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Molecular dynamics simulation of primary radiation damage in vanadium and alloy V-4Ti

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Abstract. In the framework of the molecular dynamics method, simulation of the primary radiation damage in crystallites of bcc both V and alloy V-4Ti was carried out. The initial temperature of the crystallites was 700 K, which corresponds to the operating temperature of the alloy when used as the material of the first wall of a thermonuclear reactor. The interatomic interaction in V and alloy V-4Ti was described on the base of modern potentials of interatomic interactions which took into account the interaction of screened ions at small interatomic distances and allowed to simulate correctly radiation damage. The impact of the decay particle on the atoms of the simulated crystallites, as a result of which a cascade of atomic displacements was generated, was simulated by assigning a pulse to one of the lattice atoms, the primary knocked out atom. The main characteristics of atomic displacement cascades in simulated crystallites were calculated: the number of defects at different stages of cascade development, the size of the radiation-damaged regions, and an analysis of the estimation of the number, types and sizes of the surviving radiation defects in crystallites. The results obtained are compared for vanadium and alloy V-4Ti.

1. Introduction

Alloys based on the V–Ti system are known for their low radiation swelling, which is achieved through the addition of 4–5% titanium. The influence of titanium on the radiation damage of vanadium was studied by computer simulation methods in [1–6], but the influence of titanium on generation of point defects at the stage of development of atomic cascade displacements (ballistic stage in [7]) has not been considered so far. At this stage the kinetic energy of incident particle is redistributing among the lattice atoms through the elastic interaction. The number of lattice atoms displaced from the nodes increases in an abrupt way and reaches a maximum. The result of the second (recombination) stage, whose time scale is several picoseconds, is the formation of a set of point and clustered defects formed by a cascade of atomic displacements known as the primary state of the material after radiation damage. In the third stage, the defects that "survived" after recombination continue to evolve as a result of the diffusion displacements of the atoms (main state). In [8], the first stage of damage in pure vanadium was studied by molecular dynamics (MD) methods using interatomic potentials calculated in the framework of the centrally symmetric approximation. The authors of this paper [8] showed that vacancies remain in the central part of the simulated cell in the resulting structure, while interstitials

leave the periphery. At this time, small vacancy and interstitial clusters are formed, which are distributed along the simulated cell, mainly as point defects. In this paper we carried out a study of the influence of titanium on the formation and evolution of defects in the alloy V–Ti formed as a result of the development of atomic displacement cascades at the atomic level by MD simulation using interatomic interaction potentials for the V–Ti system [3, 9], taking into account the angular dependence in the interatomic interactions.

2. Formalism of simulation

The simulated crystallites of V and V-4Ti had the shape of a cube of bcc lattice with periodic boundary conditions in the directions [100], [010] and [001]. The size of the crystallites was chosen proceeding from the primary knocked out atom (PKA) energy. We used 128 000-node samples (12 nm in edge length) for PKA energies 5 keV and below, and 432 000-node samples (18 nm in edge length) for higher PKA energies. The initial temperature of the simulated crystallites was 700 K, which corresponds to the operating temperature of the alloy when used as the material of the first wall of a thermonuclear reactor [10]. The crystallite of V-4Ti differs from one of pure vanadium in that 4% vanadium atoms are randomly replaced by titanium.

The V–Ti potentials [3] used in this paper correctly predict the melting temperature of vanadium, the thermal expansion of vanadium, and the interaction of titanium atoms with intrinsic point defects in the bcc lattice of vanadium. These properties of the potentials are important for the correct simulation of the radiation damage, since the effects of radiation swelling essentially depend on the homological temperature and characteristics of point defects and their complexes.

We used an original MD program package optimized for Message Passing Interface (MPI) parallel calculations on the basis of our interatomic potentials. During MD simulation, firstly, each sample was kept at a given temperature and zero pressure using a Nose–Hoover thermostat [11] and Berendsen barostat [12], respectively, at 700 K during 20 ps (NPT ensemble). Next we set a vanadium atom in the center of the crystallite a velocity corresponding to PKA energy with a random vector orientation. To obtain the statistics, for every value of PKA energy we used 10 samples with a random orientation of the velocity vector of PKA. Then we continued kept our samples using NPT ensemble with changing the MD time step.

The MD time step changed depend on the maximum velocity of the atom in the model crystallite based on the position that PKA can not pass a distance greater than 0.02 Å in one step. Based on the estimate, minimal time step was chosen 0.02 fs for PKA energies 10 keV and below, and 0.005 fs for greater PKA energies. Maximum time step was 1 fs for all values of PKA energy.

We analyzed the evolution of damage regions in the crystallites by visualization using the OVITO package [13, 14] with Wigner–Seitz defect analyze modifier.

3. Results and discussion

From the results of simulation, we obtained the dependence of changes in the number of Frenkel pairs with time during the 0.5–20 keV cascades of atomic displacements. The observed general trends and differences of the displacement cascades in the crystallites of pure vanadium and the alloy V-4Ti are illustrated in figure 1 by the example of the PKA energies of 1, 10, and 20 keV.

As can be seen in figure 1, both pure vanadium and the alloy V-4Ti tend to increase the number of surviving Frenkel pairs at the end of the cascade with increasing energy of PKA. The presence of titanium does not affect the amount of these pairs. A small influence of titanium takes place in the decrease in the maximum number of Frenkel pairs during the peak of the cascade at high energies considered in this paper, as seen in figure 1 in for the case of 20 keV displacement cascade. The absence of strong differences in the numbers of Frenkel pairs in the

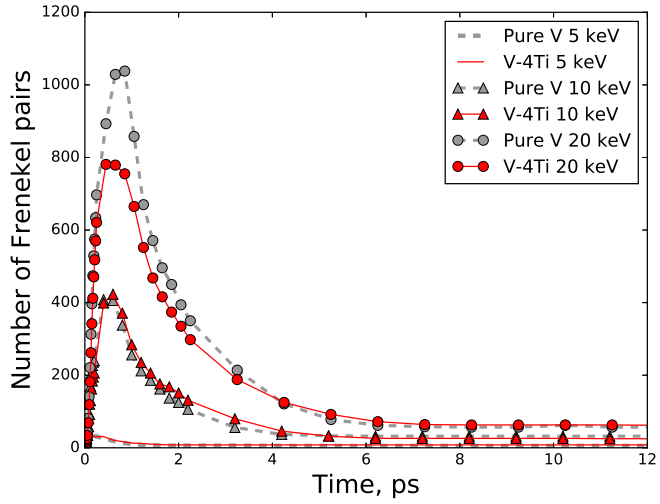

Figure 1. The number of Frenkel pairs in crystallites of pure V and alloy V-4Ti as a function of time for a PKA energy of 1, 10 and 20 keV. Results were averaged over the 10 simulated crystallites with random orientation of the PKA velocity vector.

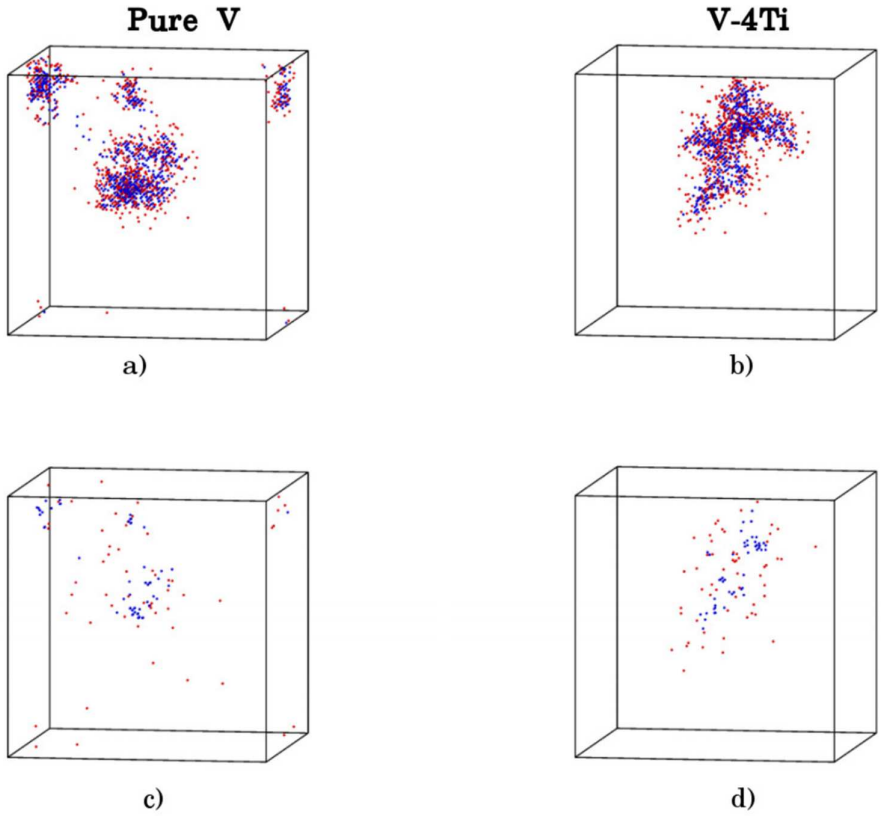

Figure 2. Point defects in the simulated crystallite containing 432 000 atoms in pure vanadium (a) and in alloy V-4Ti (b) at the peak time and at the time of main state in 12 ps for pure vanadium (c) and alloy V-4Ti (d). Vacancies and SIAs are shown blue and red, respectively. PKA energy is 20 keV.

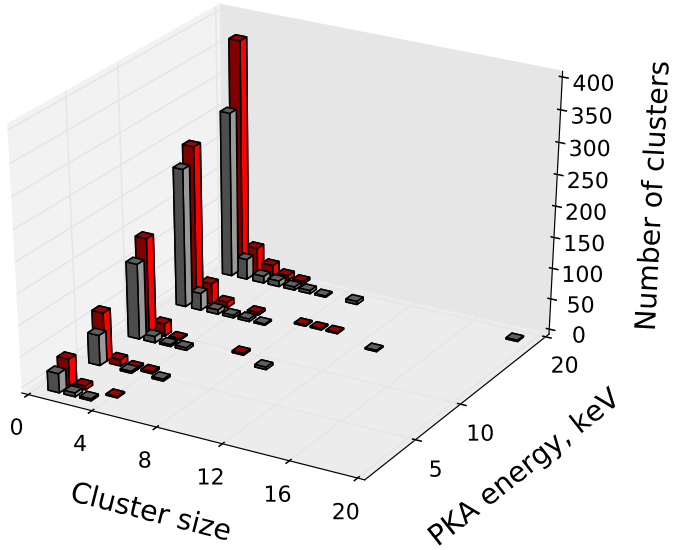

Figure 3. Distribution of vacancy clusters by their sizes in pure vanadium (grey color) and in alloy V-4Ti (red) for PKA energies of 1, 5, 10, 15, and 20 keV. The total number of clusters for 10 crystallites is given for each energy of PKA.

case of pure vanadium and alloy V-4Ti at the same energy can be attributed to the proximity of the masses of these elements and to the relatively small concentration of titanium in the alloy.

A more noticeable effect of titanium is manifested in the structural differences of the radiation damaged region. Figure 2 presents a comparison of the structures of pure vanadium and alloy V-4Ti in the peak time and by the time of 12 ps (main state after the displacement cascade) by the example of the crystallites with a maximum energy of 20 keV considered in this work.

As can be seen in figure 2, in the alloy V-4Ti at a main state, the radiation damaged region is more compact, interstitial atoms are located closer to the center of the damage region, and in pure vanadium they go to large distances, which on average are 2 times larger. This difference is due to the higher mobility of interstitial atoms in pure vanadium.

One of the characteristic features of the structure of the radiation damaged region is the formation of the vacancy complexes and complexes of self-interstitial atoms (SIA). Figure 3 shows the histogram of vacancy clusters size distribution as a function of the PKA energy. Clusters were determined by the cluster analysis method implemented in the software package OVITO. The cutoff parameter selected a certain threshold value, which is equal to the distance to the second coordination sphere in vanadium (3.03 Å [15]).

As can be seen from the results of the analysis of the vacancy clusters presented in figure 3, the effect of titanium leads to a systematic decrease in the size of the surviving vacancy clusters in comparison with pure vanadium. In the latter, clusters are formed up to the size of 19 vacancies at the energy of 20 keV. However, most survived vacancies do not form complexes. This agrees with the results of modeling cascades in pure vanadium using other interatomic potentials [8]. In the case of the alloy V-4Ti, the number of monovacancies is greater than in pure vanadium, despite the fact that the total number of surviving Frenkel pairs is practically the same in pure V and alloy V-4Ti, as noted earlier (also see figure 1). This is explained by the high binding energy of vacancies with titanium atoms in the bcc lattice of vanadium [6]. The vacancy trapping

by titanium constrains the formation of vacancy complexes. As for interstitial atoms, in both materials they are in most cases in free form, or form clusters of two or three atoms.

4. Conclusion

In this paper, MD simulations of cascades of atomic displacements for pure vanadium and alloy V-4Ti were carried out. Comparison of simulation results allowed revealing common features and differences of stages of cascades for the investigated materials. Doping of 4% titanium does not affect the number of surviving Frenkel pairs in the bcc lattice of vanadium for all of the considered PKA energies in the interval 0.5–20 keV. The differences are manifested in the atomic structure of the region of the cascade development. In the case of the alloy V-4Ti, a large fraction of vacancies are in small-sized clusters, mainly remaining in the form of monovacancies. Interstitial atoms, in both pure vanadium and alloy V-4Ti, practically do not form clusters, except for a small number clusters containing 2 or 3 SIAs. Moreover, interstitial atoms in pure vanadium propagate to larger distances from the center of the cascade region, in comparison with the alloy V-4Ti.

Acknowledgments

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