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Gap discrete breathers in strained boron nitride

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ABSTRACT

Linear and nonlinear dynamics of hexagonal boron nitride (*h*-BN) lattice is studied by means of molecular dynamics simulations with the use of the Tersoff interatomic potentials. It is found that sufficiently large homogeneous elastic strain along zigzag direction opens a wide gap in the phonon spectrum. Extended vibrational mode with boron and nitrogen sublattices vibrating in-plane as a whole in strained *h*-BN has frequency within the phonon gap. This fact suggests that a nonlinear spatially localized vibrational mode with frequencies in the phonon gap, called discrete breather (also often termed as intrinsic localized mode), can be excited. Properties of the gap discrete breathers in strained *h*-BN are contrasted with that for analogous vibrational mode found earlier in strained graphene. It is found that *h*-BN modeled with the Tersoff potentials does not support transverse discrete breathers.

1. Introduction

Among nonlinear lattice excitations of particular interest are nonlinear spatially localized vibrational modes called either discrete breathers or intrinsic localized modes, first discovered in simple 1D nonlinear chains [1–3]. A transition from solitons to discrete breathers with the change of relative strength of interparticle and on-site interactions was described in [4]. Discrete breathers have been modeled in a number of crystals [5] including metals [6–10], covalent crystals [11,12], ionic crystals [13,14], and in low-dimensional materials such as graphene [15–23,25,24,26], graphane (fully hydrogeneted graphene) [27–31], and carbon nanotubes [32–35].

Undoubted success in various technological developments of graphene has generated a growing interest of researchers to other two-dimensional crystalline materials such as hexagonal boron nitride (*h*-BN), silicene, phosphorene, molybdenum dioxide, and others [36–48]. Very little is known about the existence and properties of discrete breathers in these new materials.

In the present study we consider *h*-BN, whose properties are often compared to that of graphene, because both these materials have hexagonal lattice. It is even possible to achieve pressure-induced commensurate stacking of graphene on *h*-BN [49]. In spite of similarities in their structure, many properties of *h*-BN are different from that of graphene: graphene is a semimetal with no gap in the electron spectrum, while the *h*-BN sheet is a wide-band-gap (about 6 eV) electrical insulator. Graphene and *h*-BN possess interesting thermal properties [50,51] and high strength [52–54].

Elastically strained graphene supports discrete breathers and breather clusters with frequencies within the phonon gap [23,26]. Unstrained graphene modeled with the AIREBO potential supports transverse discrete breathers with frequencies within the phonon spectrum but above the phonon spectrum of out-of-plane vibrations [15–17]. Such discrete breathers have a very long lifetime because the large-amplitude out-of-plane vibrations weakly interact with the in-plane phonons. It is tempting to check if *h*-BN can support similar nonlinear excitations and this is the subject of the present study.

2. Simulation setup

Atoms in *h*-BN form a two-dimensional hexagonal lattice with a primitive translational cell containing one B and one N atoms.

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Atom mass of boron is equal to $m_B = 10.8$ atomic mass units, while for nitrogen it is $m_N = 14.0$ atomic mass units. Let the x and the y axes of the Cartesian coordinate system are directed along the zigzag and armchair directions of the lattice. This cell is generated by the vectors $\mathbf{a}_1 = (a, 0, 0)$ and $\mathbf{a}_2 = (a/2, a\sqrt{3}/2, 0)$, where $a = 2.497$ Å is the equilibrium lattice parameter. For definiteness, boron atom is located at the origin, while nitrogen atom at the middle of the primitive translational cell. The computational cell of $N \times N$ primitive cells is considered with periodic boundary conditions.

The large-scale atomic/molecular massively parallel simulator (LAMMPS) [55] is employed to conduct the molecular dynamics simulations with the use of the Tersoff-like interatomic potential [56,57]. Fourth-order scheme with the time step of 0.1 fs is used to integrate numerically the equations of atomic motion.

Phonon density of states (DOS) is calculated as the Fourier transform of the autocorrelation functions of trajectories of atoms at a temperature of 10 K. The results are compared for different computational cell sizes, $N = 10$, 20, and 40. It is found that $N = 20$ is sufficient and this size is used also for simulation of the extended vibrational modes and discrete breathers.

In order to induce a gap into phonon spectrum, we apply in-plane tensile elastic strain $\varepsilon_{xx} > 0$ along zigzag direction. The equilibrium positions of atoms in uniformly strained lattice are found by minimizing the potential energy of the crystal.

The initial conditions used to excite the extended vibrational modes and the discrete breathers are described below. Thermal vibrations are not introduced in the study of extended vibrational modes and discrete breathers. Frequency and amplitude of the extended modes and discrete breathers are found by averaging over the simulation run of 0.6 ps which covers more than a dosen of the oscillation periods.

3. Results

3.1. Effect of elastic strain on phonon DOS

The phonon density of states (DOS) for unstrained h-BN is shown in Fig. 1. Panels (a)–(c) give the x, y, and z-components of DOS, while in (d) the cumulative DOS is presented. It can be seen that maximal frequency of in-plane small-amplitude vibrations is about 47 THz, while for out-of-plane phonon modes it is at 26 THz. A narrow gap in phonon DOS (width of about 2 THz) can be seen around 35 THz.

Similar results but for elastically stretched h-BN along zigzag direction with $\varepsilon_{xx} = 0.3$ can be seen in Fig. 2. Maximal frequencies for in-plane and out-of-plane phonons have been reduced down to 40 THz and 15 THz, respectively. More important for our discussion is the appearance of the wide gap in the phonon spectrum ranging from 23 to 36 THz. This makes it possible for in-plane DBs to exist with frequencies inside the gap, as it has been shown for strained graphene [26].

We have also calculated phonon DOS for $\varepsilon_{xx} = 0.1$ and 0.2. For 10% strain, due to breaking of the lattice symmetry, the gap exists only in the x-component of DOS and no gap in the cumulative phonon spectrum is found. For 20% strain the gap does exist in the frequency range from 26 to 34 THz.

3.2. Extended nonlinear vibrational modes

Symmetry of h-BN lattice under homogeneous strain along zigzag direction allows one to excite at least two extended short-wavelength vibrational modes [58]. The first one (in-plane mode) is obtained when, say, boron sublattice is shifted as a whole along the armchair direction relative to the nitrogen sublattice by $2A$. Initial velocities of all atoms are equal to zero. The second one

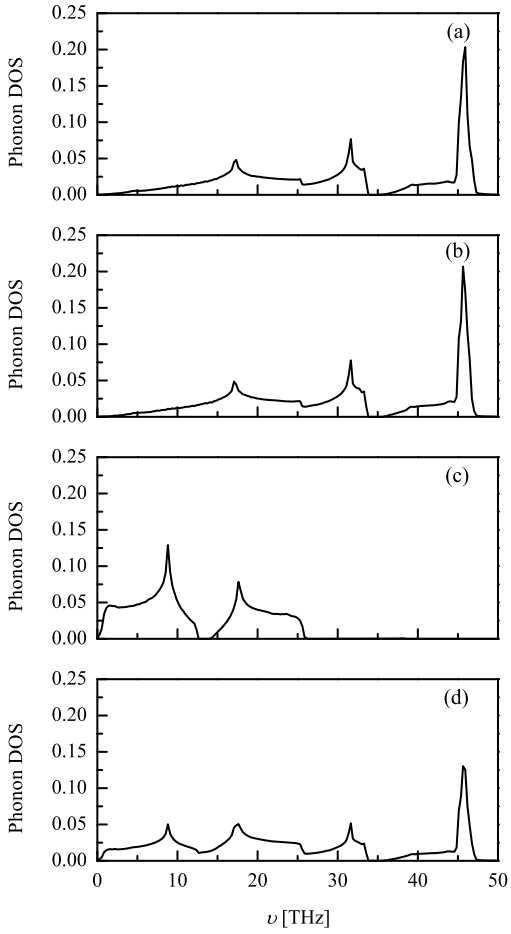

Fig. 1. Phonon DOS for unstraind h-BN.

(transverse mode) is obtained by the relative shift of, say, boron sublattice relative to the nitrogen sublattice by $2A$ in the direction normal to the sheet. In both cases the two sublattices will oscillate out-of-phase along the corresponding direction with the amplitudes A_B and A_N satisfying $A_B + A_N = A$. The amplitudes A_B and A_N are not equal because B and N have different atomic masses and because stiffness of B-N-B valence angle is different from that for N-B-N valence angle.

These extended vibrational modes are the lattice symmetry dictated exact solutions to the equations of atomic motion, no matter what kind of interatomic potential is used and for any amplitude. Typically such modes demonstrate the effect of modulational instability [59–68] with the critical exponent growing with the increase of the amplitude. If frequency of an extended vibrational mode at large amplitudes lies outside the phonon spectrum, one can attempt to excite a discrete breather by applying a bell-shaped localization function [15,69].

Frequency as a function of amplitude A_B for the in-plane mode is shown in Fig. 3. It can be seen that frequency of this mode bifurcates from the upper edge of the gap in the phonon spectrum (shown by the horizontal dashed line) and decreases with increasing amplitude being in the phonon gap. The same picture was observed for strained graphene in [26]. We thus conclude that h-BN, similar to graphene, can support gap discrete breathers, and in the following it will be shown that this is true.

As for the transverse extended mode, its frequency also decreases with amplitude (see Fig. 4), bifurcating from the upper edge of the z-component of phonon DOS (see Fig. 1). This result is for unstrained h-BN, but the same is observed for h-BN under elastic strain $\varepsilon_{xx} = 0.2$ and 0.3. Since the transverse mode has fre-