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Breathing subsonic crowdion in Morse lattices

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ABSTRACT

Based on molecular dynamics simulations, we discuss dynamics of nonlinear localized excitations in two-dimensional crystal with Morse interatomic interactions and without on-site potential. It is shown that supersonic solitons (SupS) or supersonic crowdions (SupC) can be excited by kicking one atom with initial velocity along a close-packed atomic row. The difference between SupS and SupC is that the former is excited with the kicking velocity insufficient for Frenkel pair (vacancy and interstitial atom) creation, while the latter one is formed with initial momentum sufficient for creation of two such defects and while propagating, SupC carries a mass of one atom. It is shown that, in a range of kicking velocity, SupC soon after its formation transforms into a pair of excitations, one is SupS and another one is subsonic crowdion bearing internal vibrational mode. The latter one is called here breathing subsonic crowdion (BSubC). BSubC is localized in the close-packed atomic row on a dozen of atoms that vibrate out-of-phase with the nearest neighbors along the row, and it carries one atom. To the best of our knowledge such excitation has not been reported before. We offer a physically motivated ansatz to set initial conditions for excitation of BSubC in molecular dynamics simulations. With this ansatz BSubC was successfully excited also in three-dimensional fcc Morse lattice. Our results contribute to a deeper understanding of nonlinear excitations in crystals.

1. Introduction

Point defects play a very important role in processes of energy dissipation in crystals subjected to plastic deformation, irradiation, plasma treatment, etc. [1–16]. Their basic properties can be studied in frame of simplified crystal models.

Localized modes in one-dimensional (1D) lattices (chains) of particles bound by nonlinear potential forces have been well studied. In chains without an on-site potential, solitons (kinks) propagating at supersonic speed can be excited [17–20]. Chains with a strong on-site potential support immobile or mobile discrete breathers (DB) also called intrinsic localized modes [21–26]. It has been also shown that in a chain with nonlinear on-site potential and nonlinear coupling potential (both Morse), a supersonic soliton (SupS) is first transformed into a mobile DB and then into an immobile DB when relative strength of the on-site potential increases from zero value [27]. DB can exist in monoatomic chains without on-site potential [28–30], but nonlinear coupling should be of hard-type anharmonicity, while realistic interatomic potentials with soft tails, e.g., Lennard-Jones and Morse, do not support DB in 1D case [31]. On the other hand, 2D and 3D monoatomic crystals with Morse potential and without on-site potential do support DB [32–34]. In Ref. [35] a 2D close-packed lattice with on-site potential was offered and it has been shown that the lattice supports highly localized moving breathers [36–39]. In a close-packed atomic row of a triangular lattice (without on-site potential), mobile and immobile DB can be excited (sometimes also called quodons) [40,41]. DB possess the property of solitary waves, they interact with each other almost elastically, preserving their identities [42].

2D densely packed Morse lattice without on-site potential

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supports localized quasi-1D modes propagating in a close-packed row of atoms. They are excited by an initial kick of single atom along the row. If kicking velocity is below a threshold value, SupS is excited, which has almost the same profile as kink in a 1D chain, in spite of the fact that the particles of the row interact with particles in adjacent rows [43–45]. SupS constantly radiates its energy and eventually disappears without creating a lattice defect. The mean free path of SupS is up to many tenths of interatomic distances [48]. For a larger initial kicking velocity, the Frenkel pair is formed with the interstitial atom moving away from the vacancy as a supersonic crowdion (SupC) [46,47]. SupC is highly localized on one-two atoms. Propagation of SupC can be self-focusing or defocusing and this largely defines its mean free path [46,49]. SupC constantly radiates energy and transforms into a subsonic crowdion (SubC), which is localized on a dozen of atoms. Further radiation reduces its velocity and eventually it stops. Note that standing crowdion is unstable in 2D Morse lattice and the extra atom leaves the close-packed atomic row and becomes an immobile interstitial atom. However, in 3D Morse lattice standing crowdion is stable.

From the literature analysis it can be concluded that DB, SupS, SupC, and SubC are the known localized nonlinear excitations in 2D and 3D lattices. In this study we report on numerical experiments which, quite surprisingly, have produced excitations in the form of subsonic crowdion bearing internal vibrational mode. It is termed as breathing subsonic crowdion (BSubC).

2. Numerical setup

Cartesian coordinate system is used in the simulations. We consider 2D close-packed lattice generated by the translation vectors $(a,0)$, $(a/2, a\sqrt{3}/2)$, where a is the interatomic distance. We also study 3D fcc crystal with translational cell generated by the vectors $(2a,0,0)$, $(0,2a,0)$, and $(0,0,a\sqrt{2})$. The cell contains 8 atoms in the positions $(0,0,0)$, $(a,0,0)$, $(0,a,0)$, $(a,a,0)$, $(a/2, a/2, a/\sqrt{2})$, $(3a/2, a/2, a/\sqrt{2})$, $(a/2, 3a/2, a/\sqrt{2})$, and $(3a/2, 3a/2, a/\sqrt{2})$. Note that with this choice, in 2D and 3D cases, the x axis is along a close-packed direction.

The interatomic interactions for both 2D and 3D crystals are described by the Morse pair potential, determined as [50].

$$U(r) = D\left(e^{-2\alpha(r-r_m)} - 2e^{\alpha(r-r_m)}\right) \tag{1}$$

Here U is the potential energy of two atoms placed at a distance r and 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 rigidity of the bond. 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. Let $\alpha = 4/r_m$ and we set the cut-off radius to be equal to $5r_m$. Then the equilibrium interatomic distance is $a^{2D} = 0.9315$ and $a^{3D} = 0.9014$ for 2D and 3D crystals, respectively. Note that due to the long-range interactions $a < r_m$.

Equations of atomic motion are integrated with the use of the Stormer method of order six with the time step $\tau = 10^{-3}$.

Computational cell in 2D case includes 200×200 primitive translational cells and thus, it contains 4×10^4 atoms. In 3D case a block of $40 \times 10 \times 10$ translational cells is considered, which includes 3.2×10^4 atoms.

Periodic boundary conditions are used in 2D and 3D cases.

Phonon density of states (DOS) is calculated by solving the eigenvalue problem for the equations of atomic motion linearized in the vicinity of equilibrium positions. The first Brillouin zone is scanned with the step 0.01π in all reciprocal directions.

Very simple initial conditions are used to excite SupS and SupC. Namely, initial velocity v_0 is given to one atom along the close-packed atomic row parallel to x axis. 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 excited atom at $t = 0$,

$$T_0 = \frac{Mv_0^2}{2}. \tag{2}$$

Recall that atom mass $M = 1$ in our model.

Such trivial initial conditions in a particular range of T_0 have produced BSubC, as it will be shown later for 2D crystal. After careful examination of this numerically found nonlinear mode, the following ansatz was offered for its excitation in a close-packed atomic row parallel to x axis both in 2D and 3D crystals

$$x_n(t) = \frac{a}{2}\{1 - \tanh[\beta(n - x_0 - Vt)]\} + \frac{(-1)^n A\cos(2\pi\omega t)}{\cosh[\gamma(n - x_0)]}, \tag{3}$$

$$y_n(0) = 0, \quad \dot{y}_n(0) = 0. \tag{4}$$

Here n numbers atoms in the considered close-packed row. The first term in the right-hand side of Eq. (3) produces the soliton (kink) of inverse width β and V defines its velocity. The second term sets the soliton's internal vibrational mode of amplitude A, inverse width γ, and frequency ω, which is above the phonon band of the lattice. Initial position of the BSubC is x_0. All other atoms in the computational cell have zero initial displacements and velocities. It should be pointed out that the initial conditions Eq. (3) and (4) do not correspond to an exact solution. Subsonic velocity V, vibrational mode amplitude A, and initial position x_0 are free parameters, while β, γ, and ω were defined by the try and error method [33] in order to achieve a long-lived excitation with less radiation of energy.

3. Simulation results

3.1. Phonon DOS and sound velocities

Phonon DOS is presented in Fig. 1 by thin (thick) line for 2D (3D) crystal. For further discussion it is important to note that maximal phonon frequency is $\omega_{\max}^{2D} = 2.66$ and $\omega_{\max}^{3D} = 4.23$ for 2D and 3D cases, respectively. From dispersion curves it is also possible to calculate the velocity of sound as $\mathrm{d}\omega/\mathrm{d}q$ in the limit $q \to 0$, where q is the wave vector. In 2D crystal the longitudinal sound waves

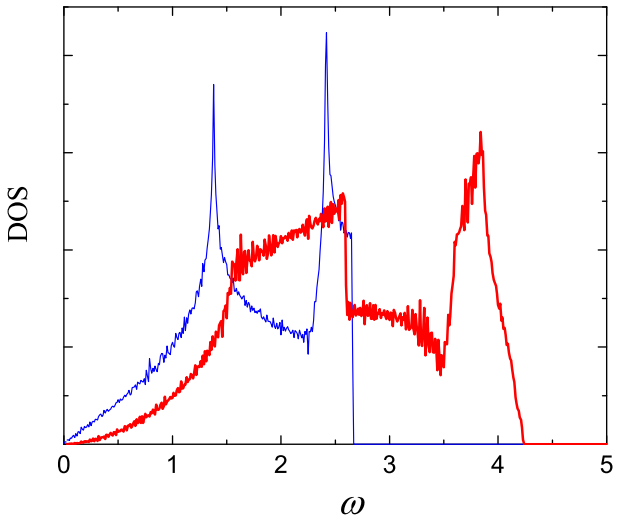

Fig. 1. Density of phonon states for the considered 2D (thin blue line) and 3D (thick red line) Morse crystals. Maximal phonon frequency is $\omega_{\max}^{2D} = 2.66$ for 2D and $\omega_{\max}^{3D} = 4.23$ for 3D case. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

propagate with the velocity

$$v_l^{2D} = 6.31. \quad (5)$$

Unlike 2D crystal, 3D one is elastically anisotropic and the velocity of sound depends on the crystallographic direction. Since propagation of nonlinear excitations along close-packed atomic row is studied here, the speed of longitudinal sound is calculated along this direction, and it is found to be equal to

$$v_l^{3D} = 8.29. \quad (6)$$

3.2. Evolution of the trivial initial excitation in 2D case

Let us present dynamics of atoms in the close-packed atomic row $m = 100$ of the 2D crystal when only one atom is kicked along the row with velocity v_0 and kinetic energy T_0 given by Eq. (2). It was found that for $T_0 < 40$ ($v_0 < 9$) a SupS is formed. In Fig. 2, propagation of SupS initialized by kicking the atom $n = 90$ with $T_0 = 32$ is shown by plotting atomic displacements as the functions of time, $X_n(t) = x_n(t) - x_n(0)$, (upper panel) and atomic coordinates as the functions of time, $x_n(t)$, (lower panel). It can be seen that the atoms do not overcome the potential barrier at $X_n = 0.5a$ and return to their equilibrium positions giving momentum to the neighbors. SupS constantly radiates its energy in the form of small-amplitude waves. Its initial velocity is about 16, which is nearly $2.5v_l^{2D}$. It propagates 22 interatomic distances and disappears without formation of any crystal lattice defect.

For $T_0 > 72$ ($v_0 > 12$) a vacancy and a SupC is formed. We do not present here dynamics of SupC because it has been studied (see Refs. [46,49] and references therein).

The most interesting results are obtained for the initial kinetic energy of the excited particle in the range $40 < T_0 < 72$. For example, for $T_0 = 45$ the results are shown in Figs. 3 and 4 in different time scales. In Fig. 3, upper panel, one can see that the first three particles overcome the potential barrier at $X_n = 0.5a$ but then they return to their equilibrium positions. The following particles in the row overcome the potential barrier and occupy the positions of the $n + 1$ particle creating a vacancy at the site $n = 93$. Propagation of SupS can be seen with the initial velocity of 17.5, which is about $2.8v_l$. However, SupS does not carry an atom, but since vacancy is formed, the question is where is an extra atom? This can be seen in Fig. 4, which shows the same dynamics for a longer time. Apart from the SupS, one more excitation can be clearly seen (two straight lines are added as the guides for the eye in the lower panel). Its propagation velocity is estimated as 1.6, which is subsonic ($0.25v_l^{2D}$), and its width is about 8–10 atoms. This slowly propagating excitation is a subsonic crowdion, it carries one atom which becomes an immobile interstitial at $n = 124$ after the crowdion stops. On the other hand, as it can be seen from the upper panel, trajectories of particles show oscillations. Frequency of the oscillations can be estimated as 2.8, which is above the phonon band (see Fig. 1). Naturally this excitation can be called BSubC.

3.3. Breathing subsonic crowdion in 2D case

From the analysis of atomic motion in the core of BSubC excited as described in Sec. 3.2, the ansatz Eq. (3) was offered for setting initial conditions. Here we apply the ansatz placing the kink at initial position $x_0 = 80$, taking for the parameter $V = 1.0$, 2.0, and 3.0, and setting the amplitude of the vibrational mode $A = 0.025$. By try and error method we found that the dynamics of BSubC is stable for the inverse width of $\beta = \gamma = 0.3$ and frequency $\omega = 3.0$, which is above the phonon spectrum (see. Fig. 1). With such parameters we observe dynamics of atoms in the close-packed atomic row till $t = 25$. In Fig. 5, the initial profile of BSubC is shown by open squares and its profile at $t = 25$ is plotted by circles, triangles up, and triangles down for $V = 1$, 2, and 3, respectively. This excitation moves

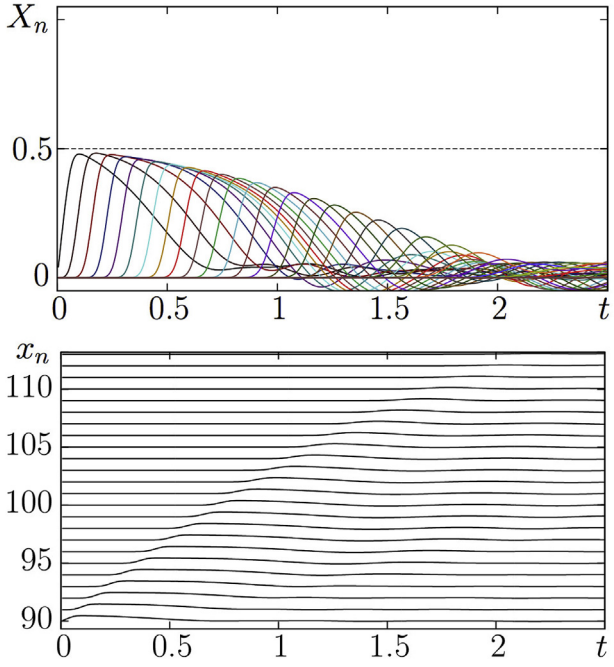

Fig. 2. Propagation of SupS initiated by kicking the particle $(n,m) = (90,100)$ with initial kinetic energy $T_0 = 32$ along the atomic row. Initial propagation velocity is about 16 (nearly $2.5v_l$). Upper panel: displacements as the functions of time, $X_n(t) = x_n(t) - x_n(0)$, for the atoms with $n = 90$, 91, 92... in the close-packed atomic row with $m = 100$. Bottom panel: coordinates of the corresponding atoms as the functions of time, $x_n(t)$.

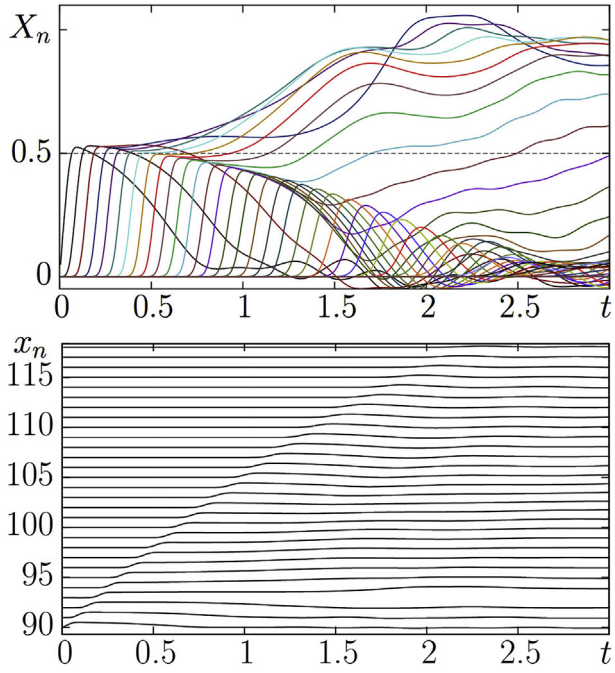

Fig. 3. Same as in Fig. 2, but for $T_0 = 45$. Propagation of SupS at speed of 17.5 (about $2.8v_l$) and formation of a vacancy at $n = 93$ can be seen.

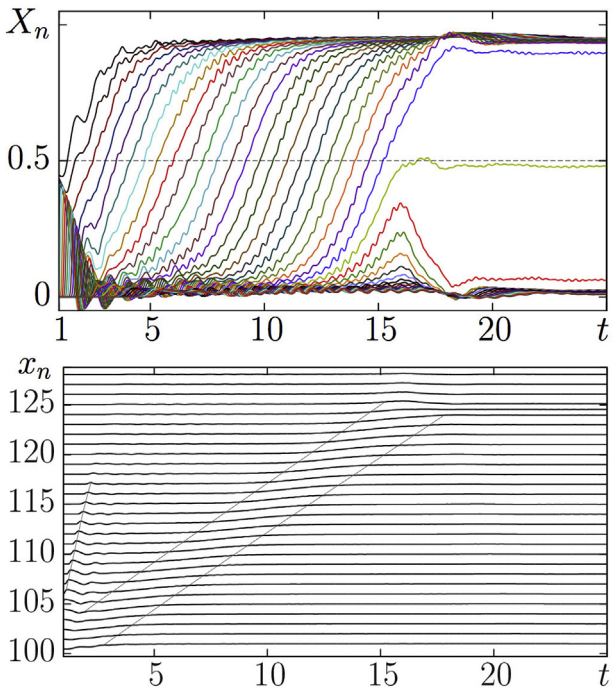

Fig. 4. Same as in Fig. 3, but for longer time. BSubC moves, as highlighted by two straight lines, and eventually transforms into immobile interstitial at $n = 124$.

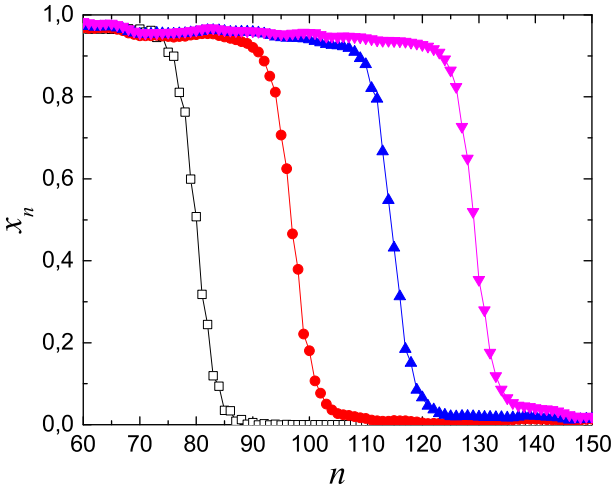

Fig. 5. Results for 2D Morse lattice. Initial profile of BSubC (open squares) and profiles at $t = 25$ for BSubC excited with $V = 1$, 2, and 3 (circles, triangles up, and triangles down, respectively). Other parameters of the ansatz Eq. (3) are: kink initial position $x_0 = 80$, inverse width $\beta = \gamma = 0.3$, amplitude of the vibrational mode $A = 0.025$, and frequency $\omega = 3.0$.

along the close-packed atomic row with velocity 0.64, 1.36, and 2.00 for $V = 1$, 2, and 3, respectively. Propagation velocity is about 1.5 times smaller than V because initial momentum is given only to the atoms in the close-packed atomic row, and a part of it is spent to excite the atoms in the neighboring rows. Atoms in the core of BSubC oscillate out-of-phase with the nearest neighbors along the close-packed atomic row with frequency about 3.8 (higher than the set value of 3.0). This can be seen in Fig. 6, where x-displacements of the particles in the close-packed atomic row are shown as the functions of time.

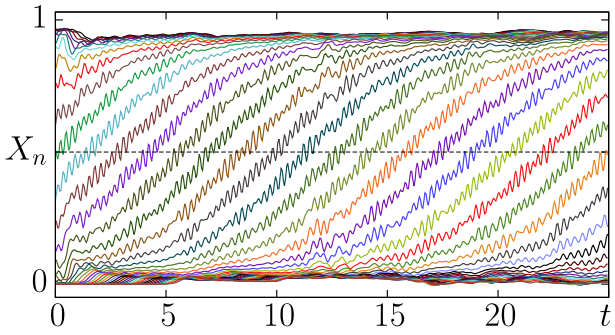

Fig. 6. Results for 2D Morse lattice. Displacements as the functions of time, $X_n(t) = x_n(t) - x_n(0)$, for the atoms in the close-packed atomic row where BSubC is excited using ansatz Eq. (3) with $V = 1$, $x_0 = 80$, $\beta = \gamma = 0.3$, $A = 0.025$, and $\omega = 3.0$.

3.4. Breathing subsonic crowdion in 3D case

The ansatz Eq. (3) can be used to excite BSubC in close-packed atomic rows of 3D crystals and here we demonstrate this for fcc Morse crystal. Parameters of the ansatz are taken as follows: kink initial position $x_0 = 15$, inverse width $\beta = \gamma = 0.33$, amplitude of the vibrational mode $A = 0.025$, and its frequency $\omega = 4.5$, which is above the phonon band of the 3D crystal, see Fig. 1. For V three values are considered, 1, 2, and 3.

In Fig. 7 we plot the profile of BSubC at $t = 0$ as set by the ansatz (open squares) and profiles at $t = 25$ for $V = 1$, 2, and 3 by circles, triangles up, and triangles down, respectively. It can be estimated that BSubC moves along the close-packed atomic row with velocity 0.56, 1.24, and 1.83 for $V = 1$, 2, and 3, respectively. The propagation velocity is 1.6–1.8 times smaller than the set value of V. Note that in comparison to 2D case the reduction of the velocity with respect to the set value is larger, which can be explained by a larger number of atoms surrounding the close-packed atomic row where BSubC moves. Momentum of the initial excitation given to only one row is now sheared by a larger number of neighboring rows than in 2D case.

Comparison of Fig. 5 with Fig. 7 reveals that in 3D case BSubC is localized somewhat stronger. Again, this is because in 3D crystal

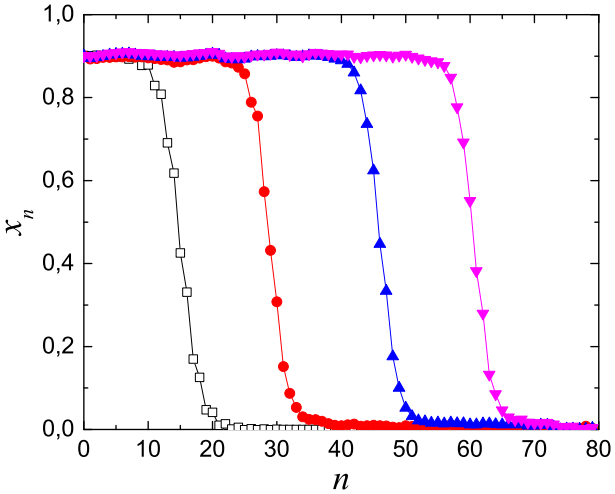

Fig. 7. Same as in Fig. 5, but for 3D Morse lattice. Open squares show initial profile of BSubC. Circles, triangles up, and triangles down show profiles at $t = 25$ for BSubC excited with $V = 1$, 2, and 3, respectively. Other parameters of the ansatz Eq. (3) are: kink initial position $x_0 = 15$, inverse width $\beta = \gamma = 0.33$, amplitude of the vibrational mode $A = 0.025$, and frequency $\omega = 4.5$.

the atomic row where BSubC propagates, is surrounded by a larger number of atoms than in 2D case, and they create a deeper on-site potential. When strength of the on-site potential increases relative to the coupling energy between atoms in the row, the degree of spatial localization of kinks increases [51].

In Fig. 8 displacements of atoms as the functions of time are plotted for the atoms in the atomic row hosting BSubC. One can estimate the frequency of the vibrational mode localized on BSubC to be equal to 5.7 (higher than the set value of 4.5). This frequency is above the phonon spectrum of the considered fcc crystal, $\omega_{\max}^{3D} = 4.23$, (see Fig. 1).

4. Conclusions

By using molecular dynamics, is was shown that a very simple initial excitation of 2D Morse lattice, in the form of one atom kicked along a close-packed atomic row with supersonic velocity, can produce a crowdion localized on a dozen of atoms, moving with a subsonic speed, and bearing large-amplitude vibrational mode. This counterintuitive transformation of a highly localized initial excitation into a long-lived propagating excitation with much smaller degree of spatial localization uncovers a new mechanism of energy and mass transport in crystal lattice. The subsonic crowdion bearing internal vibrational mode is termed here breathing subsonic crowdion (BSubC).

Analysis of atomic motion in the core of BSubC lead us to formulation of the ansatz Eq. (3) for setting initial conditions producing BSubC in molecular dynamics simulations. This ansatz was successfully applied to excitation of BSubC in 2D and 3D Morse lattices.

It is shown that BSubC in 3D lattice has somewhat higher degree of spatial localization than in 2D case. While propagating, BSubC constantly radiates its energy in the form of small-amplitude waves. As a result, its velocity slowly decreases and eventually it stops being trapped by the periodic on-site potential (see Fig. 4). In 2D crystal moving crowdion is stable, while standing crowdion is unstable and the extra atom leaves the close-packed atomic row being transformed into an immobile interstitial. In 3D case standing crowdion is stable and it preserves its kink-like profile after BSubC stops.

In 2D and 3D cases vibrational frequency of BSubC is above the phonon spectrum, that is why, it does not resonate with phonons and does not lose its energy for their excitation.

The fact that lattice defects can support localized vibrational modes is not new, but here it was shown that they can naturally emerge as a result of evolution of trivial excitations produced, e.g., by plasma treatment from the surface or by irradiation in the bulk.

The ansatz Eq. (3), offered in this study, can be applied to excitation of BSubC in close-packed atomic rows of various crystals including fcc, bcc, and hcp metals. Comparative analysis of BSubC properties in such metals is in progress and will be reported elsewhere. Our results can be of particular interest for the community studying the properties of irradiated crystals [52].

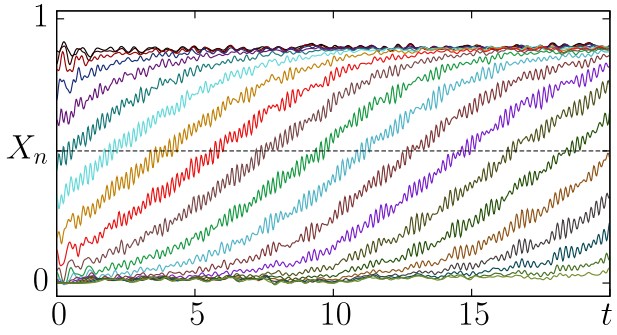

Fig. 8. Same as in Fig. 6, but for 3D Morse lattice. Displacements as the functions of time, $X_n(t) = x_n(t) - x_n(0)$, for the atoms in the close-packed atomic row where BSubC is excited using ansatz Eq. (3) with $V = 1$, $x_0 = 15$, $\beta = \gamma = 0.33$, $A = 0.025$, and $\omega = 4.5$.

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