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HIGH-VELOCITY MASS TRANSFER IN FCC-METALS CONTAINING CHAINS OF VACANCIES AND INTERSTITIAL ATOMS

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Using the method of molecular dynamics simulations, the dynamics of structure rearrangement in the course of relaxation in a three-dimensional aluminum is investigated via introduction of one-dimensional chains containing equal number of vacancies and interstitial atoms and located in close-packed positions along the <101> directions. This model represents a starting material structure possessing regions with differing mass densities: m^+ and m^-. The process of relaxation is shown to proceed via a number of phases: generation of shock waves, nucleation of vortex displacements of atoms, transformation of shock waves into acoustic waves, and correlated high-velocity collective displacements of atoms from interstitial into vacancy positions. The latter displacements are developed at velocities much higher than acoustic velocity.

Keywords: mass transfer, structure defects, simulations.

INTRODUCTION

In condensed matter physics there is a currently increased interest in condensed systems with extraordinary properties and structure heterogeneities of a nanoscale level. Primarily, these are semiconducting systems that could in the future provide a basis for a new type of electronics – nanoelectronics. Other promising systems are metals and their alloys, which exhibit unique properties in nanostructured state for application as structural and functional materials. From the research perspective, of great interest are metals and ordered alloys with long-period structure [1–10], in which the defect structure is provided by an anti-phase boundary (APB) [1, 11–21]. Of special interest are metals and alloys with anomalous properties, including high-rate mass transfer [22].

Point defects play a critical role in structure-energy changes taking place in materials under high-energy impact. Vacancies and interstitial atoms are the simplest representatives of point defects, which are easy to investigate. Under external action an atom can move from a site in the crystal lattice to an interstitial space, leaving behind a vacancy and forming a Frenkel pair, and the regions adjacent to the vacancy and interstitial atom are the regions of local density changes (Δm^- and Δm^+, respectively) [23]. In the course of structure relaxation, a large number of vacancies formed as a result of, e.g., radiation damage, recombine with interstitial atoms, with the "ideal" density of the crystal being restored. The other part of defects migrates towards interfaces in the region of the local density variation [24]. This recombination, especially at short-range distances between the vacancy and interstitial atom occurs sufficiently fast to prevent experimental investigation of these processes, especially in metals.

Vacancies and interstitial atoms can appear in the crystal lattice as a result of external high intensity action such as ion implantation. They give rise to local density variation and result in elastic stress fields. Further non-linear relaxation processes can in turn generate relaxational background vibrations in the crystal. At comparatively high

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temperatures they are suppressed by thermal chaotic atomic vibrations. In [25, 26] the authors addressed the peculiarities of generation of relaxational displacement waves in the vicinity of vacancies and the respective interstitial atoms in a number of fcc-metals. They simulated pulsed introduction of a vacancy or interstitial atom, followed by structure relaxation at a predetermined initial temperature close to 0 K. It was found out that in the first stage the atoms displace with respect to the point defect, these displacements being discrete along the close-packed directions. After that, the displacements involve other directions, which could be treated as shock displacements. Still further these displacements become collective in the form of a spherical wave propagating from the point defect as a center. The initial atomic displacements with respect to the central interstitial atom turn out to be nearly two orders more intensive over similar displacements with a central vacancy. Note that the spherical-wave propagation velocity is initially much higher than the speed of sound, while approximating the latter over time.

The purpose of this work is using the method of molecular dynamics simulations to study the features of structure-energy transformations taking place in a bulk fcc-metal nanocrystal in the course of stress relaxation via atomic displacements under the condition of introduction of one-dimensional chains containing an equal number of vacancies and interstitial atoms located along close-packed <110> orientations of the fcc-lattice.

COMPUTER EXPERIMENT MODEL AND PROCEDURE

In this work we investigate the mechanisms of structure-energy rearrangements in a metal nanocrystal with an fcc-lattice in the course of stress relation via atomic displacements and by introduction of one-dimensional chains, containing equal number of vacancies and interstitial atoms, oriented along close-packed directions of <101>-type.

A simulation grid was formed as a rectangular containing 50 layers of atoms along <101> and <211> 12 layers of atoms oriented along <111> in the crystallography of an fcc-lattice. Periodic boundary conditions were set at the grid boundaries along <111>, and rigid boundary conditions were prescribed in the other two orientations. Let us use the Morse method of pair-potential functions [22–29], since our interest lies in the principal physical mechanisms of structure transformations. The selected values of the Morse functions [27] correspond to aluminum. The use of a straightforward semi-empirical potential is reasonable since the interaction characteristics are controlled by the elastic modulus with which the potential parameters were fitted. The cutoff radius for pair interaction between atoms was reduced to the first six coordination spheres. Use was made of the method of molecular dynamics [30–32]. In order to solve a system of ordinary differential equations, use was made of the Euler method in a half-step run.

Two chains were introduced into the computational grid, which contained vacancies and interstitial atoms. After that, a relaxational procedure was initiated by heating to the temperature close to 0 K. In predetermined time intervals we registered the crystal structure changes taking place in the course of relaxartion without energy dissipation beyond the computational grid.

The following parameters were computed and analyzed: the energy change per single atom as a function of relaxation time and the time of complete annihilation of the vacancy and interstitial atom, in other words, the time within which the sources of local density variation disappear.

RESULTS AND DISCUSSION

The computer simulation demonstrated that during relaxation there is a pulsed heating of the crystal to a certain temperature in all experimental runs irrespective of the number of interstitial atoms and vacancies introduced; shock waves are developed, which further transform into acoustic waves and vortex displacements of atoms. These phenomena are most conspicuous in the vicinity of interstitial atoms [33]. Given a random distribution of vacancies and interstitial atoms in the crystal, in the final relaxation phase we observe chains of non-correlated displacements from the interstitial atom towards the respective vacancy. The chains are oriented along close-packed directions <101> and can be polygonal. The vacancy – interstitial atoms pairs annihilated at a considerable distance between them. If the equal number of vacancies and interstitial atoms turned out to be equal, their annihilation was not complete. In the latter case, the crystal still contained the regions of local density variation (denoted as m^+ or m^-, depending on the excessive defect

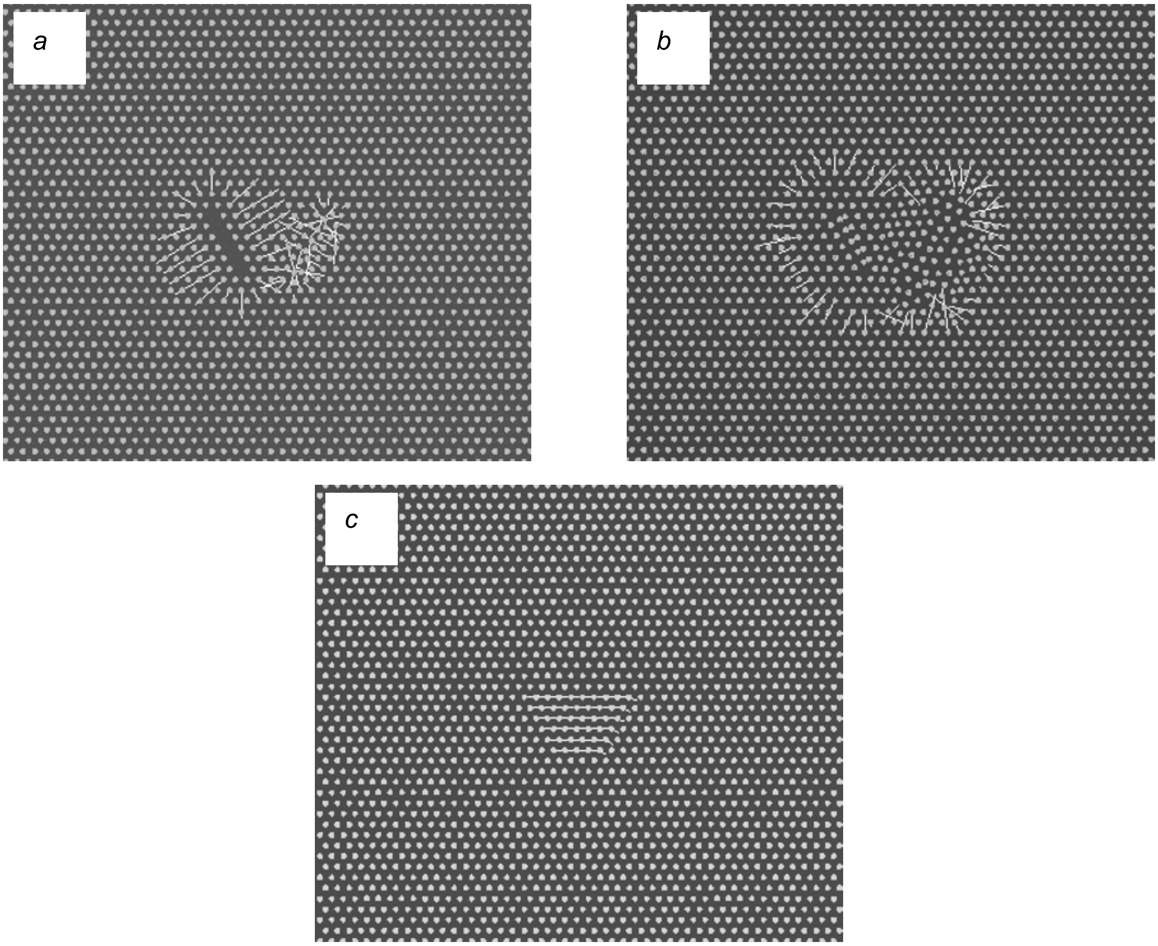

Fig. 1. Atomic lattice configuration in the {111} plane at different relaxation times: 0.01 ps (*a*), 0.09 ps (*b*), and 0.7 ps (*c*). The displacement pattern in Figs. 1*a* and *b* are enlarged; large displacements are cut off.

type). For very large spacings between the structure defects and their low concentration, the energy released during relation was not enough to excite collective displacements of atomic pairs resulting in annihilation of the vacancy – interstitial atom pair. The most dynamic relaxation process was observed in the cases where interstitial atoms and vacancies formed chains, in particular, along close-packed orientations. When the spacing between the chains is increased, the rate of formations of collective displacements is decreased, while with increased number of point defects in the crystal system the rate is increased. The intensity of the initial wave shocks, which are developed in the course of relaxation, behaves in a similar manner. The displacement velocity and the trajectories change with the orientation angle of a vacancy and interstitial atom. For the disorientation angles 0, 2π/3, and π, the displacement trajectories are found to be polygonal, while at a disorientation angle of π/3 they are rectilinear. The cooperative displacement velocities in this case are found to be maximal.

Let us consider an experimental run in which we introduced 6 vacancies and six interstitial atoms into the computational grid, which were positioned symmetrically with respect to each other at the angle π/3. Figure 1 shows the patterns of dynamic structures formed in the course of relaxation at different time points of our computer experiment.

At the onset of relaxation, shock waves of atomic displacements are generated in certain crystallographic directions (Fig. 1*a*). Then the shock wave begins to transform into an acoustic wave (Fig. 1*b*). Later in the process, regions of vortex displacements of atoms are generated in the interference regions. Due to these, a mechanism is

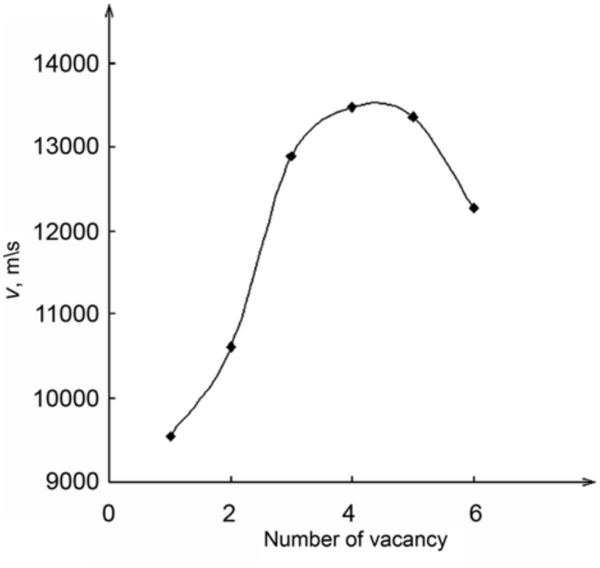

Fig. 2

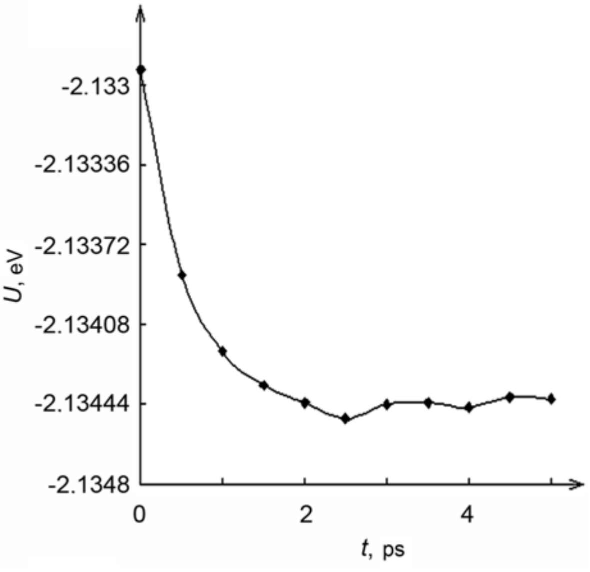

Fig. 3

Fig. 2. Velocity of cooperative atomic displacements versus the number of a vacancy (interstitial atom) in the lattice.

Fig. 3. Energy of a single atom versus experimental time.

switched on, which in a relay-race mode displaces a collection of interstitial atoms towards the positions occupied by the lattice atoms. The latter push out the entire row of atoms chain by chain towards the vacant sites via the crowdion mechanism (Fig. 1*c*). The cooperative displacements of a crowdion group, corresponding to the number of interstitial atoms, are energetically more favorable than single displacements. The relaxation process clearly demonstrates self-organization of the system from chaos into an ordered displacement of a collection of atoms. As a result, the regions of non-uniform distribution of the local density m^+ and m^- in the crystal block under study disappear. The initiation of shock waves, their transformation into acoustic waves, and the development of vortex atomic displacements were shown earlier [33] using the atomic structure of a two-dimensional crystal during single vacancy formation. The nonlinear high-rate mass transfer was already reported in [34].

SUMMARY

The investigations made in this work have revealed that stress relaxation in a bulk structure, wherein regions of local material density variation are generated using point defects, involves a few stages. The initial stage represents "shock" displacements of atoms treated as a shock wave generated in the material, which is later on transformed into a longitudinal wave. The final stage of relaxation has been found to represent cooperative atomic displacements following the crowdion mechanism, which eventually result in defect annihilation. We have also shown that the momentum transfer by the atoms during these displacements occurs at the rate much higher than the speed of sound for this material.

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