Properties of discrete breathers in 2D and 3D Morse crystals

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Based on the results of molecular dynamics simulations the characteristics of discrete breathers (DB) in two-dimensional (2D) and three-dimensional (3D) crystals with Morse long-range interatomic interactions are compared. It is demonstrated that DB in 3D crystal have higher frequencies and higher degree of localization than in 2D crystal.

Keywords: two-dimensional crystal, three-dimensional crystal, Morse potential, discrete breather.

Introduction

Recently, in many areas of modern physics, there has been growing interest in the study of nonlinear, spatially localized vibrational modes in defect-free lattices in the form of discrete breathers (DB) [1—3]. Existence of DB is provided by the anharmonicity of interatomic forces leading to the amplitude dependence of the oscillation frequency of atoms. DB have the oscillation frequencies outside the phonon spectrum of crystals. For this reason DB do not resonate with phonons and hence, they do not excite them and have very long lifetime [4,5].

DB can demonstrate soft or hard nonlinearity. In the former (later) case DB frequency decreases (increases) with increasing amplitude. Decrease of the soft nonlinearity DB frequency with growing amplitude can result in entering the phonon spectrum gap, if it exists. For the hard type nonlinearity DB the frequency growing with increasing amplitude can cross the upper edge of the phonon spectrum. A concept of quasibreather having finite lifetime and not satisfying the exact time-periodicity condition, introduced by Chechin *et al.* [6] is very important for variety of physical applications.

Not a few theoretical studies involve the concept of DB for explanation of a series of physical effects. Thus, the concept of the polaron has been generalized to the concept of solectron, which is the electron-DB coupled state [7,8]. Considerable energy (about 1 eV [9,10]) localized by DB can cause defect formation in carbon nanotubes [11] or facilitate the detachment of dislocations from stoppers, explaining the effect of electro-plastic deformation of metals [12—14]. DB have been successfully modeled by means of molecular dynamics simulations in the NaI crystal [15], in Si and Ge [16], in the NaCl structure crystal [9,17—19], in carbon nanotubes [11], in elastically deformed graphene [20,21] and graphene nanoribbons [22], as well as in graphane [23,24].

In the theoretical work by Kiselev et al. [25] it has been shown that the 1D chains with atoms interacting via classical pairwise potentials (Toda, Born-Mayer, Lennard-Jones and Morse) cannot support DB with frequency above the phonon spectrum. It can be demonstrated that introduction of the on-site potential in that model makes the existence of DB with frequency above the phonon spectrum possible by suppressing the dc displacements of the atoms and increasing the contribution of the hard core of the potential into atomic dynamics.

Until recently it was believed that in real crystals interatomic interactions tend to exhibit a soft type of nonlinearity, and DB can only exist within a gap in the phonon spectrum of the crystal [26]. However, in [27] a possibility of existence of DB with hard type nonlinearity and with frequencies above the phonon spectrum was demonstrated by means of molecular dynamics modeling for Ni and Nb. Later the possibility of the existence of DB with frequencies above the phonon spectrum was confirmed for the case of two-dimensional (2D) monoatomic crystal with Morse interatomic potentials [28—31]. Note that the Morse potential has been successfully used in many studies on DB in ordered alloys [32—42].

In this work the possibility of existence of DB with frequency above the phonon spectrum in 2D and 3D crystals with long-range Morse interactions is analyzed.

Simulation details

We consider the 2D close-packed and the 3D FCC monoatomic crystals. Without loss of generality, the mass of atoms is considered to be unity. The interaction between atoms is described by the pairwise Morse potential:

$$V(r) = D(e^{-2\alpha(r-r_m)} - 2e^{-\alpha(r-r_m)}), \qquad (1)$$

where r - is the distance between two atoms and D, α, r_m are potential parameters. The function $V(r)$ has a minimum at $r=r_m$, the minimum depth (bond energy) is D, and the parameter α determines the bond stiffness. Without the loss in generality one can set $r_m=1$ and $D=1$, selecting the

appropriate units of distance and energy. For the parameter α determining the rigidity of the interatomic bond the value α=5 was considered for both 2D and 3D crystals. Thermal vibrations of atoms are not introduced so that the properties of DB are investigated here at 0 K.

For the selected *cut*-off radius of 7.5 Å, the equilibrium interatomic distance is 0.988 Å for the 2D crystal and 0.961Å for the 3D case.

The Morse potential (1) has an inflection point and to the left of the inflection point the potential is had, while to the right of the point it is soft. Since the interatomic distance in the 3D crystal is smaller than in 2D crystal, one can expect that the 3D crystal will demonstrate a larger stiffness.

The computational cell with periodic boundary conditions contained 160×160 atoms for the 2D crystal and 32×32×16 atoms for the 3D case.

Excitation of discrete breathers

Atoms of one of the close packed rows of 2D or 3D crystal were numbered by the index n as is shown in Fig. 1a and b respectively. The initial conditions for the standing discrete breather were taken as follows [28]:

$$x_n^0 = T_n + S_n, \; \dot{x}_n^0 = 0, \; y_n^0 = 0, \; \dot{y}_n^0 = 0 \qquad (2)$$

where y_n^0, x_n^0 and $\dot{x}_n^0$, $\dot{y}_n^0$ - are the components of initial displacement vectors and initial velocities of atoms in the considered row. All other atoms had zero initial displacements and zero initial velocities. Functions T_n and S_n in (1) describe the amplitudes and the displacements of the centers of vibrations of atoms, respectively. In other words, $T_n=(x_{n,max}-x_{n,min})/2$, $S_n=(x_{n,max}+x_{n,min})/2$ where $x_{n,max}$ and $x_{n,min}$ -
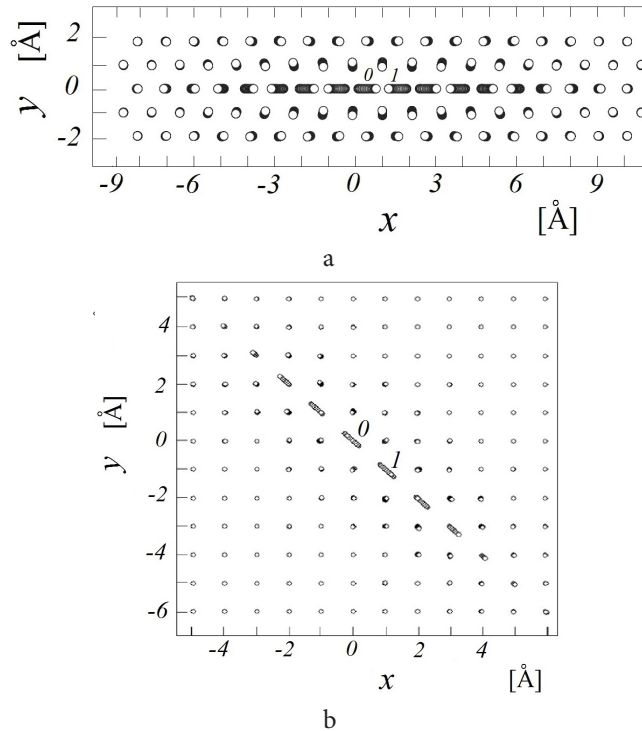

a

b

Fig. 1. Stroboscopic picture of atomic motion showing the DB excited in a close-packed atomic row in (a) 2D and (b) 3D crystal. The atomic displacements are increased by a factor of 4 for clarity.
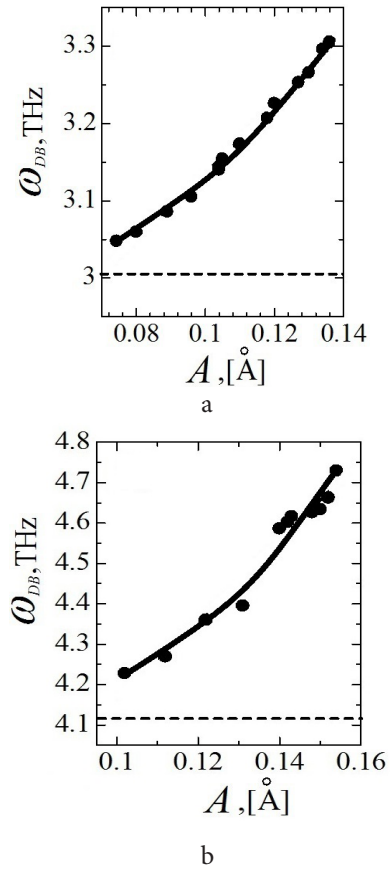

a

b

Fig. 2. DB frequency as the function of DB amplitudefor (a) 2D and (b) 3D monoatomic crystals with long-range Morse interactions. The horizontal dashed lines mark the upper edge of the phonon spectrum for each case.

are maximal and minimal values of (quasi) periodic function xn(t), describing the vibrational motion of the *n*-th atom. The functions are

$$T_n = \frac{(-1)^n A}{\cosh\left[\beta(n-x_0)\right]} \qquad (3)$$
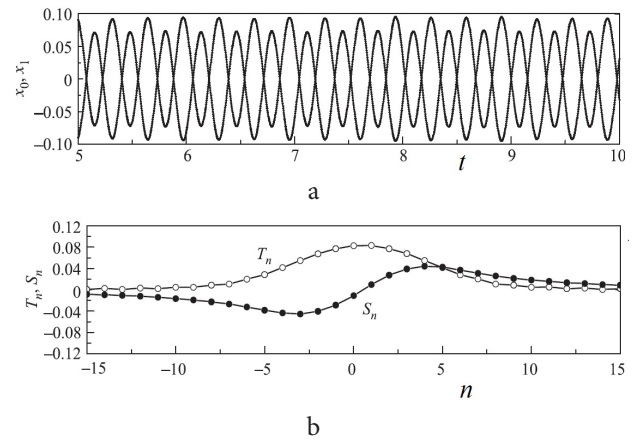

a

b

Fig. 3. Example of stationary DB excited with the help of the ansatz (2), (3) and (4) in a close-packed row of the 2D crystal. Ansatz parameters are indicated in the text. (a) Time dependence of the atomic displacements for the central DB atoms marked as 0 and 1 in Fig.1a. (b) Amplitudes, T_n, and displacements of the atom vibration centers, Sn, in the close-packed row where the DB is excited.
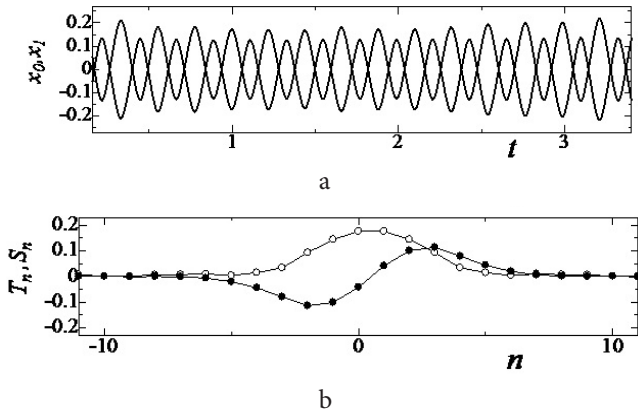
a

b

Fig. 4. Same as in Fig. 3, but for the 3D crystal.

$$S_n = \frac{-B(n - x_0)}{\cosh\left[\gamma(n - x_0)\right]} \qquad (4)$$

where A is the DB amplitude, B is the amplitude of displacements of the center of vibration of atoms, the parameters β and γ specify the degree of spatial localization of DB, and x_0 is its initial position. At $x_0=0$ and 1/2, the discrete breather is centered on the atom and in the middle between two neighboring atoms, respectively.

Simulation results

In Fig.2 the DB frequency as the function of DB amplitude is shown for (a) 2D and (b) 3D crystals. The horizontal dashed lines mark the upper edge of the phonon spectrum.
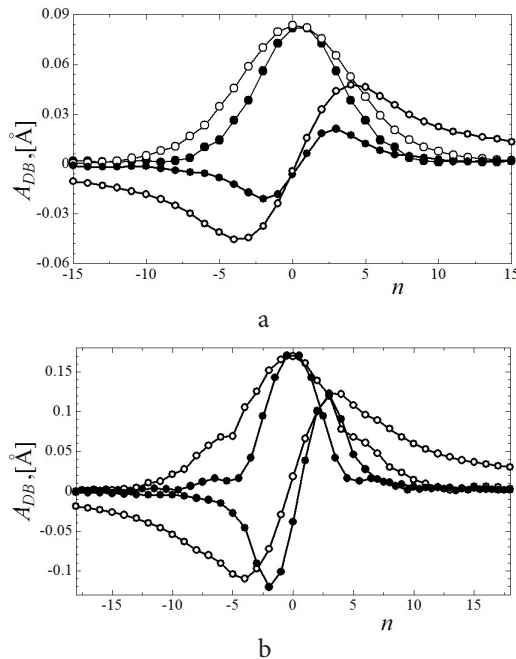

a

b

Fig. 5. Comparison of DB in 2D and 3D crystals excited with different ansatz parameters. The initial conditions of the DB excitation parameters for cases (a) and (b) are presented in the text. The open circles show the displacement of DB atoms in the 2D crystal, black circles stand for those in 3D case.

In both cases the DB frequency increases with the increase in its amplitude revealing the hard type of nonlinearity of the DB. Note that the DB in 3D crystal have higher frequencies which is due to the smaller interatomic distance in this case and hence, larger contribution of the hard core of the Morse potential into the DB dynamics.

In Fig.3 an example of stationary DB excited with the help of the ansatz (2), (3) and (4) in the 2D crystal is presented. The following parameters of the anzats were used: A=0.0945Å, B=0.011Å, β=γ=0.22, x_0=1/2. Fig.3a presents the time evolution of displacements $x_0(t)$ and $x_1(t)$ of the two central DB atoms marked as 0 and 1 in Fig.1a. The functions T_n and S_n, shown in Fig.3b, indicate the amplitudes and atomic shifts from the lattice positions for the atoms in the close-packed atomic row where the DB is excited.

Figure 4 presents the same as Fig.3, but for the 3D crystal. Parameters of the ansatz (2), (3) and (4) are as follows A=0.21, B=0.07, β=γ=0.6, x_0=1/2. It should be noted that the amplitude of atomic vibrations in the example shown for the 3D crystal are almost twice higher than those for the DB in 2D crystal.

DB excited with different initial conditions in 2D and 3D cases are shown in Fig.5. Ansatz parameters (2), (3) and (4) used for DB excitation were A=0.24, B=0.014, β=γ=0.22, x_0=1/2 - for 2D crystal, A=0.19, B=0.04, β=γ=0.65, x_0=1/2 for 3D for the case demonstrated in Fig.5a. Figure 5b present a case of A=0.4, B=0.016, β=γ=0.22, x_0=1/2 for 2D crystal; A=0.23, B=0.07, β=γ=0.65, x_0=1/2 for 3D crystal.

Atoms in 2D crystal are shown by open circles, in 3D by filled circles. Let us note that the degree of localization of the DB in 3D crystal is higher than in 2D case. Different parameters of the ansatz do not show any considerable effect on the degree of DB localization.

Conclusions

Stationary DB in 2D and 3D monoatomic crystals with long-range Morse interaction potential are investigated by means of molecular dynamics simulation.

Amplitude — frequency dependence of analyzed DB revealed a hard type of nonlinearity for both crystals. It was shown that localization degree in 3D crystal is higher than that in 2D one. This can be explained by the smaller lattice parameter of the 3D crystal that results in a higher stiffness of the 3D crystal.

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