Dynamics of supersonic $N$-crowdions in bcc tungsten

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Abstract. An interstitial atom placed in a close-packed atomic row of a crystal is called a crowdion. Such defects are highly mobile; they can move along the close-packed row at subsonic and even supersonic speeds, transferring mass and energy. In this paper, we consider the initial conditions for excitation of $N$-crowdions, in which $N$-atoms move simultaneously with high speed. The most efficient methods for initiating supersonic $N$-crowdions with $N=2$ and 4 are demonstrated using molecular dynamics modelling for bcc tungsten.

1. Introduction

Migration of point defects in metals contributes to the mass and energy transfer during plastic deformation, heat treatment, irradiation, etc. Interstitial atoms, as compared to vacancies, have a higher energy but much lower mobility [1-4], with the exception of crowdions – interstitials embedded in a close-packed atomic rows [5], that are highly mobile. Crowdions can propagate along its close-packed atomic row transferring mass of an atom with subsonic or even supersonic speed [6-10].

Moving crowdions are difficult to identify experimentally, that is why, molecular dynamics is a very popular and reliable method of their investigation. This method proved to be an effective approach in analysis of surface voidions [11], discrete breathers [12,13] and recently discovered 2D nanomaterials [14-17]. Molecular dynamics is a suitable tool for the study of crowdions because they have nanometer size, corresponding to several interatomic distances, and they travel fast, so that the computational cell and the simulation time can be relatively small. Since crowdions move in a close packed atomic rows, their motion can be considered as quasi one-dimensional and can be described by the chain models, such as the Frenkel-Kontorova model [18,19]. In the frames of this model it was shown that crowdions initiated by a molecule impact on the surface have smaller energy threshold required for crowdion initiation in comparison to the initiation with single atoms [19]. This effect has been confirmed for Pt crystal, where the crowdion was found to emerge at lower energies and propagate longer distances, when it was excited by a molecule impact rather than by single atom impact [20]. The results of the work [21-23] show that clusters larger than three to four self interstitial atoms in Cu and Fe can demonstrate one-dimensional motion. Moving subsonic crowdions can bear a vibrational mode with the frequency lying well above the phonon spectrum [9].

In molecular dynamics simulations, crowdion dynamics is determined by the initial conditions. In this work, we study the effect of initial conditions used for crowdion initiation in the crystal structure of bcc W. Note that supersonic crowdions in bcc tungsten are poorly studied.

2. Simulation setup

A three-dimensional bcc lattice of tungsten is considered, the equilibrium interatomic distance of
which is $x_0 = 3.16 \, \text{Å}$. As shown in figure 1, the $x$ axis is directed along the close-packed atomic rows parallel to the [111] direction. For modelling, the EAM interatomic potential for tungsten is used, which is included in the molecular dynamics software package LAMMPS. The size of the computational cell is $543.7 \times 51.3 \times 44.4 \, \text{Å}$ and it included 80,000 atoms. Periodic boundary conditions were used along all three axes.

To launch a crowdion, the following initial conditions are used: the equal initial velocity $V_x$ is given to two or four neighbouring atoms in a close packed row parallel to the $x$-axis, as shown in figure 1 (a) and (b), respectively. The initial displacements and velocities of all other atoms in the structure are equal to zero. Thus, the total energy of the system is equal to the initial kinetic energy of excited atoms, $E=NMV_x^2/2$, where $N$ is the number of excited atoms and $M$ is the atom mass. As a result of application of such initial conditions for sufficiently large $V_x$, supersonic 2- or 4-crowdions are formed. In our simulations we take different values of $V_x$ and the dynamics of supersonic 2- and 4-crowdions.

![Figure 1](image)

**Figure 1.** Initial conditions used for excitations of supersonic (a) 2- and (b) 4-crowdions. Equal initial velocity $V_x$ is given to two or four neighbouring atoms in a close packed row parallel to the $x$-axis.

3. Simulation results

In figure 2, as the function of time, we plot normalized displacements of atoms in the close-packed atomic row where the supersonic $N$-crowdion moves. The left column is for 2-crowdion and the right column for 4-crowdion. Initial velocities of the atoms are from $V_x=40$ to $70 \, \text{Å/ps}$, as indicated for each of the four rows. The displacements of the atoms along $x$-axis, $dx$, are normalized to the equilibrium interatomic distance, $x_0$.

In the first row of figure 2 the results for $V_x=40 \, \text{Å/ps}$ are presented. For the 2-crowdion (left column) the two first atoms loose their initial kinetic energy at $dx/x_0=0.8$, so that they do not reach the position of the neighboring atom moving with the high speed and they reach this position drifting with a small velocity. The supersonic 2-crowdion rapidly transforms into a subsonic one after travelling about a dozen of interatomic distances. The 4-crowdion (right panel) launched with $V_x=40 \, \text{Å/ps}$ has two times greater initial energy. The atoms almost reach the position of the neighboring atoms and supersonic motion is observed during the whole simulation run (1 ps). Note that the supersonic 2-crowdion carries one interstitial atom, while supersonic 4-crowdion carries 2 interstitials. One can say that the 4-crowdion transports mass more efficiently because with the double energy it carries double mass over longer distance.

In the second row of figure 2 the results for $V_x=50 \, \text{Å/ps}$ are plotted. For the 2-crowdion the atoms loose their initial momentum still a bit before reaching the positions of the neighboring atoms. On the other hand, for the 4-crowdion one can see that the atoms stop nearly at the positions of the nearest atoms, i.e., at $dx/x_0=1$. In the third row of figure 2 we give the results for $V_x=60 \, \text{Å/ps}$. This initial velocity is sufficient for the 2-crowdion to shift the atoms to the positions of the neighboring atoms. For the 4-crowdions the atoms overshoot these positions. Finally, for $V_x=70 \, \text{Å/ps}$ (see the last row of figure 2) the initial velocity is big enough for both 2- and 4-crowdions to shift the atoms to the positions beyond the energy minimu.
Figure 2. Normalized displacements of atoms, in the close-packed atomic row where the supersonic \textit{N}-crowdion moves, as the functions of time. The left column is for 2-crowdion and the right column for 4-crowdion. Initial velocities of the atoms are from $V_x=40$ to 70 Å/ps, as indicated for each of the four rows.
4. Conclusions

According to the results of our simulations, the supersonic 4-crowdion transports mass more efficiently than the supersonic 2-crowdion because with the double initial energy it carries double mass over longer distance. The initial velocity of $V_x = 60 \text{ Å/ps}$ is sufficient for the 2-crowdion to shift the atoms to the positions of neighbouring atoms. For the 4-crowdion, $V_x = 50 \text{ Å/ps}$ is sufficient.

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