallite were investigated. The calculations were based on the molecular dynamics method. It was found that the number of surviving defects at the generation of atomic displacement cascades near the free surfaces is almost twice their number than in case of cascade generation far away from the various interfaces. Besides it the cascades can knock out some atoms from the free surfaces and form some specific structural defects: craters, adatom islands, dislocation loops of vacancy type. The crystallographic orientation of the irradiated surfaces has a significant influence on the features of the material damage. Craters are much more frequently formed at the irradiation of the (111) surface. There is a correlation between the size of the vacancy loops and the number of adatoms on the free surface. The size of the vacancy loops formed by the irradiation of the (111) surface is slightly larger than the number of adatoms. The inverse relationship was found at the irradiation of the (110) surface of Fe-Cr crystallite.

1 INTRODUCTION

The primary radiation damage of materials is determined by the evolution of cascades of atomic displacements, which are generated in collisions of the decay particles with lattice atoms. The internal structure of the material, as well as the chemical composition has a significant impact on the nature of radiation damage. So, the survived radiation defects near the free surfaces, interfacial and grain boundaries differ in the amount and type from radiation defects in the material with ideal structure [1-4]. Grain boundaries accumulate in their regions the greatest number of the generated radiation defects [5,6]. They formed the largest clusters of point defects. Features of the radiation damage evolution near the free surfaces associated with the formation of craters and adatom islands on the surface of the irradiated material, as well as the escape of the generated defects onto the surface. As a result of collision of the decay particles and atoms of the surface layer, usually a certain number of atoms is knocked out from a sample.

It is expected that the generation of atomic displacement cascades with energies less than 50 keV in the surface region most significantly affects the radiation damage of the material. This is due to the fact that the evolution of the cascade occurs in the vicinity of the surface. The aim of this work is investigation of peculiarities of the radiation defect evolution in the atomic displacement cascades in the Fe-10Cr crystallite near free surfaces with different crystallographic orientations.

2 FORMALISM

Primary radiation damage near free surfaces of the Fe-10Cr alloy was studied on the base of the molecular dynamics method [7-9]. Simulations were performed in the LAMMPS package [10]. The interaction between atoms was described by the many-body potential constructed according to the concentration-dependent embedded atom method [11]. The collision of decay particle with the crystallite was simulated by setting a momentum to the one of surface atoms – the primary knocked atom (PKA). Direction of PKA momentum was perpendicular to the free surface. Periodic boundary conditions were applied in other two directions. The PKA energy was equal to 20 keV. Simulated crystallites had the cubic shape with 20 nm edges. The irradiated free surface had the (110) or (111) indices. The temperature of the crystallite before irradiation was 300 K. Concentration of Cr was 10 at.% which is close to concentrations for majority of steels applied in nuclear power plants. About 40 calculations with different PKA positions for each irradiated surface were made. The occupancy of Wigner-Seitz cells was calculated to identify point defects in irradiated crystallites. Analysis of extended defects, such as craters and dislocation loops was based on the Common Neighbor Analysis [12] and the Dislocation Extraction Algorithm [13]. Visualization of investigated structures was performed in the OVITO software [14].

3 RESULTS AND DISCUSSION

The evolution of cascades of atomic displacements can be characterized by three stages. The ballistic stage lasts from the generation of cascade of atomic displacements until a number of defects in the cascade reaches its maximum size. At the recombination stage, the number of radiation defects decreases as a result of annihilation of the formed self-interstitial atoms (SIAs) and vacancies. It finishes when the number of radiation defects reaches saturation. At the steady stage, the number of radiation defects is subject to weak fluctuations, associated only with thermal and diffusion processes in the material.

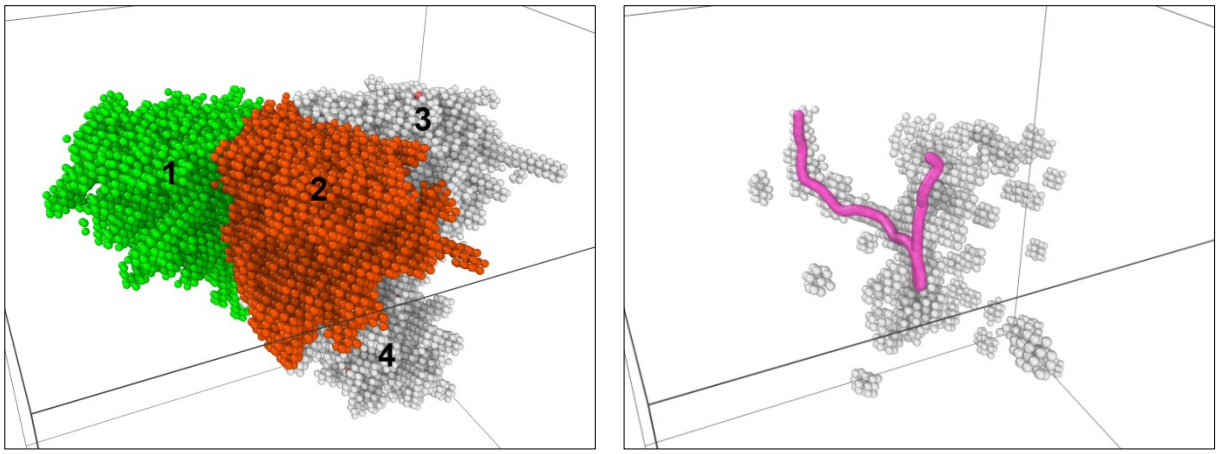
Calculations showed that twice more radiation damage is formed at the steady stage of cascade with an energy of 20 keV near the free surface, than at the same energy cascade in the volume far from the interfaces. This is due to the knockout of atoms from the surface of the sample and the formation of a number of specific structural defects: craters, dislocation loops of a vacancy type, adatom islands. Approximately 250 point defects survive (this is without taking into account surface defects such as adatoms and craters) in the near-surface region of the material. In the case of cascade generation in the material bulk, approximately 110 point defects survive and some of which form small clusters.

The Table 1 presents the calculation results of the number of survived radiation defects at the generation of cascades of atomic displacements in the volume of the material and in the regions of the (111) and (110) free surfaces. The number of vacancies, without taking into

account vacancy loops, is approximately the same for cascades near irradiated surfaces, and for cascades in the bulk of the material. The number of SIAs survived in the free surface regions is approximately half that in the volume of the material. This is explained by the SIAs escape onto the free surfaces and by the knocking out of atoms from the irradiated surface at the ballistic stage of the cascade. It can be seen from the table that the number of adatoms on the (110) surface is somewhat higher than on the (111) surface.

Table 1: The number of radiation defects in the steady stage formed by cascades of atomic displacements with energy of 20 keV in different regions of Fe-Cr crystallite

Cascade type	Number			Average size, vacancies		
	Vacancies	SIAs	Adatoms	Crater	½<111> loop	<100> loop
Bulk cascade	54±3	54±3	-	-	-	-
(110) surface cascade	46±3	26±2	176±26	-	63±8	101±12
(111) surface cascade	53±3	28±2	127±18	105±16	113±18	75±9



a) b)

Figure 1: The defect structure of the crystallite with the irradiated (110) surface at different stages of cascade evolution: a) the end of the ballistic stage, b) the steady state. Only atoms which symmetry of the nearest environment is different from the bcc lattice are shown. Subcascades are numbered by digits. The pink line shows the <100> dislocation

The simulation results showed that near-surface cascades lead to the formation of sufficiently large vacancy loops with the 1/2 <111> and <100> Burgers vectors. When the (110) surface is irradiated, the <100> vacancy loops are mainly formed in the material. In the case of the (111) surface, the 1/2 <111> vacancy loops are formed. The loop size was determined by the number of vacancies from which they are consisted. The average size of vacancy loops depends on the orientation of the irradiated surface. It should be noted that the cascades of atomic displacements generated in the bulk of the material do not lead to the formation of vacancy loops (Table). Calculations showed that craters, as a rule, are formed

during the generation of cascades of atomic displacements on the (111) surface. The formation of craters on the (110) surface is much less frequent. The results of the simulation are in good agreement with experimental [15,16] and theoretical data [1,2].

A cascade of atomic displacements near the (110) free surface at different stages of evolution is shown in Fig. 1. At the ballistic stage, the cascade consists of four subcascades (Fig. 1a). The displaced atoms in the region of the main subcascades, whose energy exceeds 50% of the kinetic energy of the whole cascade, are colored green and orange. At the end of the recombination stage, the largest vacancy loop is formed in this region (Fig. 1b).

The character of the radiation damage of the crystallite structure after the cascade generation on the (110) and (111) free surfaces is shown in Fig. 2. It is clearly seen that the crater is formed on the (111) surface and the vacancy loops arise in the near-surface regions.

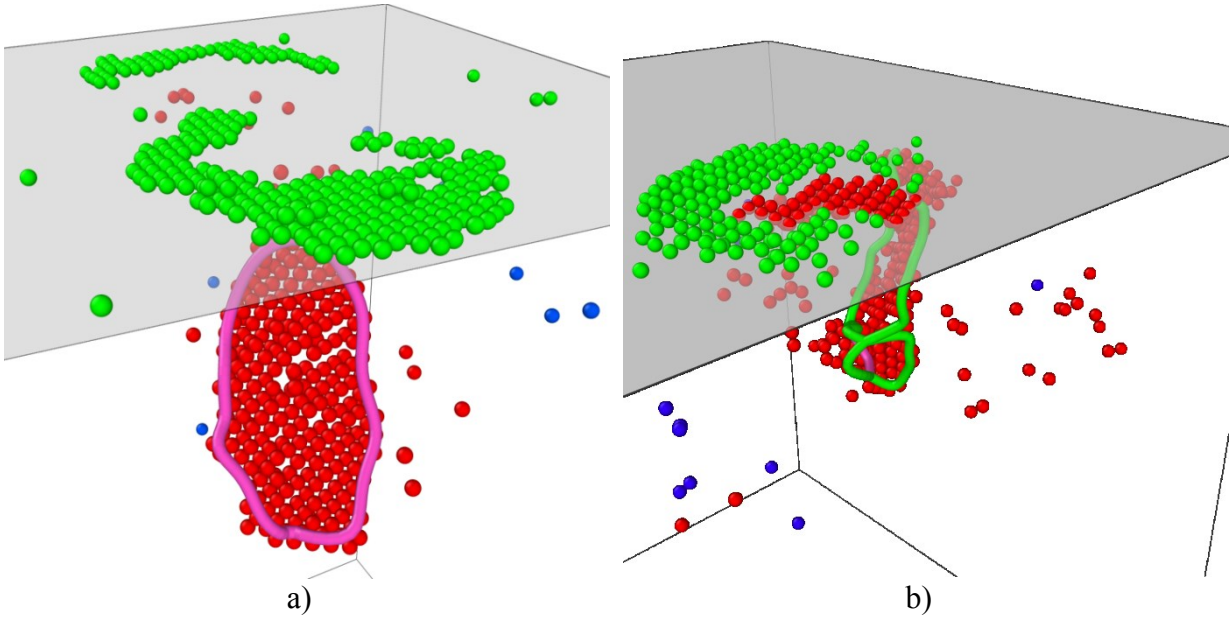


Figure 2: Radiation damage in the crystallite on the (110) (a) and (111) (b) surfaces. Adatoms are shown in green, vacancies in red, and SIAs in blue. The pink and green lines show the <100> and 1/2 <111> dislocations, correspondingly. The free surface is colored by grey

Analysis of the results of calculations shows that there is a correlation between the size of the vacancy loops and the number of adatoms. Thus, the number of adatoms on the free surface is approximately equal to the size of the vacancy loop (Fig. 3). Deviations from this ratio are associated with a small number of surviving point defects and clusters formed from them in the crystallite bulk. It is found that the number of adatoms on the (110) surface is slightly larger than the number of vacancies that make up the loop. The number of adatoms on the (111) surface is, as a rule, smaller than the size of the loop. A sufficiently large number of loops left the (111) free surface in the process of crystallite relaxation.

It follows from the calculations that there is a correlation between the sizes of the surviving vacancy loop and the crater on the free surface. So, the smaller the size of the surviving vacancy loop, the larger the crater size on the free surface. It was found that the higher the kinetic energy of the main subcascade of atomic displacements, the larger the size of the

vacancy loop.

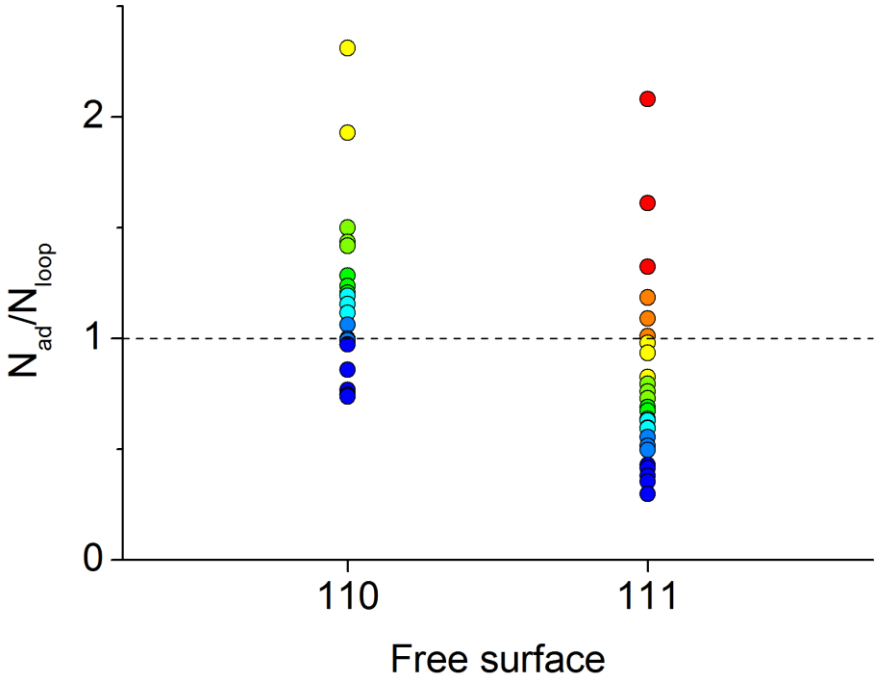


Figure 3: The ratio between the number of adatoms and the size of dislocation loops at the steady stage of cascade development near the (110) and (111) surfaces. Colors mean different calculations

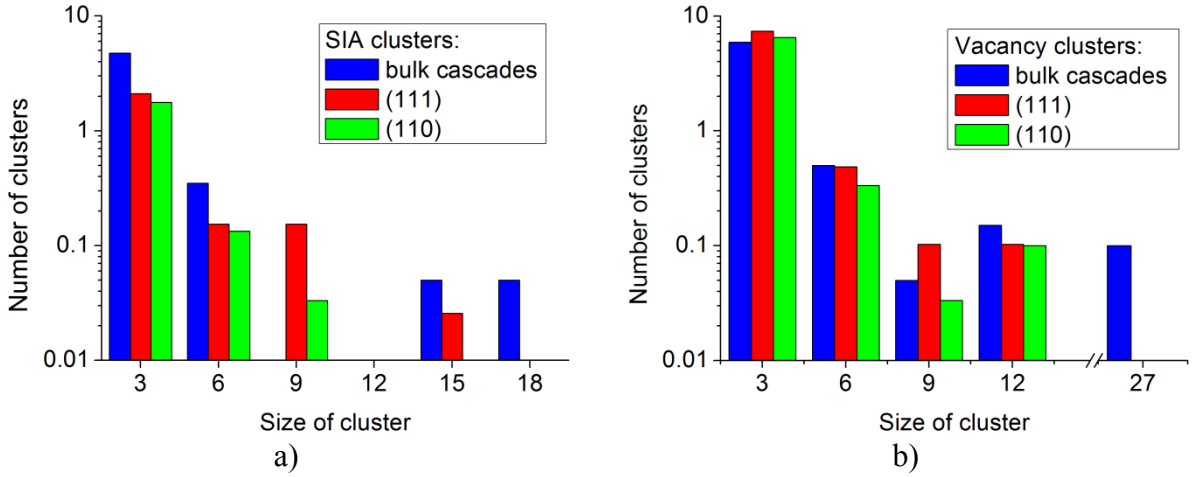


Figure 4: Distribution of survived SIA (a) and vacancy (b) clusters by their size for cascades generated near the (111) и (110) free surfaces and in the bulk

Since free surfaces are a region of a point defect sink, the number of survived clusters consisting of SIAs at irradiation of free surfaces is less than when cascades of atomic displacements develop in the bulk of the material (Fig. 4a). Note that the largest clusters are

formed by cascades of atomic displacements which are far from free surfaces. In this case clusters with size up to 18 SIAs can survive in the bulk of the material. This is almost twice the size of clusters in the near-surface regions. The number of clusters of SIAs larger than 6 is always less for the (110) surface than for the (111) one. The number of single dumbbells is the same for both surfaces. The number of survived vacancies and vacancy clusters with size of ≤12 is approximately the same for the generation of cascades in the near-surface region and in the bulk. This is due to their low mobility. Figure 4b shows that the largest vacancy clusters (except dislocation loops) are formed in the bulk of the material. It should be noted that an increase of the atomic volume at constant temperature and pressure can lead to a change in the phase composition of the region [17].

4 CONCLUSION

The cascades of atomic displacements near the free surface generate twice as many radiation defects as cascades developing in the bulk far from different interfaces. This is due to the fact that the generation of cascades of atomic displacements in the near-surface region leads to knockout of atoms from the free surface, as well as the formation of craters, adatom islands and dislocation loops of the vacancy type. The nature of the radiation damage of the near-surface region depends on the crystallographic orientation of the irradiated surfaces. In the samples with the (111) irradiated surface, as a rule, craters are formed. In the (111) near-surface region, the 1/2 <111> dislocations are mainly formed, and <100> dislocations arise in regions with the (110) orientation. There is a correlation between the number of adatoms on the free surface and the size of the vacancy loops. When the (111) surface is irradiated, the size of the vacancy loop is somewhat larger than the number of adatoms, while for the (110) surface the inverse ratio is observed. A greater number of vacancy loops from the radiation-damaged region escape on the (111) free surface than on the (110) surface.

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