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Dynamics of supersonic *N*-crowdions in fcc metals

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ABSTRACT

Crowdion is an interstitial atom located in a close-packed atomic row. It is an important point defect participating in relaxation processes occurring in metals and alloys under irradiation, effectively transferring mass and energy. In recent works of the authors, the concept of a supersonic crowdion was extended to a supersonic *N*-crowdion, in which not one, but *N* atoms move with high speed along a close-packed row. An experimental study of interstitial atoms moving along a crystal lattice at supersonic speeds encounters serious technical difficulties, and the most effective method for studying them is the molecular dynamics method. In this regard, a numerical study of dynamics of supersonic crowdions in metals is very important. In the present study, the molecular dynamics method was used to analyze the motion of supersonic 1- and 2-crowdions in fcc metals Ni, Al, Cu. The calculations were carried out using the LAMMPS software package and many-body potentials. The *N*-crowdion was excited by setting the same initial velocity to *N* neighboring atoms along a close-packed row. It was found that the mean free path of a 2-crowdion in pure metals can reach values that are 3 times greater than the mean free path of a 1-crowdion having the same initial energy. The results obtained indicate a higher efficiency of 2-crowdions in mass transfer in the studied metals. In further works, the possibility of launching supersonic 2-crowdions by bombarding the crystal surface with biatomic molecules will be analyzed.

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1.Introduction

In the course of operation or technological processing, modern materials are often subjected to extreme influences, leading the material to a far from equilibrium state (Turnage et al., 2018). Such effects include laser irradiation (Kiss et al., 2019), intense plastic deformation (Korznikova et al., 2006, Korznikova et al., 2012), impact loads (Wei et al., 2008, Shepelev et al., 2020), ion and neutron irradiation (Terentyev et al.,2008, Terentyev et al., 2007, Zhang et al., 2016, Zhou et al., 2014), plasma treatment (Nordmark et al., 2009) and others. Another important fact is that under such external conditions, the nonlinear nature of the interatomic bonds inevitably manifests itself. One of the consequences of this effect is the presence of an abnormally high

concentration of point defects, which was previously observed in metals subjected to all types of the abovementioned treatments.

The scenario for the development of a defect structure in the far from equilibrium states usually involves the formation of Frenkel pairs, that is, vacancies and interstitial atoms. Since the interstitials migrate much faster than vacancies due to the lower potential barriers, they tend to annihilate during or shortly after creation, which makes their experimental analysis difficult. Both types of point defects can exist in several configurations, the main difference being the degree of spatial localization and structure of their clusters. The interstitial atom in the fcc lattice can be located in an octahedral or tetrahedral pore, or it can be embedded in a close packed atomic row, forming a crowdion with a very low migration energy and, therefore, high mobility, playing an important role in mass transfer and structure evolution in non-equilibrium states (Fitzgerald et al., 2018). A defect of the opposite topological sign, a vacancy, is characterized by a much higher migration energy and, therefore, is less mobile. As such, it is often observed in the structure of materials by various experimental methods (Korznikova et al., 2006, Xu et al., 2017, Xu et al., 2019). Like an interstitial atom, a vacancy can exist in a delocalized form called voidion, which, however, has a very low probability of existence due to some features of nonlinear interatomic interactions (Marjaneh et al., 2018) and, to date, a limited number of works have been devoted to voidions (Mazilova et al., 2018, Uche et al., 2009). It has been demonstrated that both vacancy clusters (Mazilova et al., 2018, Matsukawa and Zinkle, 2007) and interstitial atom clusters (Terentyev et al., 2007, Kononenko et al., 2016, Fitzgerald et al., 2018) can exhibit cooperative one-dimensional motion.

The low-temperature migration of interstitial atoms in bcc metals can be explained from the point of view of diffusion of crowdions (Indenbom 1970), where the one-dimensional motion of crowdion clusters can have a greater effect on the development of a defect structure, since it is associated with overcoming the potential barrier several orders of magnitude lower than that for an isolated crowdion (Fitzgerald et al., 2018). Supersonic 2-crowdions are much more efficient in mass transfer than supersonic 1-crowdions, which was numerically confirmed for crystals with Morse and Lennard-Jones interatomic potentials (Korznikova et al., 2019, Dmitriev et al., 2017, Chetverikov et al., 2017), pure metals (Babicheva et al., 2019, Bayazitov et al., 2018) and Ni_3Al intermetallic compound (Bayazitov et al., 2019).

Another important issue that needs to be studied is the effect of the configuration of a crowdion cluster on the dynamics of propagation and the formation of the structure of the resulting defects. It was shown that vacancies and crowdion clusters can lead to the formation of vacancy and dislocation prismatic loops (Korznikova et al., 2018). It was shown in (Shepelev et al., 2020) that the evolution scenario of a defect structure caused by the excitation of supersonic *MN*-crowdions strongly depends on the initial conditions, that is, on the values of *M* and *N* and the initial velocities of the excited atoms.

One of the problems of studying the motion of supersonic crowdions in metals and ordered alloys by the molecular dynamics method is the search for the initial conditions leading to their initiation. It was found that one interstitial atom can move at a supersonic speed along a close-packed atomic row in two different ways, either in the form of a 1-crowdion or in the form of a 2-crowdion (Korznikova et al., 2019, Dmitriev et al., 2017, Chetverikov et al., 2017). The difference is that in the first case only one atom moves at a high speed, and in the second - two atoms move at a high speed at the same time. The next important issue is the establishment of a range of atomic velocities at which the stable dynamics of supersonic crowdions takes place. If the initial atomic velocity is too small, a supersonic crowdion will not be initiated, since the interstitial atom will not be able to overcome the potential barrier to move into the neighboring interstitial position. If the initial velocity of the atoms is too high, the condition of self-focusing propagation of an interstitial atom will be violated (Dmitriev et al., 2017). In addition to the above issues, there are also problems of visualization and analysis of the obtained numerical results. Crowdions are divided into subsonic and supersonic ones depending on the speed with which they move. In this work, we study supersonic crowdions in the crystal structure of fcc metals Ni, Al and Cu.

2. Simulation setup

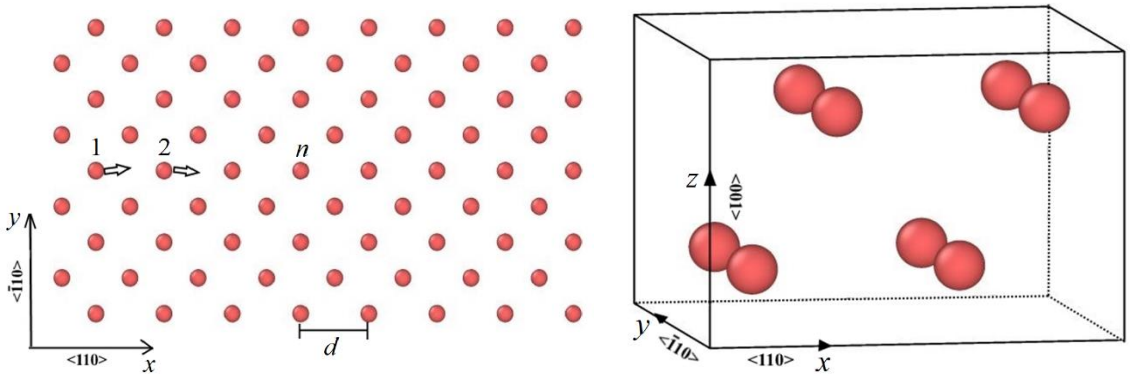
In this work, we consider fcc metals Ni, Al, and Cu with lattice parameters a_{Ni} = 3.524 Å, a_{Al} = 4.050 Å, and a_{Cu} =3.615 Å, respectively, and with an interatomic distance $d = a/\sqrt{2}$. The *x* and *y* axes are oriented along the close packed directions [1 1 0] and [$\overline{1}$ 1 0], and the *z* axis is oriented along the [0 0 1] direction (Figure 1). The *x* axis is directed along a close-packed atomic row; *d* is the interatomic distance or diameter of the atom. Atoms in one close-packed row are numbered by the index *n*. In Figure 1 (b), a parallelepiped-shaped translation cell containing 8 atoms is shown. The computation cell includes 30 such cells along the *x* axis, 4 cells along the *y* axis, and 2 along the *z* axis. The total number of atoms is 1920.

Only supersonic regime of crowdion motion is studied, when any disturbance created by the crowdion remains in a certain cone behind it. Periodic boundary conditions were used. No thermal vibrations are

introduced, i.e., modeling is carried out at a temperature of 0 K. The supersonic 1- and 2-crowdions were excited by setting the initial velocity V_x to one and two atoms, respectively, as shown in Figure 1 (a). A small component of velocity in lateral direction, V_y=$\mathbf{10^{-5}}$ V_x is introduced in order to analyze the stability of crowdion propagation. The initial velocities of all other atoms and the initial displacements of all atoms in the computational cell are equal to zero. The total energy of the system is equal to the kinetic energy of the excited atoms at t=0:

$$T_0 = \frac{NMV_x^2}{2}. \quad (1)$$

The contribution from the small transverse component of the initial velocity is not taken into account in (1). The mass M of Ni atom is 59 amu, the mass of Al atom is 27 amu, while the mass of Cu atom is 64 amu. In the simulations, we use the LAMMPS software package with the many-body interatomic potentials constructed with the help of the embedded atom method.



(a) (б)

Figure 1. (a) The atoms occupying the sites of the fcc lattice projected onto the *xy* plane, where the axes of the Cartesian coordinate system *x*, *y* and *z* are aligned with the crystallographic directions [110], [$\bar{1}$10] and [001]. (b) A translational cell in the form of a parallelepiped containing 8 atoms.

3. Results and discussion

With the use of molecular dynamics modeling of supersonic 1- and 2-crowdions in fcc lattices of Ni, Al and Cu the numerical data was obtained, which was used to construct the dependences of the mean free path on the initial velocity (Figures 2 and 3) and the initial kinetic energy (Figure 4) of the excited atoms. Figure 2 shows the dependences of the mean free path of the 1-crowdions in the three studied metals on the velocity of the initial excited atom. Figure 3 shows the dependences of the mean free path for 2-crowdions on the initial velocity. In the panels (a) of Figures 2 and 3 the mean free path (ordinate) is given in the units of the equilibrium interatomic distances, while in the panels (b) in angstroms. Metals have different values of the interatomic distance d, but normalization of the mean free path by d does not change the order of metals in terms of the crowdion's mean free path. Maximal initial velocity presented in Figure 2 is 150 Å/ps and in Figure 3 it is 80 Å/ps. For higher initial velocities cowdion dynamics becomes unstable since the minimal distance between the atoms becomes less than d/2 (Dmitriev et al., 2017). It can be noted that for both 1-crowdions and 2-crowdions, for the same initial velocity, the largest mean free path is observed in Cu, and the shortest one in Al. This is because Cu atom has the largest mass and the Al atom the smallest mass. Atoms with the greater mass gain larger kinetic energy having the same velocity, according to Equation (1).

Based on the results presented in Figure 4(a), we can conclude that for 1-crowdion the mean free path in all three metals increases linearly with the initial kinetic energy. The slope of the linear dependence is somewhat higher for Cu and it is almost same for Ni and Al. On the other hand, as it is seen from Figure 4(b), for 2-crowdion the mean free path grows with the initial kinetic energy faster than linearly. Remarkably, 2-crowdions having same initial energy travel greater distances than 1-crowdions. Supersonic 2-crowdions with the same initial energy travel longest distance in Cu and shortest distance in Al.

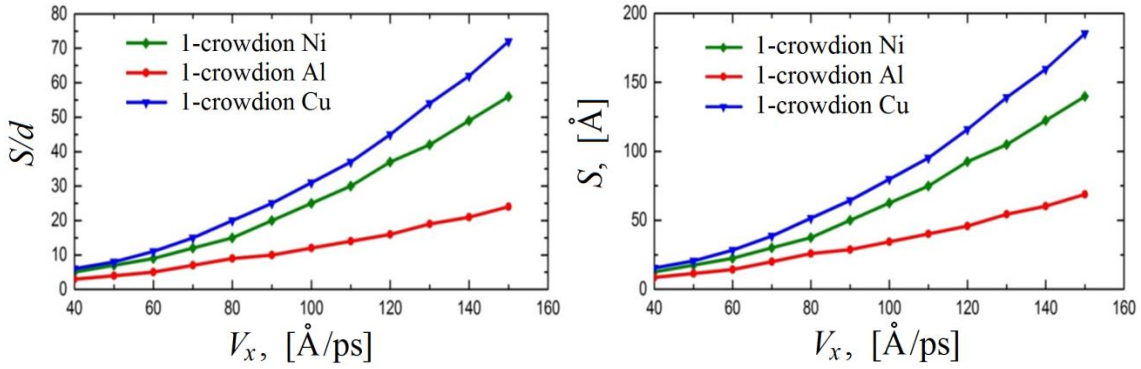


Figure 2. Dependence of the mean free path of the 1-crowdion on the initial velocity of the excited atom for Ni (green rhombuses), Al (red circles), and Cu (blue triangles). In (a) the mean free path is normalized to the equilibrium interatomic distance *d*, while in (b) it is given in angstroms.

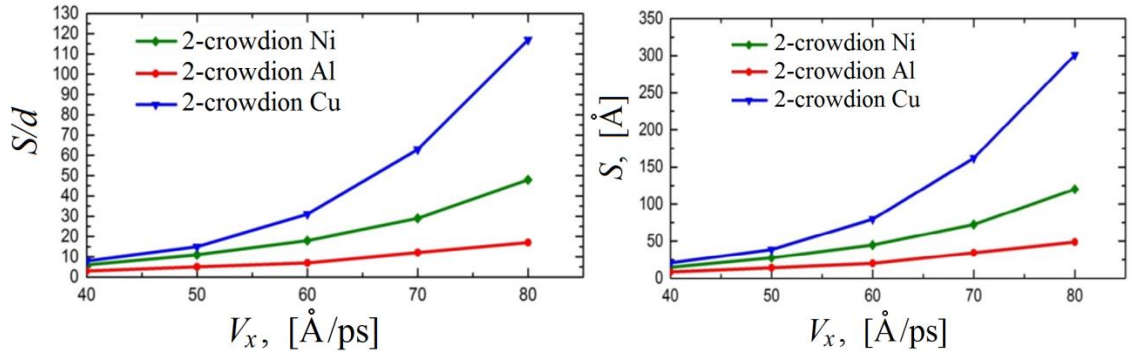


Figure 3. Same as in Figure 2, but for 2-crowdion.

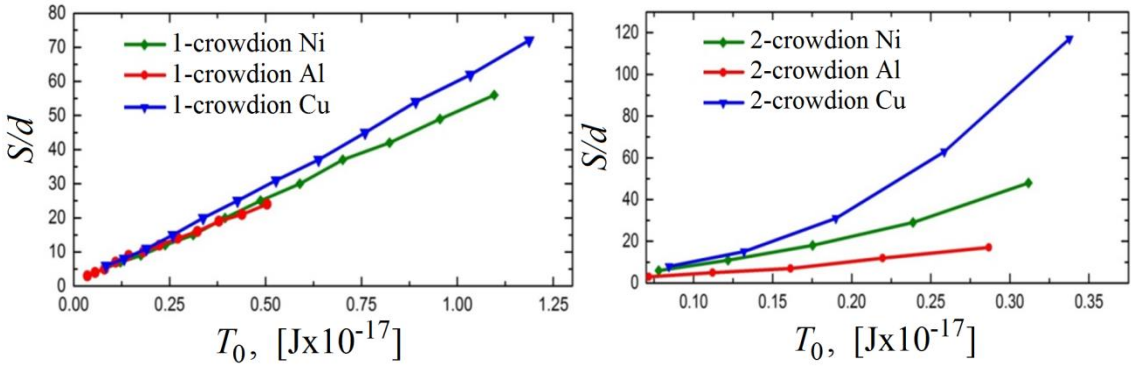


Figure 4. Dependence of the mean free path on the initial kinetic energy of atoms for Ni, Al, and Cu. In (a) the results for 1-crowdion are presented, while in (b) for 2-crowdion.

4. Conclusions

Molecular dynamics modeling of supersonic 1- and 2-crowdions in fcc lattices of Ni, Al and Cu was performed. The mean free path of the crowdions was presented depending on the initial atomic velocity and initial kinetic energy. 1-crowdions demonstrate stable dynamics if the initial velocity of excited atom does not exceed 150 Å/ps. For 2-crowdions maximal initial velocity of excited atoms is 80 Å/ps. Excitation with greater initial velocity leads to the minimal interatomic distance of colliding atoms less than *d*/2, which violates the condition of self-focusing propagation (Dmitriev et al., 2017).

It was demonstrated that the mean free path of a 1-crowdion increases linearly with the increase in the initial kinetic energy. The slope of the linear dependence is somewhat higher for copper, as compared to Ni and Al demonstrating nearly same slope. On the other hand, the mean free path of a 2-crowdion increases with the initial energy faster than linearly. This can be explained by the fact that the maximal velocity of the atoms in 2-crowdion is $\sqrt{2}$=1.414 times smaller as compared to the maximal velocity of the atom in 1-crowdion having same energy. Smaller atomic velocities result in slower energy radiation by propagating 2-crowdion and it travels longer distance.

The largest mean free path was observed in copper, and the shortest in aluminum. Based on the simulation results, it was revealed that in all three studied metals excitation of a supersonic 2-crowdion with the same mean free path requires less energy than excitation of a supersonic 1-crowdion.

In further works, it is supposed to study the possibility of launching supersonic 2-crowdions by bombarding the crystal surface with biatomic or other molecules, following the preliminary study (Babicheva et al, 2019).

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