Aggregatization of Frenckel Pairs in Metallic Materials at External High-Energetic Impulsive Influences

M.D. Starostenkov, N.N. Medvedev*, G.M. Poletaev, O.V. Pozhidaeva

Altay State Technical University, Lenin Street, 46, City Barnaul, 656038, Russia, Phone (8-3852)36-85-22, Fax(8-3854)36-78-64, E-mail: genphys@agtu.secna.ru
** Biysk Pedagogical State University, Korolenko Street, 53, City Biysk, 659333, Russia*

Abstract – The peculiarities of annihilation and aggregatization of Frenckel pairs in pure metals Ni, Al and Ni_3Al intermetallide at low temperatures are studied by the method of molecular dynamics. Intensive formation, recombination and aggregatization of interstitials and vacancies take place at an impulsive heating to the temperature, which is near the temperature of phase transition crystal-melt.

1. Introduction

The influence of radiation on a solid state of any nature (dielectric, semiconductor, metal) leads to the appearance of so-called Frenckel pairs – vacancies and interstitial atoms (IA). The processes of accumulation of Frenckel defects and their further evolution determine radiation stability of a material. It is of great interest for radiation Material Science.

It is known [1–2] that chaotic distribution of defect pairs over the volume in irradiation process change into more ordered distribution. As a result, heterogeneous distribution local density of non-interacting defects of the same type takes place. It is shown in essential deviation of pair centers consentration on the value corresponding to chaotic distribution [1]. Defect consentration owing to aggregates formation can exceed consentration during their chaotic spatial distribution in several times [2]. But the studies devoted to evolution of Frenckel defects in metals are not known to the authors.

2. Model

The paper presents the results of two-dimensional simulated experiment. Frenckel pairs in metals without any admixtures (in Ni, Al) and alloy Ni_3Al were simulated, and their evolution was observed during the interval of time. Molecular dynamics method was used as the method of computer simulation. It was considered low temperature case, where diffusion was insignificant (order 400 K). The cell contained 3250 atoms, periodical boundary conditions were applied. Interaction between atoms was given by Morse potential.

The definite number of Frenckel pairs was placed in the calculated block of crystal arbitrarily. Then, relaxation of the system by an impulsive heating near 0 K took place. It was made to determine a start configuration and energy of the complex formation. Further, the crystal was subjected to an impulsive heating to the temperature of a computer experiment. It was kept at that temperature during some interval of time. Then it followed a hardening of the sample to 0 K by energy dissipation outside the crystal block under study.

The relaxation of the investigating system was held by the method of molecular dynamics. The atomic displacement in the cell was calculated by the solving of the system of ordinary differential equations of Newton's movement.

The interactions of atoms were limited by the distance 8 E (first 5 coordination spheres in 2D system). The temporal step of recalculation of movement equations system was equal to 10^{-14} seconds. In all the experiments, the temperature of the calculated block was equal to 1500 K. The temperature was given by the initial velocities of atoms: every atom of the calculated block had the initial velocity equal to root-mean-square velocity in the correspondence with Maxwell distribution multiplied by $\sqrt{2}$. The directions of the velocities were given as accidental ones, but on condition that total impulse of atoms in the calculated block was to be equal to zero [3,4].

3. Results and discussion

It was found an effect in the result of the experiment. Interstitial atoms were moving to each other and then united. They formed another defect-a dipole of an elastic stress or so-called dislocation dipole. Vacancies interact neither with the removed IA nor with each other and they left relatively stable.

Fig. 1 shows a fragment of the cell (Al), where we can see six Frenckel pairs and temperature of the cell-150 K. Also all possible variants of interstitial displacements can be noticed. IA annihilates with a vacancy, it can be observed in the upper part of the figure. In the middle, IA diffusion is seen. Four IA unite in an "association" forming a dipole of an elastic stress. A new defect is observed near a vacancy, but no one atom occupies it. It can be seen in the figure that an initial interstitial atom does not displace (the displacement of atoms takes place in the result of the displacement of the nearest neighbour by it), it displaces the nearest neighbour. In this connection, the displaced atom in turn displaces the other atom and so on.

In Fig. 1, it can be seen an interstitial atom which does not recombine with a vacancy (because of the

removal of the last one) and does not unite with a dislocation dipole. It can be explained by it's removal from the other IA or by the effect of saturation of a dislocation dipole by interstitial atoms. It is obtained a unification consisting of the dozen of IA. Interaction between interstitial atoms is spread to 20-th neighbouring.

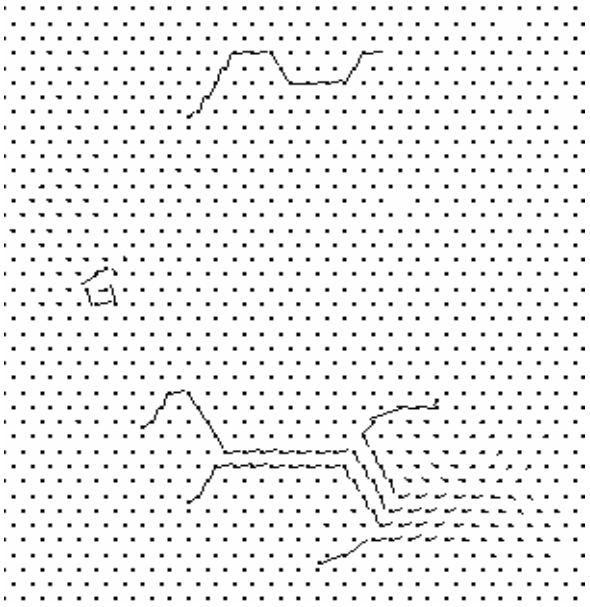

Fig. 1. Trajectories of the movement of atoms displaced from their places by an IA (Al)

Fig. 2 depicts the result of 10 IA unification (further one of them recombine with a vacancy).
The trajectories show the unification of atoms (Fig. 2). The defect has a good mobility, the movement direction can be changed during the interval of time arbitrarily (see Fig. 2).

When an interstitial atom meets a vacancy, further processes depend on the place of it's occupation. If a vacancy is situated at the edge of united IA flow, the recombination takes place at any condition (marked by the square, Fig. 2). When a vacancy appears at the distance of 3 atoms from the edge of a dislocation dipole (marked by a little cross, Fig. 2), recombination takes place in the dependence on temperature. For Al, recombination occurs at the temperature higher 115 K. For Ni – at the temperature higher 360 K (increment of numerical integration – h = 0.01 ps).

It is evident that when a vacancy is removed from a dislocation, conditions for recombination appear at a higher temperature. The number of interstitial atoms uniting a defect is not limited, because only dislocation nucleus can be the center of the attraction of free IA.
The effect of IA unification in a dislocation dipole is observed nearly in all simulated experiments of metals with Frenckel defects. The defects leave stable at low temperatures. But all vacancies recombine with interstitial atoms at the temperatures from 100 K to 800 K in the dependence on metal type. Not only single IA recombine with vacancies but also IA of the structure of a dislocation dipole.

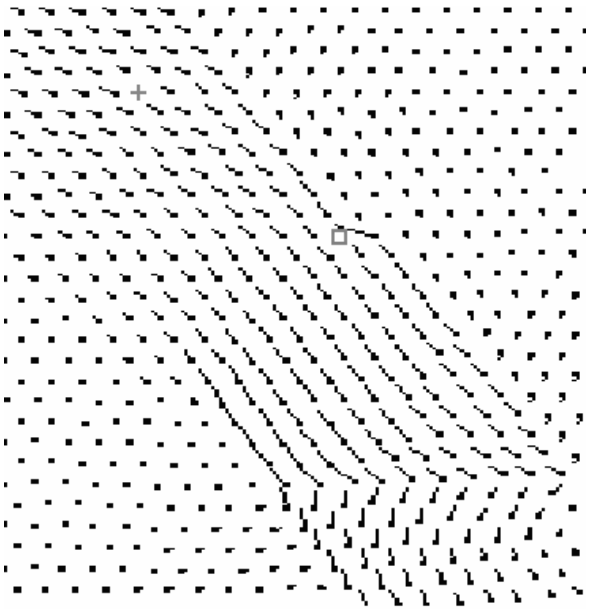

Fig. 2. Trajectories of the movement of the unified IA (Ni, T=135 K)

It is obvious that IA uniform in dipoles because such unification is more profitable. It can be explained also from the point of view of dynamics. Neighbouring atoms influencing on each atom of crystal lattice site with some forces. These forces are compensated at low temperature because of the symmetry of a crystal lattice. This circumstance does not allow an atom to move from it's place. IA are in the other conditions. They are influenced by not compensated forces of the other IA. It makes them to move to each other, i.e. IA move to a neighbouring atom having occupied it's place. The atom in turn occupies the place of the other atom and so on. The process continues until all neighbouring interstitial atoms unify in a dislocation dipole.

At low temperatures, atoms having united in a dislocation dipole are not able to overcome a potential barrier and occupy a vacancy, even if it is situated not far from it. The probability of the barrier overcoming increases at the increasing of temperature.

Aggregates of interstitial atoms appear to be less mobile in comparison with other defects. They begin to recombine with vacancies at high temperatures. At the same time, it is found intensive formations and annihilation of new Frenckel pairs to the temperatures which is near to melting temperature, at an impulsive heating. Interstitial atoms of new pairs join to the existing aggregates. Free vacancies unite in divacancies complexes.

To our opinion, intensive formation, annihilation and aggregatization of Frenckel pairs at the tempera-

tures preceding take place to melting. Such defects and their aggregates should contribute in phase transition crystal-melt.

Redistribution of local densities over the volume is connected with the formation of dynamical Frenckel pairs. The density is high in the areas having interstitial atoms. The density is low in the areas with the increased concentration of vacancies and their complexes.

Aggregatization of interstitial atoms in Frenckel pairs of Ni_3Al intermetallide blocks thermo activated diffusion and alloy disordering process.

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