Subsonic $M,N$-crowdions in 2D Morse crystal

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Abstract. Crowdion is a zero-dimensional defect of the crystal lattice in the form of an extra atom in a close-packed atomic row. Crowdions can be at rest or move with subsonic or supersonic velocity. A moving crowdion transports the mass of one atom. Recently it has been revealed that crowdion clusters can be more efficient in mass transfer as compared to single crowdions. For example, in our recent work it has been shown that a supersonic $N$-crowdion can be excited by giving a sufficiently large equal initial momentum to $N$ neighbouring atoms in a close-packed row along the row. This work presents an extension of the concept of $N$-crowdion to $M,N$-crowdion, the latter one is excited in a 2D crystal by the initial kick of a block of $M \times N$ atoms along a close-packed direction. The effect of the initial velocity on the dynamics of $M,N$-crowdions is analysed for various values of $M$ and $N$. It is revealed that the initial velocity affects not only the propagation length, but also the resulting defect configurations. It is suggested that $M,N$-crowdions can be initiated from the surface by bombardment with nanoparticles.

1. Introduction

Highly mobile crystal defects, such as crowdions and prismatic dislocation loops, exhibit anomalous temperature independent mobility [1]. Due to this fact, their possible role in mass transfer in various crystals has been a subject for numerous studies [1-10]. For example, in [2] it was shown that the in-plane migration of self-interstitials in $\alpha$-zirconium was dominated by one-dimensional crowdion motion along $<11-20>$ directions, from time to time interrupted by off-line or out-of-plane jumps. Another analysis of the crowdion contribution to the mass transfer in the biatomic structure of W-He was performed in [3]. During the formation of helium clusters, interstitial tungsten atoms were produced and evolved into bundles of $<111>$ crowdions, which were reported to stay constrained around the helium clusters for a long time [3].

Crowdions can demonstrate different types of mobility. They can move with supersonic or subsonic velocity or be at rest. An increase in the crowdion velocity usually results in a growth of its degree of spatial localization. The concept of a supersonic an $N$-crowdion was introduced in [9]. In this case, not one, but $N$ atoms in a close-packed atomic row move simultaneously at a high speed, and the defect propagation length increases considerably.

A subsonic crowdion can bear a localized vibrational mode [10], and, thus, it has features of both a crowdion and a discrete breather. Numerous investigations of localized excitations, such as crowdions [1-10] and discrete breathers [11-20], have shown that they carry energy and/or mass thus contributing...
to the evolution of the crystal structure. An analysis of the crowdion dynamics performed in [10], showed that it was strongly dependent on the initial velocity. In this work, our aim is to study the effect of the configuration and the initial velocity of the crowdion on its dynamics, the mass propagation length, and the resulting defect structure.

2. Simulation details
We consider a 2D close-packed triangular lattice with an interatomic distance equal to $a$. Interatomic interactions are described by the Morse pair potential

$$V(r) = D(e^{-2\alpha(r-r_m)} - 2e^{-\alpha(r-r_m)})$$

where $r$ is the distance between two atoms, $D$, $\alpha$, $r_m$ are the parameters. The function $V(r)$ has a minimum at $r=r_m$. $D$ is the depth of the potential (bond breaking energy) and $\alpha$ is the parameter defining the bond stiffness. By a proper choice of units of energy, distance, and time, one can set $D$, $r_m$, and atom mass $m$ to be equal to 1. For the bond stiffness, a typical value of $\alpha=4$ is taken. We choose the cut-off radius $r_c=5r_m$ and find the equilibrium interatomic distance to be equal to $a=0.9656$. The computational cell includes 300×100 atoms. Periodic boundary conditions are used in the simulation.

Initial conditions are set as follows (see figure 1). The initial velocity $v_0$ is given to a block of $M\times N$ atoms (colored in figure 1) along the close-packed direction, where $N$ is the number of neighboring atoms in one close-packed row, and $M$ is the number of neighboring rows. Thermal fluctuations are not taken into account, which means that initially the crystal has zero temperature, with only $N\times M$ atoms having an initial momentum. Cases for $M$ from 1 to 5 and $N$ from 1 to 4 are investigated. For every $M$ and $N$ we have found the minimal velocity required to initiate a moving subsonic $M,N$-crowdion. The structure evolution induced by kicking a group of atoms was visualized with the OVITO software package [21].

3. Results and discussion
Figure 2 demonstrates the evolution of the energy distribution for the cases $M=1$, $N=1$ (figure 2, a-c) and $M=3$, $N=1$ (figure 2, d-e). Here blue (red) atoms have minimal (maximal) potential energies. The launch of one atom with the initial velocity $v_0=10$ results in the formation of a vacancy (a) and a moving breathing crowdion (b), which loses stability when its velocity becomes below the threshold value and transforms into an immobile interstitial atom (c). For the case of $M=3$, $N=1$ one can observe the formation of a three-vacancy complex (d) and a crowdion complex, which includes three extra atoms, one extra atom in each of the three neighboring rows (e). Figure 3 represents the evolution of the defect structure after launching of (a, b) $M=5$, $N=1$ and (c, d) $M=2$, $N=4$ crowdions. Detailed features are given in the figure caption. It should be noted that (i) in case of $M>4$, the vacancy loop and the crowdion cluster transform into prismatic dislocation loops of the opposite topological charge (a, b); (ii) for $M=2$, $N=4$ a 2×2 vacancy complex and two 1,2-crowdions are formed, one of them
moving in the close-packed direction different from the direction of the initial kick (c) and another one along this direction (d).

Figure 2. The potential energy distribution in a 2D Morse crystal after the launch of (a-c) 1,1- crowdion with $v_0 = 9.05$ and (d,e) 3,1- crowdion with $v_0 = 10$. The launch of one atom leads to the formation of (a) a vacancy, simulation time $t=4.5$, (b) a moving breathing crowdion, $t=4.5$, and (c) an immobile interstitial atom, $t=10$. The launch of three atoms results in (d) the formation of a three-vacancy complex, $t=4$ and (e) the propagation of a stable crowdion with three extra atoms, $t=4$.

Figure 3. The potential distribution of energy in a 2D Morse crystal after the launch of (a, b) 5,1- crowdion and (c, d) 2,4-crowdion, both with $v_0 = 9.0$. The launch of five atoms results in the formation of prismatic dislocation loops of the opposite topological sign, namely (a) a five-vacancy agglomerate and (b) a crowdion cluster with five extra atoms shown at the simulation time $t=17$. Initiation of the 2,4-crowdion results in the formation of a 2×2 vacancy complex and two 2,1-crowdions, one moving along the close-packed rows tilted by 60° with respect to the initial kick direction (c) and the other one along the direction of the initial kick (d).

The propagation of a 3,1-crowdion is shown in figure 4 a. The atomic displacement as a function of time, $X_n(t) = x_n(t) - x_n(0)$, is plotted for the atoms of the middle atomic row among the three rows along which the crowdion propagates. One can notice high frequency vibrations on the trajectories of atoms. The vibration frequency is above the phonon spectrum of the considered crystal [10,12] that allows us to claim that in this case we are dealing with a breathing subsonic crowdion similar to that analyzed in [10]. A detailed analysis of atomic displacement plots allows one to estimate the propagation length $S$ of crowdions. The results are shown in figure 4 b as a functions of $M$ for $N=1, 2, and 4$, where $S$ is normalized to the interatomic distance $a$. One can see that an increase in $N$ from 1 to 2 results in an increase in $S$ by three (for $M=5$) to four (for $M=1$) times. For $N=1$ and $N=2$ one can observe a monotonous increase in $S$ with growing $M$. However, for $N=4$ a non-monotonous $S(M)$ dependence can be seen. This is explained by a qualitative change in the formation of defects for $N \geq 4$. In particular, crowdions propagating along directions different from the initial launch direction are observed for $N \geq 4$.

4. Conclusions

The dynamics of $M,N$-crowdions has been studied for the first time for various $M \geq 1$ and $N \geq 1$. It was found that (i) an increase in $N$ from 1 to 2 drastically increases the propagation length of crowdions (by three to four times, see figure 4 b); (ii) a further increase in $N$ weakly affects this parameter due to the formation of crowdion complexes propagating along crystallographic directions different from the initial kick direction (see figure 3 c); (iii) $M,1$-crowdions carry an internal mode oscillating with a frequency above the upper edge of the phonon spectrum (see figure 4 a). We note that $M,N$-crowdions can be initiated from the crystal surface by its bombardment with nanoparticles [22]. This process will be analyzed in a forthcoming publication.
Figure 4. (a) Propagation of the $M=3$, $N=1$ crowdion launched with $v_0=9$. Shown are the atomic displacements as functions of time, $X_n(t) = x_n(t) - x_n(0)$, for atoms in the middle row of three rows along which the crowdion complex moves. (b) Distance of mass transfer as a function of $M$ for $N=1, 2, 4$, for the initial velocity $v_0=9$. The distance is normalized to the interatomic distance $a$.

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