Dynamics of dislocation loops in radiation-damaged Fe-10Cr crystallites

K P Zolnikov, A V Korchuganov and D S Kryzhevich
Institute of Strength Physics and Material Science of the Siberian Branch of the Russian Academy of Sciences, Akademicheskii 2/4, Tomsk 634021, Russia

E-mail: kost@ispms.tsc.ru

Abstract. Molecular-dynamics study of the mobility of dislocation loops formed at irradiation of two surfaces with different orientations of Fe-10Cr crystallite is carried out. The simulated crystallite had the form of a cube. In two directions, periodic boundary conditions were used, in the third direction, one of the faces was simulated as a free surface, and on the opposite face the atoms were fixed. The temperature of the simulated crystallite was 300 K. Interatomic interactions were described on the basis of the embedded atom method. It is shown that the mobility of vacancy loops for each of the free surfaces depends on their size, the Burgers vector and the distance from the free surface. Loops of large sizes in subsurface layer almost do not reach the free surface. Exceptions are loops of short length 80–110 Å. The mobility of the \( \frac{1}{2} \langle 111 \rangle \) dislocations is greater than the mobility the \( \langle 100 \rangle \) dislocations at 300 K of crystallite. With an increase in temperature to 600 K, the \( \langle 100 \rangle \) dislocations begin to escape to the (110) free surface more intensively, and the mobility of the \( \langle 111 \rangle \) dislocations decreases substantially.

1. Introduction

Dislocation mobility is a fundamental property that determines the plasticity of materials under mechanical, thermal influences, irradiation with high-energy flows. The influence of shear stresses and temperature on the mobility of edge dislocations in bcc materials was studied in papers [1,2]. The studies were carried out in the framework of molecular dynamics calculations. The authors calculated the critical shear stresses of dislocations, proposed analytical expressions for the dislocation velocity as a function of temperature and applied shear loads, described in detail the mechanisms of structural rearrangements responsible for dislocation displacement, etc.

It is known that the irradiation leads to a significant decrease in the plasticity of the material. In this case, materials with a bcc structure show better resistance to radiation embrittlement and swelling in comparison with fcc materials at high radiation doses [3]. This quality makes them promising construction materials for atomic power engineering. The change in the plastic behavior of materials during irradiation is caused by the formation of point defects (vacancies and self interstitial atoms) that can be assembled into dislocation loops.

Generated point defects, interacting with structural features (dislocations, interfaces), can lead to a significant change in the physical-mechanical properties of the irradiated material. Thus, in [4,5] it was shown that grain boundaries are barriers to the propagation of cascades of atomic displacements and accumulate in their region the largest clusters of radiation defects.

Molecular dynamics simulation has shown that cascades of atomic displacements near the dislocations promote their creeping, facilitating the movement of point defects in the direction...
of the dislocation creep [6]. Depending on position, direction and energy of the primary knocked out atom (PKA), as well as the width of dipoles of edge dislocations, a cascade can cause displacements of such dipoles.

The paper [7] shows that irradiation of stainless steel 304 changes the movement and mobility of dislocations. Their motion becomes irregular and jump-like, the mobility slowly increases as the radiation defects locally annihilate.

The effect of Cr on the radiation-stimulated hardening of ferrite Fe–Cr alloys was studied on the basis of computer simulation of atomic scale in [8]. It was shown that the hardening of the alloy is associated with chromium segregation on dislocation loops. In this case, the Cr atoms are segregated in the region of tensile deformation of the loop. Local microchemical changes near the loop reduce its mobility and increase the strength of the material. In general, the effect of chromium enrichment on vacancy loops on their interaction with dislocations decreases with increasing temperature. This indicates the thermal activation nature of the effect.

Dislocation mobility in alloys can be significantly reduced compared to pure metals [9]. This is due to the fact that mobility of dislocations is determined by local fluctuations in the energy of the defects, related to changes in the local stoichiometric composition. Despite significant advances in this field, the influence of the radiation effect on dislocation mobility has been studied rather poorly.

The present work is devoted to the study of the effect of free surfaces with different crystallographic orientations on the mobility of dislocation loops in the near-surface layer in the Fe-10Cr alloy under irradiation.

2. Formalism of simulation
Dislocation mobility upon irradiation of free surfaces of Fe-10Cr alloy was studied on the basis of molecular dynamics method. This method allows one to study the evolution of materials on the atomic level even in nonequilibrium conditions [10–13]. The LAMMPS package was used for calculations [14]. The interatomic interactions were described by a potential constructed according to the concentration-dependent embedded atom method [15]. The collision of the decay particle 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 200 Å edges. In the direction of the two edges periodic boundary conditions were used, in the third direction the irradiated face was modeled as a free surface. On the opposite face, several atomic layers were rigidly fixed to prevent displacement of the sample as a whole. The positions of the Cr atoms were set using a random number generator by replacing Fe atoms at the bcc lattice sites. Indices of the irradiated free surfaces were (110) or (111). The crystallite temperature was 300 K. For each irradiated surface 40 calculations with different PKA positions were made. The occupancy of Wigner-Seitz was calculated to identify point defects in irradiated crystallites. Structural analysis of extended defects, such as dislocation loops based on the Common Neighbor Analysis [18] and the Dislocation Extraction Algorithm [19]. Visualization of obtained structures was performed in the OVITO software [20]. After the generation of cascades of atomic displacements, the samples were maintained at a temperature of 300 K for 350 ps. Then, for 50 ps the samples were heated to a temperature of 600 K and held for an additional 250 ps. Samples were allowed to change their sizes in all directions at heating.

3. Simulation results
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 the most formed after irradiation of the (110) surface, and the 1/2 (111) vacancy loops after irradiation of the (111) surface. The features of their generation are described in [21], and the mechanisms for the formation of such loops were proposed in [22,23].
Figure 1. Typical configurations of dislocations on irradiated surfaces: loops under surfaces (a), loops that escape to surfaces (b), bound loops under surfaces with different Burgers vectors (c), loops escaping to surfaces, two segments of which are connected by a dislocation with another Burgers vector, (d), connected loops escaping to surfaces with different Burgers vectors (e). Magenta and green lines corresponds to the $\langle 100 \rangle$ and $1/2 \langle 111 \rangle$ dislocations, respectively.

The results of MD 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 of the loop from the free surface. The typical dislocation structures formed in 50 ps after the generation of cascades of atomic displacements are shown in figure 1. Analysis of the results allowed identifying 5 types of vacancy loops, based on their Burgers vector and position relative to each other and/or the free surface. In the case of irradiation of the surface (111), dislocations are most often formed in its vicinity, as shown in figure 1(a, b, d). The dislocations shown in figure 1(a, b, c, e) are more often formed at irradiation of the (110) surface.

One of the important characteristics of the dislocation behavior in irradiated crystallite is the change of the total dislocation length as a function of time. The length of dislocations changes because of their escape to free surfaces, absorption of point defects, transformations of one type of dislocation to another one. In general, the main contribution to changes of the dislocation length gives their escape to free surfaces. The remaining processes give a small contribution. Results of simulation showed that for the (111) surface, the length of the $\langle 100 \rangle$ dislocations increased insignificantly due to the transformation of the $\langle 111 \rangle$ dislocation into the $\langle 100 \rangle$ ones. At 300 K for both irradiated surfaces, mobility of the $\langle 111 \rangle$ dislocations is greater than the mobility of the $\langle 100 \rangle$ ones. With an increase in temperature to 600 K, the $\langle 100 \rangle$ dislocations begin to escape to the (110) free surface more intensively (figure 2). It is found that the mobility of dislocations with different Burgers vectors for the (111) surface at 600 K is practically the same. Despite heating to 600 K, the mobility of dislocations with the Burgers vector $\langle 111 \rangle$ decreased after 400 ps (green curves in figure 2). 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 length of different dislocations as a function of time in samples with free surfaces of (111) and (110) facets. The average length of dislocation based on 40 calculations had a standard deviation less than 10%.

Figure 3. The structure of the ⟨100⟩ edge dislocation near the (111) free surface (a–c) and the 1/2 ⟨111⟩ dislocation near the (110) surface (d–f) at different time instants. Magenta and green lines correspond to the ⟨100⟩ and 1/2 ⟨111⟩ dislocations, respectively.

When several dislocations cross, their mobility depend on the orientation of their Burgers vectors. The formation of a mixture of dislocations with different Burgers vectors, as shown in figure 1(c, d, e), significantly diminishes their mobility. It is possible when all edge dislocations change their Burgers vector, forming one dislocation. This occurred by emitting a screw dislocation or its bounding with a boundary dislocation. The characteristic structural rearrangements occurring in both cases are shown in figure 3. The transformation of the ⟨100⟩ dislocation into the ⟨111⟩ one with the emission of the ⟨111⟩ screw dislocation in vicinity of the (111) surface is shown in figure 3(a–c). The rearrangement of the screw and edge dislocations...
into the (100) edge dislocation on the (110) free surface is shown in figure 3(d–f). We note that in both cases the dislocations change the Burgers vector.

We note that the vacancy loops shown in figure 1 do not escape to the free surface. The exceptions are small loops, the length of which does not exceed 80–110 Å. The calculations showed that only one out four the 1/2 ⟨111⟩ loop, which was 86 Å in size, escaped to the (111) free surface. In this case, all 8 loops formed on the ⟨100⟩ surface did not escape. During the estimated time, a single 1/2 ⟨111⟩ loop of size 89 Å escaped to the free surface (110) (there were no other such loops). In addition, one of the three ⟨100⟩ loops with a size of 109 Å escaped to this surface.

The results of the calculations are in agreement with the work [24] in which it is shown that the shape and size of the loop significantly influence on the critical depth of their position from the surface. At depths greater than the critical depth, loops practically do not escape to free surfaces.

4. Conclusions

A molecular dynamics study of the mobility of dislocations formed in the region of the (110) and (111) free surfaces of Fe-10Cr alloy by cascades of atomic displacements with PKA 20 keV is carried out. It was found that the ⟨100⟩ vacancy loops are mainly formed after the (110) surface irradiation, and 1/2 ⟨111⟩ vacancy loops after the (111) surface exposure. It is shown that the mobility of vacancy loops for each of the free surfaces depends on their size, the Burgers vector and their distance from free surface. Large loops under the surface almost do not escape to free surfaces. Exceptions are loops of short length 80–110 Å.

A mixture of intersecting dislocations with different Burgers vectors does not escape to the free surface. The dislocations in this mixture can rearrange their structure and transform into single dislocation. This can occur as a result of the emission of a screw dislocation or its combination with an edge dislocation.

Mobility of the 1/2 ⟨111⟩ dislocations is greater than the mobility of the ⟨100⟩ ones at 300 K. As the temperature increases to 600 K, the ⟨100⟩ dislocations begin to escape to the (110) free surface more intensively, and the mobility of the 1/2 ⟨111⟩ dislocations decreases substantially.

Acknowledgments

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

References

[1] Monnet G and Terentyev D 2009 Acta Mater. 57 1416–26
[2] Queyreau S, Marian J, Gilbert M R and Wirth B D 2011 Phys. Rev. B 84 064106
[3] Singh K, Robertson C and Bhaduri A K 2017 Procedia Struct. Integrity 5 294–301
[4] Psakhie S G, Zolnikov K P, Kryzhevich D S, Zheleznyakov A V and Chernov V M 2009 Crystallogr. Rep. 54 1002
[5] Psakhie S G, Zolnikov K P, Kryzhevich D S, Zheleznyakov A V and Chernov V M 2009 Phys. Mesomech. 12 20–8
[6] Fu B Q, Fitzgerald S P, Hou Q, Wang J and Li M 2017 Nucl. Instrum. Methods Phys. Res. Sect. B 393 169–73
[7] Briceño M, Fonseka J, Dadfarnia M, Sofronis P and Robertson I 2011 J. Nucl. Mater. 409 18–26
[8] Terentyev D, Bergner F and Osetsyky Y 2013 Acta Mater. 61 1444–53
[9] Zhao S, Osetsyky Y N and Zhang Y 2017 J. Alloys Compd. 701 1003–8
[10] Psakhie S G, Zolnikov K P, Skorentsev L F, Kryzhevich D S and Abdrashitov A V 2008 Phys. Plasmas 15 053701
[11] Psakh'e S G, Zol'nikov K P and Sarea D Yu 1998 Tech. Phys. Lett. 24 99–101
[12] Korshuganov A V, Zolnikov K P, Kryzhevich D S and Psakhie S G 2017 Russ. Phys. J. 60 170–4
[13] Kuksin A Y, Morozov I V, Norman G E, Stegailov V V and Valuev I A 2005 Mol. Simul. 31 1005–17
[14] Plimpton S 1995 J. Comput. Phys. 117 1–19
[15] Stukowski A, Sadigh B, Erhart P and Caro A 2009 Modell. Simul. Mater. Sci. Eng. 17 075005
[16] Korchuganov A V, Zolnikov K P, Kryzhevich D S, Chernov V M and Psakhie S G 2015 Nucl. Instrum. Methods Phys. Res. Sect. B 352 39–42
[17] Zolnikov K, Korchuganov A, Kryzhevich D, Chernov V and Psakhie S 2015 Nucl. Instrum. Methods Phys. Res. Sect. B 352 43–6
[18] Honeycutt J D and Andersen H C 1987 J. Phys. Chem. 91 4950–63
[19] Stukowski A and Albe K 2010 Modell. Simul. Mater. Sci. Eng. 18 085001
[20] Stukowski A 2010 Modell. Simul. Mater. Sci. Eng. 18 015012
[21] Korchuganov A V, Zolnikov K P and Kryzhevich D S 2018 J. Phys.: Conf. Ser. 946 012015
[22] Starikov S V, Insepov Z, Rest J, Kuksin A Yu, Norman G E, Stegailov V V and Yanilkin A V 2011 Phys. Rev. B 84 104109
[23] Osetsky Y, Calder A and Stoller R 2015 Curr. Opin. Solid State Mater. Sci. 19 277–86
[24] Fikar J and Gröger R 2015 Acta Mater. 99 392–401