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Supersonic *N*-Crowdions in 2D Morse Lattice

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Abstract– Interstitial atom embedded into a close-packed atomic row of a crystal is called crowdion. Such defects are highly mobile, they can move along the row in a random walk manner under thermal fluctuations or they can propagate ballistically at a speed higher than speed of sound, transporting mass and energy. In the present work the concept of classical supersonic crowdion is generalized to *N*-crowdion, in which not one but *N* atoms move at a high speed at the same time. Using molecular dynamics simulations for 2D Morse crystal, it is demonstrated that *N*-crowdions are much more efficient in mass transfer propagating through larger distances with smaller total energy than classical 1-crowdion.

1. Introduction

Mass transport by point defects in crystalline solids is responsible for many physical processes occurring during plastic deformation, irradiation, and other high-energy impacts [1-6]. Vacancies control thermally activated diffusion [7]. Self-interstitial atoms have higher formation energy and hence, much smaller concentration in thermal equilibrium, but their role increases in non-equilibrium processes. Self-interstitials can be immobile [8] or mobile, when they are located in close-packed atomic rows, creating so-called crowdions [9].

Note that crowdions can have lower potential energy than immobile interstitials [9]. Crowdions can be at rest or they can move with subsonic or supersonic velocity [10,11]. Standing or subsonic crowdions have a kink profile spanning over a dozen atoms in a close-packed atomic row. Supersonic crowdions are highly localized on one or two atoms [11].

Crowdions play very important role in the relaxation processes that involve mass and energy transport. It has been established experimentally that stress relaxation around corundum balls embedded into KCl single crystal, during cooling from melting point (1049 K) to room temperature, results in the mass transfer, of which not less than 50% is due to the crowdion mechanism [5]. Defects produced by irradiation are mainly clusters of the interstitials and vacancies. It has been shown that clusters of interstitials are highly mobile [12,13]. Moving excitations in crystals are actively studied also in relation to annealing of defects deep inside single crystal germanium under surface plasma treatment [14] and to the tracks of particles observed in mica [15,16]. As possible candidates for the travelling excitations in mica, discrete breathers [17-20] and crowdions [11] were considered.

Direct experimental observation of supersonic crowdions is a challenge so that molecular dynamics simulations are very helpful in their study [11,21]. Using this approach, here we report on novel type of propagating interstitials termed as supersonic *N*-crowdions.

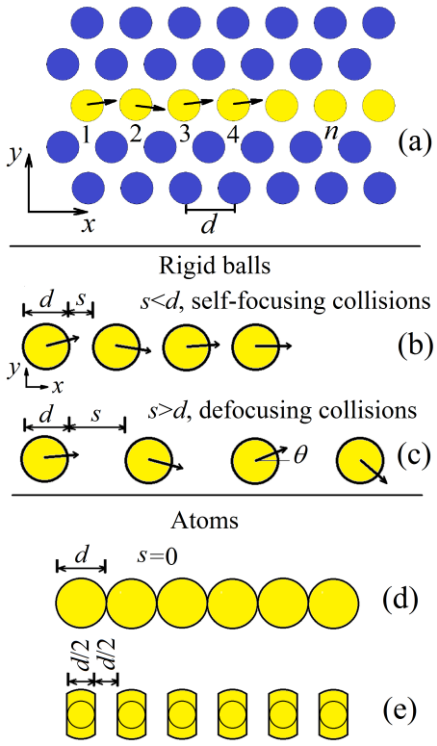

Fig. 1. (a) Atoms of triangular lattice having interatomic distance *d* with *x* axis along close-packed direction. Atoms in one close-packed row (shown in yellow) are numbered with index *n*. Example of initial conditions for initiation of 4-crowdion are shown: atoms from 1 to 4 have initial velocities with components $(V_0, \pm\varepsilon V_0)$ with "+" for odd and "–" for even *n* and ε <<1. Schematics for the condition of self-focusing collisions in the chain of (b,c) rigid balls and (d,e) atoms.

2. Numerical setup

We take triangular lattice with the interatomic distance (atom diameter) d. Cartesian coordinate system is used in the simulations with x axis oriented along close-packed direction, as shown in Fig. 1(a).

The interatomic interactions are described by the Morse pair potential

$$U(r) = D(e^{-2\alpha(r-r_m)} - 2e^{\alpha(r-r_m)}). \quad (1)$$

Here U is the potential energy of two atoms at a distance r apart; α, D, r_m are the parameters. $U(r)$ has minimum at $r = r_m$, D is the depth of the potential well, and α defines the bond rigidity. By a proper choice of units of energy, distance, and time it is possible set D, r_m, and atom mass M to be equal to 1. The cut-off radius is equal to $5r_m$. For $\alpha = 4$ the equilibrium interatomic distance is d=0.9655659 and for $\alpha = 5$ d= 0.9881329.

Dynamical equations are integrated with the help of the Störmer method of order six with the time step $\tau = 10^{-3}$. Temperature is not taken into account, i.e., simulations are carried out for 0 K.

Computational cell contains 800 atoms having dimensions $40d \times 20d\sqrt{3}/2$. Periodic boundary conditions are used. Only supersonic crowdions are studied, which means that any perturbation produced by the crowdion remains in the cone behind it. This allows to use small simulation cell, moving the window containing crowdion back by 10 interatomic distances after it reaches the middle of the computational cell. With this approach, crowdion always moves in unperturbed crystal, and very long propagation distances can be efficiently simulated.

Very simple initial conditions are used to excite N-crowdions [see Fig. 1(a)]. Namely, initial velocity with components $(V_0, \pm\varepsilon V_0)$ is given to the atoms $n = 1, 2, ..., N$ in a close-packed atomic row parallel to x axis. Here y-component of the velocity is introduced with ε <<1 to check the crowdion motion stability. We take sign "+" for odd n and "–" for even n. Initial velocities of all other atoms and initial displacements of all atoms in the computational cell are equal to zero. Thus, total energy of the system is equal to the kinetic energy of the N excited atoms at $t = 0$,

$$T_0 = \frac{NMV_0^2}{2}, \quad (2)$$

where contribution from the lateral component of the initial velocity is neglected. Recall that atom mass $M = 1$ in our model.

Crowdion velocity will be compared to the speed of longitudinal sound, which is found to be equal to

$$v_l = 6.31 \quad \text{for} \quad \alpha = 4, \quad (3)$$

$$v_l = 7.68 \quad \text{for} \quad \alpha = 5. \quad (4)$$

3. Self-focusing condition. N-Crowdions

Propagation of classical, supersonic 1-crowdion can be self-focusing (stable) or defocusing (unstable). Condition of self-focusing dynamics has been rigorously derived for a chain of rigid balls of diameter d and slit s between them, see Fig. 1(b,c) [22], and it reads $s < d$. In (c) angle

$$\theta = \arctan\frac{V_y}{V_x} \quad (5)$$

is introduced. Importantly, for rigid balls the self-focusing condition does not depend on the velocity of ball collisions.

However, atoms are not rigid and their effective diameter depends on the collision velocity. The higher velocity the smaller is the minimal distance between centers of colliding atoms. Atom diameter in equilibrium crystal is defined as interatomic distance [see Fig. 1(d)], that is why we have $s = 0$. Assuming that effective diameter of colliding atoms is equal to the minimal distance between their centers, and referring to the self-focusing condition for the rigid balls, one can formulate the self-focusing condition for atomic collisions as follows: collision velocity should not be greater than that at which minimal distance between atom centers is equal to $d/2$, see Fig. 1(e). Thus, we write the self-focusing condition for collisions in the atomic chain in the form

$$d_{\min} > \frac{d}{2}. \quad (6)$$

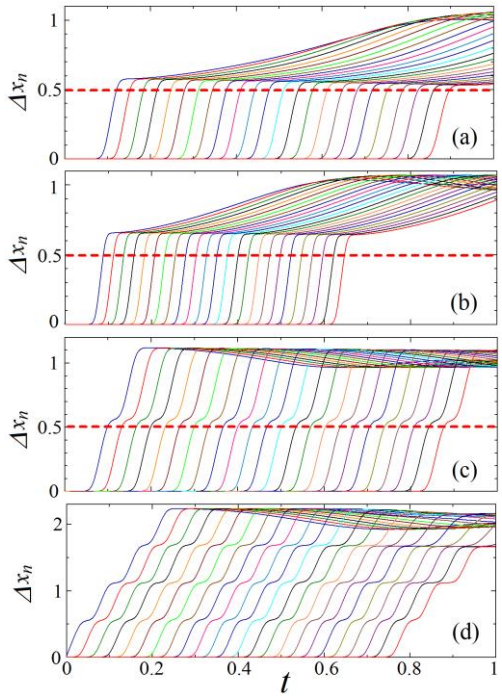

Fig. 2. Dynamics of N-crowdions in a close-packed atomic row of 2D crystal with $\alpha = 4$ shown by plotting $\Delta x_n(t)$ for $n = 1, ..., 24$. (a) N=1, V_0=19; (b) N=1, V_0=28; (c) N=2, V_0=17; (d) N=4, V_0=17. In all cases $\varepsilon = 10^{-6}$.

In Fig. 2 dynamics of *N*-crowdions is shown for $\alpha = 4$ by plotting $\Delta x_n(t)$ for $n = 1,...,24$: (a) *N*=1, V_0=19; (b) *N*=1, V_0=28; (c) *N*=2, V_0=17; (d) *N*=4, V_0=17. In all cases $\varepsilon = 10^{-6}$. In Fig. 3 the same dynamics of *N*-crowdions is shown by plotting $\theta(t)$ for atoms having maximal velocity V_x.

In Fig. 2(a) condition (6) is satisfied so that propagation of 1-crowdion is self-focusing and θ defiend by (5) does not grow with *n*, see Fig. 3(a). In Fig. 2 (b) condition (6) is not satisfied and θ deverges exponentially with *n*, as shown in Fig. 3(b). Even though initial velocity in (b) is greater than in (a), 1-crodion propagated a shorter distance due to the instability. Thus, to achieve a longer crowdion path, it is desirable to increase the energy of initial excitation without increasing initial velocity of the atoms, because at high velocities atomic collisions become defocusing. The solution is to kick not 1 but *N* atoms. In Fig. 2(c) and (d) 2- and 4-crowdions propagate in a self-focusing fassion, see Fig. 3(c) and (d).

Trajectories of atoms in Fig. 2(a-c) bring them to the new equilibrium positions at $\Delta x_n = d$. Trajectories of atoms in Fig. 2(d) bring them close to the new equilibrium positions at $\Delta x_n = 2d$, meaning that the 4-crowdion, unlike 1- and 2-crowdions, carries not one but two interstitial atoms.

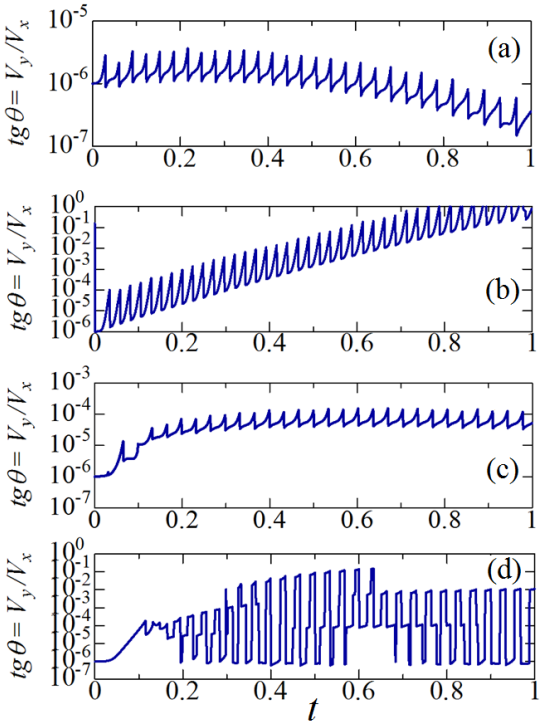

Fig. 3. Dynamics of *N*-crowdions shown by plotting $\theta(t)$ for atoms having largest velocity V_x. Parameters *N*=1 and V_0 in (a-d) are the same as in corresponding plots of Fig. 2. Note that logarithmic scale is used for the ordinate.

In all cases shown in Fig. 2, *N*-crowdions propagate faster than longitudinal sound. For example, 2-crodion in Fig. 2(c) has velocity about 31, which is almost 5 times greater the value given by Eq. (3).

It is important to note that minimal initial velocity to initiate propagation of interstitial atom is $V_0 = 9$ for $N = 1$ and $V_0 = 4$ for $N = 2$ in the crystal with $\alpha = 4$. From Eq. (2) we find that the minimal energy required to initiate mass transfer is $T_0 = 40.5$ for $N = 1$ and $T_0 = 16.0$ for $N = 2$, which is 2.5 times smaller.

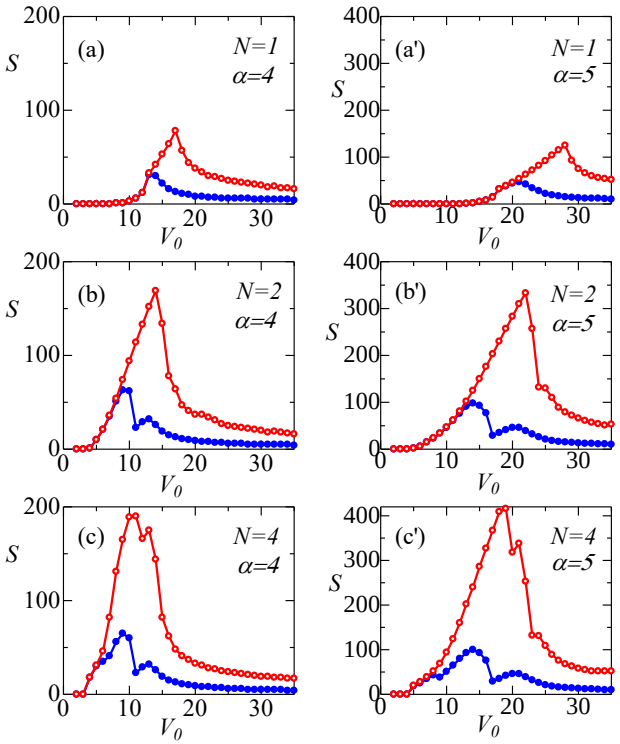

Fig. 4. Distance *S* travelled by the interstitial atom carried by (a,a') 1-crowdion, (b,b') 2-crowdion and (c,c') 4-crowdion as the functions of kicking velocity V_0 for ε=10^{-2} (filled dots) and ε=10^{-12} (open dots). In (a-c) $\alpha = 4$ and in (a'-c') $\alpha = 5$.

Let *S* be the distance travelled by the interstitial carried by a crowdion. In Fig. 4, *S* is shown as the function of V_0 for ε=10^{-2} (filled dots) and ε=10^{-12} (open dots) for (a-c) $\alpha = 4$ and (a'-c') $\alpha = 5$. In (a,a') $N = 1$, (b,b') $N = 2$, and (c,c') $N = 4$. As expected, *S* is larger for smaller perturbation parameter ε. Remarkably, 2- and 4-crowdions are able to travel through considerably larger distance than 1-crowdion and their motion can be initialized with sufficiently smaller values of the kicking velocity V_0 and smaller total energy, as it has already been mentioned.

S increases with increasing α [compare the panels at left and right in Fig. 4], which is understandable, because for larger α the interatomic potential is stiffer, minimal

distance between atoms colliding with given velocity is larger, and stability condition Eq. (6) is satisfied for larger collision velocity.

4. Conclusions

A family of new nonlinear excitations called as supersonic *N*-crowdions has been analysed with the help of molecular dynamics simulations for 2D Morse crystal. In contrast to classical supersonic 1-crowdion, not 1 but *N* atoms move at a high speed at the same time in *N*-crowdion. *N*-crowdions can travel longer distances and for their initiation smaller total energy is required than for 1-crowdion. As for the possible mechanisms of excitation, *N*-crowdions can be naturally formed in the bulk of crystals under irradiation. They can also be excited at crystal surface if it is bombarded not by a single atom ion but by ionized molecules, producing not one but a series of kicks.

It is important to continue this work by the study of properties of *N*-crowdions in metals and other real crystals. For instance, of particular importance is to consider the nuclear reactor materials. It would be also interesting to make a comparative study of *N*-crowdions in fcc Cu and Al, as two these metals have very different stacking fault energy and thus they demonstrate different mechanisms of plastic deformation.

Acknowledgments

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