Properties of one-dimensional nonlinear vibrational modes in triangular lattice with Lennard-Jones interactions

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Abstract. Crystal lattices support delocalized nonlinear vibrational modes (DNVMs), which are determined solely by the lattice point symmetry, and are exact solutions of the equations of atomic motion for any interatomic potential. DNVMs can be used for setting initial conditions to excite spatially localized vibrational modes called discrete breathers (DBs). In this study, DNVMs derived for instability can result in the formation of localized vibrational modes concentrating a significant part of the lattice energy. In some cases, localized vibrational modes can be obtained by imposing localizing functions upon DNVM.

1. Introduction

Well-known spatially localized vibrational modes in nonlinear lattices are called discrete breathers (DBs) [1–3]. It has been shown theoretically and experimentally that DBs exist in a number of discrete physical systems of different nature [4] including crystals [5] such as composed of carbon and hydrocarbon [6–14], h-BN [15], crystals with ionic [16–18] and covalent [19, 20] bonding, ordered alloys and intermetallics [21–23], various metals [24–30] and metal hydrides [31]. It is important to investigate properties of DBs because they can take part in defect structure evolution of crystalline solids [28] and affect macroscopic properties, for example, heat capacity [32], thermal expansion [33], thermal conductivity [34, 35] and stiffness [36]. DBs can be important for tribology [37].

DBs can be defined as spatially localized vibrational modes in nonlinear lattices. In most of the works on DBs it is assumed that they are localized in all spatial dimensions. However, it is clear that in a n-dimensional lattice DB can be localized in k<n dimensions and delocalized in the remaining n–k dimensions. For the first time, one-dimensional DBs (k=1) were analysed in two-dimensional lattice of graphene (n=2) by Baimova in the work [38]. Later, Bachurina has analysed linear (k=1) and planar (k=2) DBs in different metals with fcc lattice (n=3) [25, 26]. In those works, the delocalized nonlinear vibrational modes (DNVMs) were used for excitation of DBs.
Recall that DNVMs (originally called as the bushes of normal nonlinear modes [39–41]) are exact solutions of nonlinear dynamic equations, determined solely by the point symmetry of the crystal. Dynamics of $N$-component DNVM can be described by $N$ coupled equations of motion. DNVMs can be used for excitation of DBs, for example, in fcc metals [25, 26], in triangular Morse lattice [42, 43] and in graphene [44].

In the present study we reconsider the one-dimensional DBs in triangular Lennard-Jones lattice [45] excited with the help of one-component DNVMs reported in [40] for a chain of coupled particles. It is important to note that DNVMs are unstable for amplitudes above a threshold value [46–51]. In this study, parameters of the unstable DNVMs are determined before the instability develops.

2. Simulation setup
A two-dimensional triangular lattice with an interatomic distance $d$ is analyzed. Cartesian coordinate system with the $x$ axis aligned with close-packed atomic rows is used. Interatomic interactions are described by the Lennard-Jones potential

$$U_{LJ}(r) = L \left[ \left( \frac{r}{r_l} \right)^{12} - 2 \left( \frac{r}{r_l} \right)^6 \right],$$

where $L$ and $r_l$ are the parameters. Parameter $L$ defines the binding energy and $r_l$ is the equilibrium distance for a pair of atoms. We take $L = 1$ and $r_l = 1$, using them as the units of energy and distance, respectively. By a proper choice of the unit of time we also set the atom mass $M = 1$. The cut-off radius is taken to be $5r_l$. Relaxation of the triangular lattice with these parameters give the equilibrium interatomic distance $d = 0.99027777$. For solving the equations of motion the sixth-order Stormer method is employed with the time step $\tau = 10^{-3}$. Periodic boundary conditions are used. The computational cell size includes $12 \times 200$ atoms along the $x$ and the $y$-axis, respectively.

The following initial conditions are used (see figure 1). There exist four one-component DNVMs in a chain of particles. In a close-packed atomic row parallel to the $x$-axis one of them are excited by applying initial displacements along the $x$-axis as shown in figure 1(a-d). Atoms vibrating in the excited row produce kind of local thermal expansion. In order to take this thermal expansion into account, the atomic half-planes above and below the excited row are shifter as the rigid bodies by $Y$ and $-Y$, respectively. Initial velocities of all atoms in the computational cell are equal to zero. Displacement patterns in DNVMs have period $p$. Modes from 1 to 4 have the periods 2, 3, 4 and 4, respectively.

![Figure 1](image_url)

**Figure 1.** (a-d) Vibrational patterns used for excitation of one-dimensional DBs, 1 to 4, respectively, in triangular lattice. The $x$ axis is directed along a close-packed atomic row, and the $y$ axis is normal to the $x$ axis. Only atoms in one close-packed row (shown in light colour) are initially excited. In (a) and (d) all atoms vibrate, in (b) and (c) some atoms are at rest. Period of the vibrational mode in (a) is equal to 2, in (b) to 3, and in (c) and (d) to 4. The half-planes above and below the excited atomic row are initially shifted as the rigid bodies by $Y$ and $-Y$, respectively. DNVMs for the chain have been obtained and analyzed in [40,52,53].
3. Simulation results
In our simulations for each of the studied DNVMs we analyse the properties of the corresponding one-dimensional DBs. In figure 2 the following results are presented for each of the four studied DBs: (a) DB amplitude as the function of time, (b) DB frequency as the function of amplitude, (c) energy per atoms as the function of amplitude and (d) shift of the atomic half-spaces away from the excited atomic row as the function of amplitude. Curves for the modes from 1 to 4 are numbered.

As can be seen from figure 2(a), DB amplitude decreases with time because they constantly radiate energy in the form of small-amplitude phonons. Recall that the DNVMs are the exact solutions for the chain of particles, but in our simulations the chain of excited atoms interacts with the rest of the two-dimensional lattice and DBs are not the exact solutions for triangular lattice and some energy radiation takes place. In figure 2(b) one can see that all four DBs demonstrate hard-type nonlinearity with frequencies increasing with the amplitude. DB 1 has the highest frequency for given amplitude. DB 4 has the second highest frequency. DB 3 has the lowest frequency and DB 2 the second lowest frequency. DBs 1 and 4 have relatively high frequencies because in the corresponding DNVMs all atoms move, while in DB 2 one third of atoms is at rest and in the lowest frequency DB3 a half of atoms is at rest (see figure 1). From figure 2(c) we deduce that, as expected, DB energy decreases with decreasing amplitude. Finally, looking at figure 2(d), we can see that the shift of the half-planes of the crystal away from the excited row depends almost linearly on the DB amplitude. DBs 4 produces greater shift than DB 1. DB 2 produces the smallest shift.

4. Conclusions
Molecular dynamics simulations were used to analyze properties of four one-dimensional DBs in triangular Lennard-Jones lattice. DBs were excited with the help of DNVMs derived for the chain of particles by Chechin with co-authors [40]. DB amplitudes as the functions of time were calculated. DB amplitude decreases with time for all studied DBs indicating that they are not the exact solutions of the equations of motion.

A natural continuation of the presented study could be the analysis of one-dimensional DBs in 3D crystals, e.g., in fcc and bcc metals.
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