Molecular dynamics simulation of primary radiation damage in Fe–Cr alloy

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Abstract. The atomic displacement cascades generated by radiation in the iron–chromium alloy were studied using molecular dynamics simulation. Atomic displacement cascades were generated by the primary knock-on atom, which energy varied from 1 to 20 keV. The simulation of the dynamics of atomic displacement cascades and the calculation of the cascade parameters (durations of the main stages, the size of the radiation-damaged region) in the iron–chromium alloy were made for different energies of primary knock-on atom. Sizes of formed point defect clusters and their distribution in the crystallite volume were calculated. To study radiation damage in iron–chromium alloy caused by generation and evolution of displacement cascades we analyzed spatial and quantitative distribution of the generated point defects and their clusters.

1. Introduction
The study of radiation damage of metallic materials is an important fundamental problem of modern materials science. One of the primary manifestations of radiation exposure is generation of atomic displacement cascades in the material that occur during collisions of decay particles with crystal lattice atoms. Features of development of atomic displacement cascades and the formation of radiation-induced defects are determined by many factors: the type of crystal lattice of the material, temperature, energy of decay particle, the presence of extended defects in the material, etc. [1]. It should be noted that in the case of alloy presence of impurities may significantly change response of material to radiation exposure. Almost all structural materials in nuclear power plants are alloys with a complex stoichiometry and chemical composition. Therefore, it is important to study the features of the propagation of atomic displacement cascades in the crystallites consisting of more than one chemical element. Most effectively these issues can be resolved on the basis of computer simulation.

Usually, the study of the dynamics of structural changes in the materials under radiation exposure at the atomic level is carried out by the molecular dynamics method (MD) [2–11]. MD results significantly deepened the understanding of the mechanisms that govern primary radiation damage of the crystal structure, features of the defect distribution in atomic displacement cascades, and the point defect clustering in materials with different crystal lattice.

MD calculations showed that for wide range of materials the number of survived point defects in cascade for the primary knock-on atom (PKA) energy range 20–30 keV is given by the expression \( N = A(E_{PKA})^m \), where \( E_{PKA} \) is the PKA energy, \( A \) and \( m \) are the constants [5–7]. It was revealed that the amount of survived defects is weakly dependent on the initial temperature of the sample [8].
At the same time, the change in temperature significantly affects the distribution of the cluster size and its dependence on the PKA energy [1]. So, for PKA energies greater than 10 keV a fraction of self-interstitial atoms (SIAs) in the clusters increases with increasing temperature of crystallites. The fraction of vacancies in clusters decreases with increasing temperature, due to thermal instability of these clusters. Analysis of the results of atomic displacement cascade modeling in the crystallites of bcc iron showed that with an increase in both temperature and PKA energy the size distribution of SIA clusters is shifted to higher values: the number of single SIAs decreases and the number of large clusters increases [1].

Questions related to the impurity influence on the features of primary radiation damage evolution in Fe–Cr alloys were studied in [9–11]. In [9,10] the interaction of atomic displacement cascades with Cr-rich clusters was studied. It has been shown that the clusters with size $\geq 3$ nm practically don’t change the characteristics of cascades, while 1 nm clusters can be completely dissolved in the matrix by the atomic displacement cascade. The effect of Cr concentration on the number of survived point defects and the mobility of their clusters was studied in [11]. It was shown that the presence of chromium insignificantly affects the quantitative and spatial distribution of generated point defects. It was found that chromium significantly reduces the mobility of SIA clusters, and that it depends nonlinearly on the cluster size and temperature of the crystallite.

Despite advances in the modeling of primary radiation damage of materials, peculiarities of atomic displacement cascade evolution in the alloys are still not well studied. In this paper we apply MD method to investigate the features of the primary radiation damage in iron–chromium alloy, depending on the PKA energy.

2. Simulation details

The simulation of the atomic displacement cascades generated by radiation in the iron–chromium alloy was carried out on the basis of the MD method. Interatomic interactions were described in the framework of the concentration-dependent embedded atom method. Used potential [12] accurately describes many mechanical and physical properties which are very important for the atomic displacement cascade simulations, such as lattice parameters, elastic constants, point defect formation and migration energies, threshold displacement energies, etc. The simulated crystallites had a cubic shape. Initial temperature of crystallites was 300 K. Concentration of Cr was 10 at.%, which is close to concentrations for majority of steels applied in nuclear power plants [13]. The periodic boundary conditions in all directions were used at displacement cascade simulations. Atomic displacement cascades were generated by the PKA, which energy varied from 1 to 20 keV. The simulated crystallites contained from 500,000 to 2,500,000 atoms depending on the PKA energy. The direction of PKA momentum was random. For each PKA energy results were averaged by 20 calculations. Identification of point defects was based on Wigner–Seitz analysis.

3. Results and discussion

Calculations showed that after PKA generation a sequence of atomic displacements occurs, leading to the formation of point defects. The main characteristics of the atomic displacement cascade are the following: the maximum number of generated defects; the time for which they are formed; the number of survived defects; size distribution of point defect clusters; volume of the cascade region at the end of the ballistic phase.

Dependencies of the maximum number of defects and the number of survived point defects in atomic displacement cascade on the PKA energy are shown in figure 1. As can be seen in the figure, these relationships are linear. The number of point defects increases with the energy of PKA. The deviation of the maximum number of defects from the linear dependence at PKA energy of 20 keV may be associated with the generation of shock waves by a cascade. These
waves may displace the atoms from the crystal lattice sites, which leads to an increase in the number of displaced atoms.

The duration of the ballistic phase of atomic displacement cascade evolution corresponds to the time for which the number of defects in the cascade reaches maximum value (peak time). Its dependence on the value of the PKA energy is shown in figure 2a. It can be seen that the slope of the curve decreases with increasing the PKA energy. This is due to the splitting of atomic displacement cascades into subcascades which are triggered by secondary knock-on atoms with energy lower than the PKA energy. These subcascades are characterized by a shorter duration of the ballistic phase than the main cascade, and, in general, reduce the duration of the ballistic phase of the cascade development.

The analysis of simulation results showed that the volume of the atomic displacement cascade at the end of the ballistic phase is linearly dependent on the PKA energy (figure 2b). This value was calculated as follows: based on the common neighbour analysis [14] region in which atoms do not form bcc lattice is defined. Such atoms represent heated area of the crystallite in which
One of the main characteristics of the primary radiation damage of the material is the size distribution of survived point defect clusters. As a result of thermal fluctuations the generation and distribution of point defect clusters in size and spatial position in the crystallite have stochastic nature. Therefore, the determination of reliable distributions was performed on the base of the averaging of data obtained in a series of 20 calculations for each PKA energy. It was believed that the defects belong to the same cluster if the distance between SIAs is less than or equal to the radius of the first coordination sphere of the bcc lattice, and the distance between the vacancies is less than or equal to the radius of the second coordination sphere. The cluster size is defined as the number of point defects which belong to it.

The size distributions of SIA and vacancy clusters for different PKA energies are presented in figure 3a and 3b, respectively. As can be seen in the figure, with increasing of PKA energy the number and maximum size of the generated clusters of point defects increases. The number of formed vacancy clusters approximately equal to the number of clusters consisting of SIAs. Note
that for 15 and 20 keV PKA energies dislocation loops $a\{100\}\{100\}$ can be formed in the center of atomic displacement cascade. They represent clusters consisting of 25–30 vacancies (figure 4). Analysis of the simulation results show that with the increase of PKA energy the fraction of SIAs forming clusters of $\geq 2$, increased from 15 to 30%, while the fraction of vacancies decreased from 45 to 35%.

4. The main results and conclusions
Based on the molecular dynamics simulation the primary radiation damage in Fe–10Cr alloy has been studied. It has been shown that the atomic displacement cascade volume, the number of defects at the end of the ballistic phase and the number of survived defects is linearly dependent on the energy of the PKA. The peak time is dependent on the energy of PKA nonlinearly. The non-linearity of this dependence is associated with splitting of atomic displacement cascade into subcascades. It has been shown that with increasing PKA energy the number and maximum size of the generated point defect clusters increase. The number of vacancy clusters coincides approximately with the number of clusters consisting of SIAs. It has been found that for PKA energies greater than 15 keV vacancy-type dislocation loops $a\{100\}\{100\}$ can be formed. Since the average PKA energy is in the range of 15 to 20 keV for the structural materials in real operating conditions, the nucleation and growth of such dislocation loops may significantly affect the microstructure evolution of the irradiated material.

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