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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 $d\omega/dq$ in the limit $q \to 0$, where q is the wave vector. In 2D crystal the longitudinal sound waves

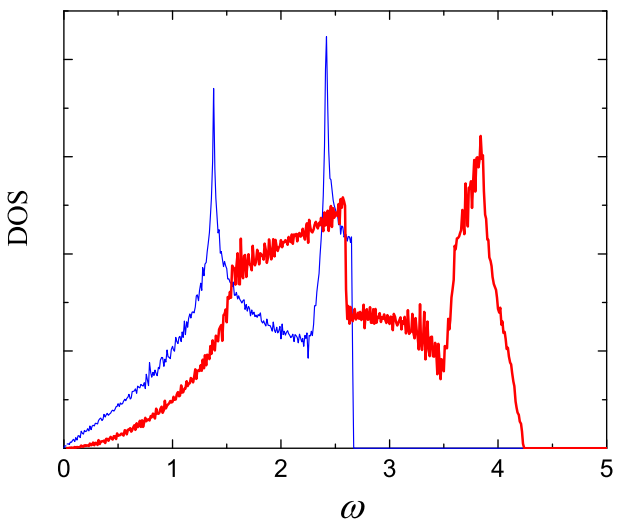

Fig. 1. Density of phonon states for the considered 2D (thin blue line) and 3D (thick red line) Morse crystals. Maximal phonon frequency is $\omega_{\max}^{2D} = 2.66$ for 2D and $\omega_{\max}^{3D} = 4.23$ for 3D case. (For interpretation of the references to colour in this figure legend, the reader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

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