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MD simulation of atomic displacement cascades in Fe–10 at.%Cr binary alloy

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ABSTRACT

Molecular dynamics simulation of atomic displacement cascades up to 20 keV has been performed in Fe–10 at.%Cr binary alloy at a temperature of 600 K. The *N*-body interatomic potentials of Finnis–Sinclair type were used. According to the obtained results the dependence of "surviving" defects amount is well approximated by power function that coincides with other researchers' results. Obtained cascade efficiency for damage energy in the range from 10 to 20 keV is ≈0.2 NRT that is slightly higher than for pure α-Fe. In post-cascade area Cr fraction in interstitials is in range 2–5% that is essentially lower than Cr content in the base alloy. The results on size and amount of vacancy and interstitial clusters generated in displacement cascades are obtained. For energies of 2 keV and higher the defect cluster average size increases and it is well approximated by a linear dependence on cascade energy both for interstitials and vacancies.

1. Introduction

Reduced activation ferritic/martesitic (RAFM) 7–10%Cr-WVTa steels are primary candidate structural materials for the first wall (FW) and breading blanket (BB) structures of the future fusion power plants. Though RAFM steels gain some advantages over commercial alloys, low temperature hardening under neutron irradiation accompanied by embrittlement, decrease of impact toughness, and ductility still remain the principle obstacles for their application. Since the beginning of 2008 Ulyanovsk State University and Joint Stock Company, State Scientific Center Research Institute of Atomic Reactors (JSC SSC RIAR) jointly with Forschungszentrum Karlsruhe have set up a significant research project "High Dose Irradiation Damage of RAFM Steels". The designated project aims at understanding of the neutron irradiation damage in RAFM steels and its influence on their mechanical properties.

The present work concerns molecular dynamics (MD) simulation of atomic displacement cascades in Fe–10 at.%Cr binary alloy. The main goal is determination of some primary radiation damage parameters taking into consideration point defects recombination and clusterization in displacement cascades. The simulation is performed at a temperature of 600 K that approximately corresponds to irradiation temperature of RAFM steel specimens in BOR-60 (JSC SSC RIAR, Dimitrovgrad, Russia) within ARBOR-1 and ARBOR-2 irradiation programmes [1,2].

MD method is the most appropriate tool of atomic displacement cascade simulation being used by different research groups for simulation of irradiation damage in various materials. Particularly, pure α-Fe has been extensively studied by using of different potentials of interatomic interaction. Cascade simulation in alloys is also being widely performed, though the problem of proper potential development for multicomponent systems still remains. Recently a number of works dedicated to Fe–Cr alloys have been published [3–6]. Malerba et al. [3] carried out a dynamic simulation of displacement cascades of Fe–10%Cr alloy for the primary knock-on atom (PKA) energies up to 15 keV. Later on Terentyev et al. [4] performed calculations for PKA energies up to 50 keV. Wallenius et al. [5] simulated cascades for Fe–5%Cr and Fe–20%Cr systems. The authors in [3–5] make use of interatomic potentials resting on embedded atom method (EAM). However, Fe potential used in [3,4] reveals the $\langle 1\,1\,1\rangle$ dumbbell structure for interstitial atoms to be more stable than $\langle 1\,1\,0\rangle$ one, that contradicts experimental data and results of ab initio calculations. The potentials used in [5] happens to yield formation energies of mixed Fe–Cr "dumbbell" in α-Fe matrix twice as large as ab initio calculations.

Shim et al. [6] had performed MD simulations of displacement cascades up to 20 keV in Fe and Fe–10 at.%Cr using two different parameterizations of Finnis–Sinclair type interatomic potentials. In particular, they had shown that the quantity of mixed Fe–Cr dumbbells is sensitive to the choice of Fe–Cr cross-potential.

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2. Simulation method and interatomic potentials

For displacement cascade simulation we made use of MD method and FRENKLOW code [7] that was developed in Tver polytechnic university and subsequently modified by our researchers. Displacement cascade simulation starts from imparting an initial velocity in a chosen crystallographic direction to one of crystallite atoms (PKA) and continues till perturbation cools down. In doing so, it is essential to consider different non-equivalent PKA momentum directions.

For the performed simulation, a semi-empirical manybody potential of interatomic interaction is applied. By using *N*-body potential each atom's energy is rather represented as some function of its local surrounding than constitutes the sum of pair interactions. Several construction schemes of such potential were developed for metals: embedded atom method [8], Finnis–Sinclair scheme [9], and Rosato–Guellopé–Legrand scheme [10]. Though physical interpretations are slightly different, all these methods yield the same analytic equation for *N* particles system's total energy.

$$E_{tot} = \sum_{i=1}^{N} F_i(\rho_i) + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \varphi_{ij}(r_{ij}), \tag{1}$$

$$\rho_i = \sum_{\substack{j=1\\(j\neq i)}}^{N} \psi_j(r_{ij}), \tag{2}$$

where E_{tot} is crystal energy, ρ_i in EAM formalism is the electron density at cite *i* generated by other atoms, $F_i(\rho_i)$ is energy of embedding of atom *i* into electron liquid with density ρ_i, $\psi_j(r_{ij})$ is electron density of atom *j* as a function of distance to its center, r_{ij} is distance between *i* and *j* atoms and $\varphi_{ij}(r_{ij})$ is pairwise interatomic potential between *i* and *j* atoms.

When constructing pairwise potential it is common to divide it into three parts (see, for instance [11]): *equilibrium*, *high-energy* and *intermediate*. The *equilibrium* part of pair potential is designated to explain interactions on interatomic distances close to or greater than the distance between the nearest neighbours in an equilibrium crystal. This part ($\varphi_{equilibrium}(r)$) may have different analytic forms for both different atoms and different methods and approaches used in potential construction.

The *high-energy* part describes interatomic interactions at short distances (typically up to 1 Å). This potential part is repulsive (i.e. decreasing with *r*) and it is usually described by the equation:

$$\varphi_{short\text{-}dist}(r) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r}\,\Phi\left(\frac{r}{a}\right), \tag{3}$$

where Z_i is atom number, *e* is electron charge, ε_0 is the dielectric constant, *a* is defined here according to Biersack and Ziegler approach [40]

$$a = \frac{0.88534 \times a_0}{\sqrt{Z_1^{2/3} + Z_2^{2/3}}}, \tag{4}$$

with $a_0 = 0.529$ Å being Bohr radius and $\Phi(x)$ being screening function given by:

$$\Phi(x) = 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x}. \tag{5}$$

The *intermediate* part is designated to smoothly join *equilibrium* and *high-energy* parts so that $\varphi(r)$ function and its first derivative should be continuous. In the present work the intermediate part is represented as:

$$\varphi_{join}(r) = e^{(B_0+B_1r+B_2r^2+B_3r^3)}, \quad r_1 \leqslant r \leqslant r_2, \tag{6}$$

where $[r_1, r_2]$ is a "join" section, B_i parameters are chosen so that the equations

$$\varphi_{join}(r_2) = \varphi_{equilibrium}(r_2),$$

$$\varphi'_{join}(r_2) = \varphi'_{equilibrium}(r_2),$$

$$\varphi_{join}(r_1) = \varphi_{short\text{-}dist}(r_1),$$

$$\varphi'_{join}(r_1) = \varphi'_{short\text{-}dist}(r_1)$$

should be satisfied.

In the present work for Fe we used *N*-body potential of Finnis–Sinclair type from Ackland et al. [12], which is derived from potential 2 from [13] by embedding function modification. The boundaries of the intermediate region for a pairwise potential part is given by $r_1 = 1$ Å, $r_2 = 2.05$ Å. High-energy and joint parts correspond to Eqs. (3)–(6). Cutting radius is 5.3 and 4.2 Å for φ and ψ functions, respectively.

It is noteworthy that, the used potential is constructed so that the more stability should be provided for ⟨1 1 0⟩ "dumbbell" configuration than for ⟨1 1 1⟩ one. The difference between corresponding formation energies is ∼0.5 eV that agrees well with experimental results on α-Fe [21].

We use Finnis–Sinclair potential [9] for Cr:

$$\psi_{\mathrm{CrCr}}(r) = \begin{cases} A^2((r-d)^2 + b(r-d)^3/d), & r \leqslant d \\ 0, & r > d \end{cases}, \tag{7}$$

$$F_{\mathrm{CrCr}}(\rho) = -\sqrt{\rho}, \tag{8}$$

$$\varphi_{\mathrm{CrCr\_equilibrium}}(r) = \begin{cases} (r-C)^2(C_0 + C_1 r + C_2 r^2), & r \leqslant C \\ 0, & r > C \end{cases}. \tag{9}$$

The potential parameters are given in Table 1. It is noteworthy that the potential yields a slightly positive Cauchy pressure $(C_{12}-C_{44})/2 \approx 1.35 \times 10^9$ Pa which disagree with experiment [22] where negative Cauchy pressure for Cr is obtained. However, as it is noted in [5] with reference to paper [23], at temperatures above 450 K chromium is paramagnetic and has a positive Cauchy pressure. For using this potential in displacement cascade simulation when the distance between atoms becomes small, it is reasonable to modify $\psi_{\mathrm{CrCr}}(r)$ function. The matter is that it increases at $r < d(1-2/(3b)) \approx 2.465$ Å and, moreover, it is negative at $r < (1-1/b)d \approx 1.74$ Å. Therefore, for $r \leqslant r_0 = 2.498$ Å we assumed.

$$\psi_{\mathrm{CrCr}}(r) = A^2((r-d)^2 + b(r-d)^3/d) + k(r_0 - r)^3, \quad r \leqslant r_0, \tag{10}$$

where $k = 11.1$ eV^2/Å^3. Original and modified curves of $\psi_{\mathrm{CrCr}}(r)$ function are given in Fig. 1. *High-energy* and *intermediate* parts of $\varphi_{\mathrm{CrCr}}(r)$ function were determined in accordance with Eqs. (3)–(6) with r_1 and r_2 values coinciding with those of Fe (i.e. 1 and 2.05 Å, respectively).

To test chosen potentials for Fe and Cr we carried out calculations of atom displacement threshold energies and performed comparison of the obtained values with the experimental data. bcc Fe and Cr crystallites comprising nearly 10,000 atoms were used to calculate displacement threshold energy (E_d). Calculations were done with periodic boundary conditions. The initial crystallite temperature was 0 K. When determining threshold energy the search of stable configurations starts from low PKA energies,

Table 1
Potential parameters for Cr (all distances are expressed in Å and energies in eV).

A	1.453418	d	3.915720	C_0	29.1429813	C_2	4.7578297
b	1.8	C	2.90	C_1	−23.3975027		