Simulation of interaction of edge dislocations with radiation defects in Fe-10Cr alloy

A V Korchuganov, K P Zolnikov and D S Kryzhevich

Institute of Strength Physics and Material Science SB RAS, 2/4 Akademichesky Ave., Tomsk 634055, Russia

E-mail: avkor@ispms.ru

Abstract. The interaction of edge dislocations with radiation-damaged regions and mobility of dislocation loops in Fe-10Cr alloy is studied. Calculations are carried out in the framework of the molecular dynamics method. Dislocation loops formed as a result of ion irradiation of the sample free surface and straight dislocations in the bulk of the material were considered. It is found that the size, direction of the Burgers vector, and the distance to the free surface significantly affect the mobility of dislocation loops. As a rule, only dislocation loops of small length escape to the free surface. It is shown that <100> dislocations are almost immobile at 300 K and begin to escape to free surface after heating the sample to 600 K. An increase of radiation induced defect concentration leads to an increase in the threshold shear stress at which the edge dislocations begin to slip.

1. Introduction

The study of mechanisms of change of physical and mechanical properties under the impact of high-energy energy flows is a pressing problem of the radiation material science. The degradation of functional properties of materials under irradiation begins with the generation of point defects (self-interstitial atoms and vacancies), which are combined in the process of evolution into dislocations, pores and other large cluster structures [1-3]. It is known that the largest clusters of point defects are formed in the grain boundary regions, which hinder the propagation cascades of atomic displacements from one grain to another [4]. In the work [5] it is shown that the generation and evolution of atomic displacement cascades can lead to the creep of dislocations, thereby facilitating the propagation of point defects in the direction of dislocations. An atomic displacement cascade can also cause the dipoles of edge dislocations to shift. The magnitude of the displacement of such dipoles depends on their width and on the energy of the primary knock-on atom (PKA) generating an atomic displacement cascade. Stainless steel 304 irradiation changes the mobility of dislocations [6]. At the same time, their mobility slowly increases with the annihilation of radiation defects. One of the main properties of materials is plasticity, which can significantly decrease under conditions of high irradiation. Metal alloys with BCC structure are less susceptible to processes of radiation embrittlement and swelling compared to FCC structures [7]. Therefore, they are the most promising structural materials for nuclear power plants. The effect of radiation-stimulated hardening of ferritic Fe-Cr alloys on the atomic scale was studied in the framework of computer simulation [8]. It was found that the hardening of the alloy is due to the segregation of chromium on dislocation loops. Cr atoms are segregated in the region of the loop tensile deformation. In this case, stoichiometric changes near the loop lead to a decrease in its mobility and increase the
strength of the material. In [9], dislocation mobility was found to be generally lower in concentrated solid solution alloys than in pure metals. The mobility of dislocations depends on the local variations of stacking fault energy which are associated with changes in the local stoichiometric composition. To date, significant progress has been made in the study of the influence of radiation exposure on the dislocation mobility of materials. However, the questions associated with the atomic mechanisms that provide dislocation mobility during irradiation are still not well understood. This work is devoted to the study of the features of the interaction of edge dislocations with radiation-damaged regions and the mobility of dislocation loops formed by atomic displacement cascades near free surfaces in the Fe-10Cr alloy.

2. Formalism of simulation
Features of dislocation mobility in radiation-damaged regions and near free surfaces of Fe-10Cr alloy were investigated on the basis of molecular dynamics method. This method explicitly takes into account the discrete structure of the material and allows obtaining detailed information about its evolution [10-13]. The LAMMPS package was used for calculations [14]. Interatomic interaction was described by potentials constructed on the basis of concentration-dependent embedded atom method [15]. The collision of decay particle with surface atoms of the crystallite was simulated by setting a momentum to the PKA [16, 17]. The PKA energy was equal to 20 keV. Simulated crystallites had the cubic shape with 20 nm edges. Indices of the irradiated free surfaces were (110) or (111). Concentration of Cr was 10 at.\% which is close to concentrations for majority of steels applied in nuclear power plants [18]. For each irradiated surface 40 calculations with different PKA positions were made. The crystallite temperature was 300 K and after 350 ps was increased linearly to 600 K during 50 ps. Structural analysis of extended defects, such as dislocation loops was based on the Dislocation Extraction Algorithm [19]. Visualization of obtained structures was performed in the OVITO software [20].

Calculations showed that the generation of cascades for both irradiated surfaces leads to the formation of large vacancy loops with the <111> and <100> Burgers vector. It is notable that the <100> vacancy loops are mainly formed after irradiation of the (110) surface, and the 1/2 <111> vacancy loops after irradiation of the (111) surface.

3. Simulation results
The results of simulations show that the mobility of vacancy loops near each of the free surfaces depends on the size of the loop, the direction of the Burgers vector, and the distance between the loop and the free surface. The schematic illustrations of typical dislocation structures formed in 50 ps after the generation atomic displacement cascades are shown in figure 1. Analysis of the results allowed identifying 5 types of vacancy loops: loops under surface (figure 1a); loops that escape to surface (figure 1b); connected loops with different Burgers vectors under surface (figure 1c); loops escaping to surface, two segments of which are connected by a dislocation with another Burgers vector (figure 1d); connected loops with different Burgers vectors escaping to surface (figure 1e). In the case of irradiation of the surface (111), dislocations are most often formed in its vicinity, as shown in figure 1a, b, d. The dislocations shown in figure 1a, b, c, e are more often formed at irradiation of the (110) surface.

![Figure 1. Schematic pictures of typical dislocation configurations near irradiated surfaces. Colors correspond to different Burgers vectors.](image-url)
Dislocation mobility in the free surface region of a material can be integrally described by the change of the total length of dislocations depending on time. The length of dislocations with a certain Burgers vector varies due to their escape to the free surface, the absorption of defects, the transformation of one type of dislocations to another. Basically, the escape to the free surface changes sufficiently the length of dislocations, other processes give a small contribution. In the case of the (111) surface it was shown that the length of the <100> dislocations increased insignificantly due to the transformation of <111> dislocations into <100>. At 300 K for both irradiated surfaces, the mobility of <111> dislocations is higher than the mobility of <100> ones (figure 2). With an increase in temperature to 600 K at time interval 350–400 ps, the <100> dislocations begin to escape to the (110) free surface more intensively. The mobility of dislocations with different Burgers vectors for the (111) surface at 600 K is practically the same (figure 2a). Despite heating to 600 K after 400 ps the mobility of dislocations with the <111> Burgers vector near the (110) surface have not changed (red curve in figure 2b). This is due to the fact that the most mobile dislocations had already escaped to the surface by this time. The remaining dislocations have configurations that diminish their escape to free surfaces.

Figure 2. Total dislocation length vs. time in samples with the (111) (a) and (110) (b) free surfaces.

If several dislocations are crossed, their mobility will depend on the orientation of their Burgers vectors. The formation of a mixture of dislocations with different Burgers vectors significantly lowers their mobility. In some cases, all edge dislocations can change their Burgers vectors and form one dislocation. This accompanied by emitting a screw dislocation or its joining with an edge dislocation. The vacancy loops in figure1 do not escape to the free surface. The exceptions are small loops with the length less than 80-110 Å. Analysis of the calculation results showed that only one out four the 1/2 <111> loop with the length 86 Å escaped to the (111) free surface. In this case, all eight <100> loops did not escape to the (111) surface. During the calculation time, only a single 1/2 <111> loop with the length of 89 Å escaped to the (110) free surface. In addition, one of the three <100> loops with a length of 109 Å escaped to this surface. It is known that the shape and size of the loop significantly influence the minimum depth from the surface at which loop stay in the sample [21]. These results are in agreement with results of our simulations. Loops practically do not escape to free surfaces, if their depths greater than the critical one.

To study the effect of radiation damage on the mobility of edge dislocations, five crystallites containing 0.0, 0.5, 1.0, 1.5, 2.0% vacancies were simulated. The threshold shear stress that cause a displacement of edge dislocations versus a vacancy concentration is shown in figure 3. It can be seen that the threshold shear stress applied to the sample increase quite rapidly with the vacancy concentration in the interval from 0.0 to 0.5%. After further increase in the concentration of vacancies, the curve in
figure 3 has a tendency to saturate. This may be due to the fact that the elastic stress fields from vacancies begin to screen the dislocation from the shear loading at vacancy concentrations of more than 1%. The position of the edge dislocation in the [112] direction perpendicular to the slip plane changes as the dislocation moves in the crystallite with vacancies (figure 4). Climb of dislocation, i.e. the decrease of its extra plane area is due to the adsorption of vacancies situated in the dislocation slip path.

Figure 3. Dependence of the threshold shear stress applied to the sample, which causes displacement of the edge dislocation, on the vacancy concentration.

4. Conclusion
It is shown that the <100> vacancy loops are mainly generated at the (110) surface and the 1/2 <111> vacancy loops at the (111) surface irradiation. The mobility of vacancy loops depends on their size, Burgers vector and distance from the free surface. The loops of small length 80–110 Å escape to a free surface, loops of greater length almost never escape to a free surface. The complexes of intersected dislocations with different Burgers vectors do not reach the free surface until the all the dislocations have the same indices of the Burgers vector. Such transformations are implemented as a result of the emission of a screw dislocation or its join with the edge one. The mobility of <111> dislocations is higher than that of <100> dislocations at 300K. At 600K the <100> dislocations more intensively escape on the (110) free surface and the mobility of the <111> dislocations is not changed. It was found that the radiation-damaged regions of the crystallite significantly lower the mobility of edge dislocations. Thus, the threshold shear stresses necessary for the beginning of the movement of an edge dislocation increase by about one and a half times when the crystallite contains 2% of vacancies.

Acknowledgments
The work was performed with financial support of Russian Foundation for Basic Research grant No. 16-08-00120 a.

References
[1] Korchuganov A V, Zolnikov K P, Kryzhevich D S and Psakhie S G 2017 Russ. Phys. J. 60 170
[2] Sand A E, Aliaga M J, Caturla M J and Nordlund K 2016 *EPL* 115 36001
[3] Zhou W, Tian J, Zheng J, Xue J and Peng S 2016 *Sci. Rep.* 6 21034
[4] Psakhie S G, Zolnikov K P, Kryzhevich D S, Zheleznyakov A V and Chernov V M 2009 *Crystallogr. Reports* 54 1002
[5] Fu B Q, Fitzgerald S P, Hou Q, Wang J and Li M 2017 *Nucl. Instrum. Methods Phys. Res. Sect. B* 393 169
[6] Briceño M, Fenske J, Dadfarnia M, Sofronis P and Robertson I M 2011 *J. Nucl. Mater.* 409 18
[7] Singh K, Robertson C and Bhaduri A K 2017 *Procedia Struct. Integr.* 5 294
[8] Terentyev D, Bergner F and Osetsky Y 2013 *Acta Mater.* 61 1444
[9] Zhao S, Osetsky Y N and Zhang Y 2017 *J. Alloys Compd.* 701 1003
[10] Zolnikov K P, Psakhie S G, Negreskul S I and Korostelev S Y 1996 *J. Mater. Sci. Technol.* 12 235
[11] Zol’nikov K P, Uvarov T Y and Psakh’e S G 2001 *Tech. Phys. Lett.* 27 263
[12] Kuksin A Y, Starikov S V, Smirnova D E and Tseplyaev V I 2016 *J. Alloys Compd.* 658 385
[13] Nikonov A Y, Zharomkhabetova A M, Ponomareva A V and Dmitriev A I 2018 *Phys. Mesomech.* 21 43
[14] Plimpton S 1995 *J. Comput. Phys.* 117 1
[15] Stukowski A, Sadigh B, Erhart P and Caro A 2009 *Model. Simul. Mater. Sci. Eng.* 17 075005
[16] Zolnikov K P, Korchuganov A V, Kryzhevich D S, Chernov V M and Psakhie S G 2015 *Nucl. Instrum. Methods Phys. Res. Sect. B* 352 43
[17] Psakhie S G, Zolnikov K P, Kryzhevich D S, Zheleznyakov A V and Chernov V M 2009 *Phys. Mesomech.* 12 20
[18] Zinkle S J and Snead L L 2014 *Annu. Rev. Mater. Res.* 44 241
[19] Stukowski A and Albe K 2010 *Model. Simul. Mater. Sci. Eng.* 18 085001
[20] Stukowski A 2010 *Model. Simul. Mater. Sci. Eng.* 18 015012
[21] Fikar J and Gröger R 2015 *Acta Mater.* 99 392