2017 International Symposium on Nonlinear Theory and Its Applications,
NOLTA2017, Cancun, Mexico, December 4-7, 2017

Interaction of Small-Amplitude Waves with Discrete Breathers in Strained Graphene

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Abstract– Nonlinear excitations in graphene and other carbon nanomaterials have been actively studied motivated by their possible applications. Of particular interest is the result of interaction of small-amplitude running waves with a large-amplitude standing discrete breather. This problem is addressed here in frame of the molecular dynamics approach. We estimate transmitted and reflected phonon energy densities as well as the energy emitted by the DB as a result of the interaction with the phonons of different frequency.

1. Introduction

Discrete breather (DB), also called an intrinsic localized mode, is a time-periodic, spatially localized vibrational mode in a defect-free nonlinear lattice. DBs were discovered by mathematicians three decades ago [1] and later they were directly observed in many macroscopic and mesoscopic systems of different physical natures [2,3]. They have also been reported by experimentalists in different crystals [4].

Mechanisms of DB excitation have been actively discussed and several nontrivial ways of their emergence have been found. Firstly, DB can appear in thermal equilibrium [5,6]. They can emerge spontaneously as a result of the modulational instability of a zone boundary vibrational mode [7-10]. They can also be excited by external driving at frequencies outside the phonon band and sufficiently large driving amplitude, the so-called supratransmission phenomenon [11-13]. In our recent study we have demonstrated that supratransmission can be observed even for rather small driving amplitudes [14]. In the theoretical work [15] the possibility of the optical creation of DBs in crystals was demonstrated.

It is well-known that graphene and other sp^2 carbon nanomaterials support DB [16]. Japanese researchers have pioneered in the theoretical studies on DB in graphene and carbon nanotubes [17-22]. DB with frequencies above the phonon spectrum were identified in their studies. It is well known that a gap can be induced in the phonon spectrum of graphene by application of homogeneous elastic strain, and then robust gap DB (having frequencies within the phonon gap) can be excited [23-26]. A DB in unstrained graphene with transverse oscillations was recently reported by Hizhnyakov et al. [27]. Later a family of DB with transverse oscillations were identified in unstrained graphene [28].

For unstrained graphene, a localized vibrational mode with in-plane atomic vibrations and frequencies above the phonon spectrum was recently reported based on the Tersoff interatomic potential [29]. This mode however is not a DB but rather a defect mode. The Tersoff potential supports in graphene a stable defect with a single valence bond longer than the other bonds, and this long bond can vibrate with frequencies above the phonon spectrum. That is why in the present molecular-dynamics study we take the Savin interatomic potential [30] and focus on the gap DB in strained graphene [23].

In our recent study, molecular-dynamics simulation of energy transport in strained graphene nanoribbon away from ac driven zigzag atomic row has been performed in a quasi-one-dimensional setting [14]. Driven zigzag atomic row was considered as the energy source, and the power of the energy source was calculated as the function of driving amplitude and frequency. It was found that nonzero power is observed when driving frequency is within the phonon gap and that even small driving amplitude is sufficient to observe energy transport. The mechanism of the energy transport in the linear regime of displacement driving is related to the excitation of two standing DB to both sides of the driven zigzag atomic row [14]. The DB amplitude is time-modulated, and due to the effect of local nonlinear lattice expansion such DB emit a low-frequency phonon wave having frequency of DB amplitude modulation. The results of work [14] suggest that DB can be a source of phonon waves. In the present study we address another important problem of how small-amplitude phonons interact with standing DB.

2. Numerical setup

Graphene is a two-dimensional hexagonal crystal with a primitive translational cell including two carbon atoms. Here a rectangular translational unit cell with four atoms is considered, as shown by the dashed lines in Fig. 1(a). To simulate a nanoribbon, a rectangular supercell with dimensions $M\times N$ was built, where M=100 and N=1 are numbers of translational unit cells along the x (armchair

direction) and y (zigzag direction) axes, respectively. The periodic boundary conditions are applied to the simulation supercell. By choosing N=1 we formulate a quasi-one-dimensional problem. Vertical atomic rows are numbered with the index k. Each translational unit cell includes four vertical atomic rows and thus, k=1,…,4M=400 [see Fig. 1(b)]. The standard set of interatomic potentials offered by Savin is used [30]. The equilibrium valent bond length in the unstrained graphene is 1.418 Å.

To induce a gap into the phonon spectrum, graphene is subjected to homogeneous elastic strain with the components ε_{xx}=-0.1, ε_{yy}=0.35, and ε_{xy}=0.

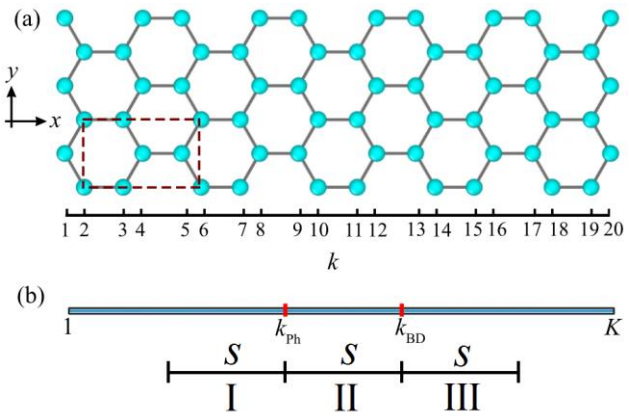

Fig. 1. (a) Graphene structure and numbering of vertical atomic rows by index k=1,…,K with K=400. Rectangular translational cell with four carbon atoms is shown by the dashed line. (b) Schematic for the numerical setup: the nanoribbon includes K =400 atomic rows, the source of phonons is at k_{Ph}=159,160 and DB is located at k_{DB}=239,240. S is the distance between phonon source and DB.

The phonon source is introduced by applying displacement ac driving to one zigzag atomic row with k=159,160 [see Fig. 1(b)] as follows

$$\Delta x_{159}(t) = \Delta x_{160}(t) = A\sin(2\pi\nu t), \qquad (1)$$

where Δx represents the displacement of atoms from their equilibrium positions in the x direction, A is the driving amplitude in angstroms, and ν is the driving frequency in THz. We always take small driving amplitude of A=0.001 Å and consider different driving frequencies within the in-plane phonon spectrum of graphene.

A large-amplitude DB centered on the valence bond connecting atomic rows k=239,240 is excited [see Fig. 1(b)]. Due to the fact that we use periodic boundary conditions and just one translational cell along zigzag direction (N=1), in fact, an infinite chain of DB is excited and the considered problem becomes quasi-one-dimensional with atoms moving along x axis only.

The distance between the phonon source and DB is denoted as S in Fig. 2(b). In our simulations S=76.6 Å. In Fig. 2(b) we also introduce the three regions I, II and III of length S each. These regions are used for the calculation of energy density around the DB as it will be described later.

Equations of atomic motion are integrated with the help of the Stormer method of order six with the time step of 0.5 fs.

3. Numerical results

In Fig. 2, we present the phonon density of states (DOS) of graphene strained with ε_{xx}=-0.1, ε_{yy}=0.35, and ε_{xy}=0. DOS is separated into DOS for phonons with in-plane atomic displacements (shaded) and DOS for transverse displacements (not shaded). Since only x-displacements of carbon atoms are considered in our quasi-one-dimensional model, only shaded DOS is important for the following discussion (note that in graphene the in-pale and the transverse waves are weakly coupled). The shaded DOS has a wide gap in the frequency range from 22.5 to 35.2 THz. The high-frequency (optic) phonon band is from 32.5 to 40.2 THz.

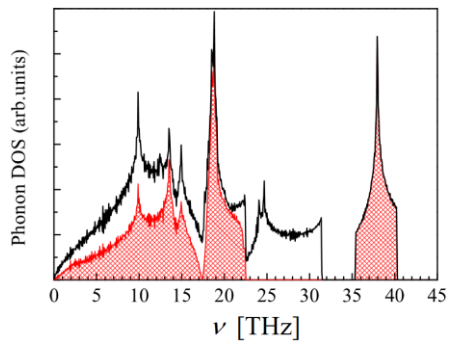

Fig. 2. Phonon DOS for graphene homogeneously strained with ε_{xx}=-0.1, ε_{yy}=0.35, and ε_{xy}=0. DOS for phonons with in-plane (transverse) atomic displacements is shaded (not shaded).

In Fig. 3 dynamics of DB centered between atomic rows k=239 and k=240 is presented by showing x-displacenets as the functions of time for the atomic rows from k=237 to k=242. It can be seen that the atomic rows k=239 and k=240 move along x-axis out-of-phase with the amplitude 0.285 Å. DB frequency is 25.6 THz. Note that the vibration centers of the atomic rows from k=239 and k=240 are shifted away from the equilibrium positions by about 0.135 Å. We note that the excited DB, when it does not interact with phonons, practically does not radiate its energy and has extremely long lifetime.

The next step in our study is to analyze the interaction of small-amplitude phonon mode excited by ac driving according to Eq. (1) with the DB shown in Fig. 3. We scan the driving frequency ranges from 0 to 18 THz (acoustic band) and from 35.5 to 40 THz (optic band). The driving starts at time t=0 and we measure the group velocity V_g of the excited phonon. The time of simulation run is

$$T = \frac{2S}{V_g}, \qquad (2)$$

which is equal to the time needed for the phonon wave to reach the DB and to come back to the energy source after being reflected from the DB.

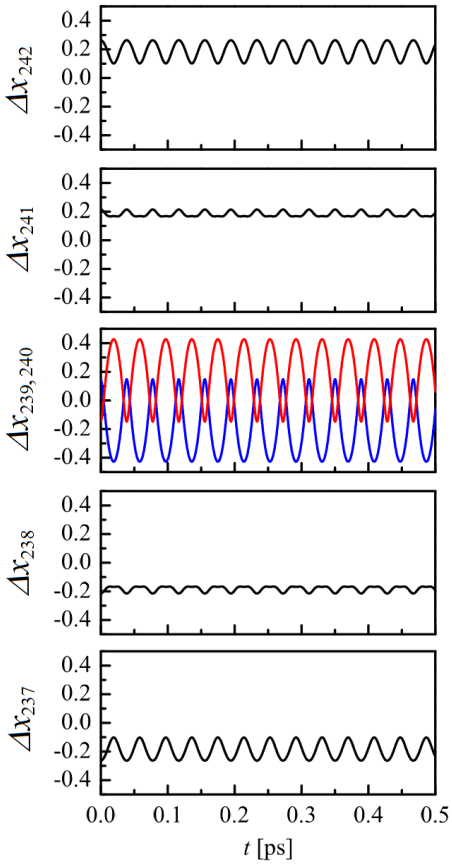

Fig. 3. Dynamics of DB centered between atomic rows k=239 and k=240. DB frequency is 25.6 THz, which is within the gap of in-plane phonon DOS (see Fig. 2).

Then we calculate total (kinetic plus potential) energy density (energy per atom) in the three regions, I, II, and III shown in Fig. 2(b). Energy density in the region I, E_I, is the incident phonon energy density. Energy density in the region II, E_{II}, is the sum of the incident and reflected by DB phonon energy densities. Then the energy density of the reflected wave is simply E_{II}-E_I. Finally, energy density in the region III, E_{III}, is the transmitted phonon energy density.

In Fig. 4 we plot E_I, E_{II}, and E_{III} as the functions of the driving frequency for (a) acoustic and (b) optic phonon bands.

As it can be seen from Fig. 4(a), ac driving with frequency ν<6 THz produces phonon which is fully transmitted by the DB with practically no reflection since transmitted and insident energy densities are equal. Within this driving frequency range DB does not radiate energy as the result of the interaction with the phonon. This is not the case for driving frequencies ν>6 THz. Indeed, here the trnasmitted energy density E_{III} is greater than the insident energy density E_I, which is only possible if the DB rediates some energy.

In the optic band [see Fig. 4(b)] the transmitted energy density E_{III} is always smaller than the insident energy density E_I and it decreases with increasing driving frequency. Thus, optic phonons are mainly reflected by the DB.

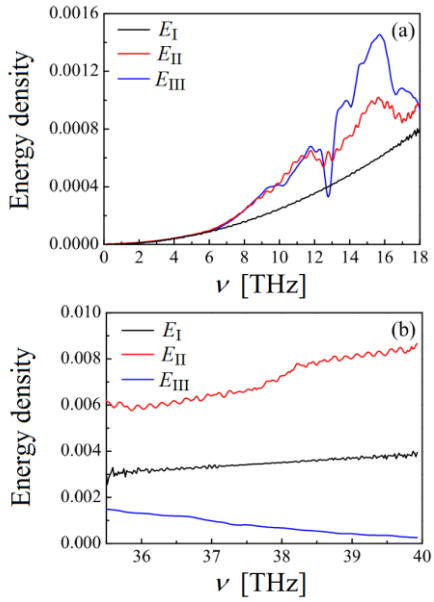

Fig. 4. Energy densities E_I, E_{II}, and E_{III} as the functions of the driving frequency for (a) acoustc and (b) optic phonon bands.

4. Conclusions

Interaction of small-amplitude phonons with standing large-amplitude gap DB was analyzed with the use of the molecular dynamics simulations based on the Savin interatomic potentials [30]. The problem is solved in the quasi-one-dimentional setting.

It is found that the acoustic in-plane phonons with frequencies smaller than 6 THz do not interact with DB being fully trnasmitted by the DB and cousing no radiation from the DB. Acoustic phonons with frequencies greater than 6 THz cause noticeable radiation from the DB.

Optic phonons are mainly reflected by the DB.

The results presented here contribute to our understanding of the relation between liner and nonlinear excitations in graphene and can be regarded as a continuation of our recent study [14].

Acknowledgments

E.A.K. and S.V.D. thank financial support from the Russian Science Foundation, grant No. 14-13-00982 and grant No. 16-12-10175, respectively. Stay of I.E. at IMSP RAS was partly supported by the Russian Foundation for Basic Research under grant No. 17-02-00984-a.

References

[1] A. J. Sievers, S. Takeno, "Intrinsic localized modes in anharmonic crystals," *Phys. Rev. Lett*. vol. 61, pp. 970, 1988.

[2] M. Sato, B. E. Hubbard, A. J. Sievers, "Nonlinear energy localization and its manipulation in micromechanical oscillator arrays," *Rev. Mod. Phys*. vol. 78, pp. 137, 2006.

[3] S. Flach, A. V. Gorbach, "Discrete breathers - Advances in theory and applications," *Phys. Rep*. vol. 467, pp. 1, 2008.

[4] S. V. Dmitriev, E. A. Korznikova, J. A. Baimova, M. G. Velarde, "Discrete breathers in crystals," *Phys. Usp*. vol. 59, pp. 446-461, 2016.

[5] M. Eleftheriou, S. Flach, "Discrete breathers in thermal equilibrium: distributions and energy gaps," *Physica D* vol. 202, pp. 142, 2005.

[6] L. Z. Khadeeva, S. V. Dmitriev, "Lifetime of gap discrete breathers in diatomic crystals at thermal equilibrium," *Phys. Rev. B* vol. 84, pp. 144304, 2011.

[7] T. Dauxois, R. Khomeriki, F. Piazza, S. Ruffo, "The anti-FPU problem," *Chaos* vol. 15, pp. 015110, 2005.

[8] Y. Doi, A. Nakatani, K. Yoshimura, "Modulational instability of zone boundary mode and band edge modes in nonlinear diatomic lattices," *Phys. Rev. E* vol. 79, pp. 026603, 2009.

[9] S. V. Dmitriev, A. A. Sukhorukov, A. I. Pshenichnyuk, L. Z. Khadeeva, A. M. Iskandarov, Y. S. Kivshar, "Anti-Fermi-Pasta-Ulam energy recursion in diatomic lattices at low energy densities," *Phys. Rev. B* vol. 80, pp. 094302, 2009.

[10] L. Z. Khadeeva, S. V. Dmitriev, "Discrete breathers in crystals with NaCl structure," *Phys. Rev. B* vol. 81, pp. 214306, 2010.

[11] F. Geniet, J. Leon, "Energy transmission in the forbidden band gap of a nonlinear chain," *Phys. Rev. Lett*. vol. 89, pp. 134102, 2002.

[12] R. Khomeriki, S. Lepri, S. Ruffo, "Nonlinear supratransmission and bistability in the Fermi-Pasta-Ulam model," *Phys. Rev. E* vol. 70, pp. 066626, 2004.

[13] P. G. Kevrekidis, S. V. Dmitriev, S. Takeno, A. R. Bishop, E. C. Aifantis, "Rich example of geometrically induced nonlinearity: From rotobreathers and kinks to moving localized modes and resonant energy transfer," *Phys. Rev. E* vol. 70, pp. 066627, 2004.

[14] I. Evazzade, I. P. Lobzenko, E. A. Korznikova, I. A. Ovid'ko, M. R. Roknabadi, S. V. Dmitriev, "Energy transfer in strained graphene assisted by discrete breathers excited by external ac driving," *Phys. Rev. B* vol. 95, pp. 035423, 2017.

[15] T. Rossler, J. B. Page, "Optical creation of vibrational intrinsic localized modes in anharmonic lattices with realistic interatomic potentials," *Phys. Rev. B* vol. 62, pp. 11460, 2000.

[16] J. A. Baimova, E. A. Korznikova, I. P. Lobzenko, S. V. Dmitriev, "Discrete breathers in carbon and hydrocarbon nanostructures," *Rev. Adv. Mater. Sci*. vol. 42, pp. 68, 2015.

[17] Y. Yamayose, Y. Kinoshita, Y. Doi, A. Nakatani, T. Kitamura, "Excitation of intrinsic localized modes in a graphene sheet," *Europhys. Lett*. vol. 80, pp. 40008, 2007.

[18] Y. Kinoshita, Y. Yamayose, Y. Doi, A. Nakatani, T. Kitamura, "Selective excitations of intrinsic localized modes of atomic scales in carbon nanotubes," *Phys. Rev. B* vol. 77, pp. 024307, 2008.

[19] T. Shimada, D. Shirasaki, T. Kitamura, "Stone-Wales transformations triggered by intrinsic localized modes in carbon nanotubes," *Phys. Rev. B* vol. 81, pp. 035401, 2010.

[20] T. Shimada, D. Shirasaki, Y. Kinoshita, Y. Doi, A. Nakatani, T. Kitamura, "Influence of nonlinear atomic interaction on excitation of intrinsic localized modes in carbon nanotubes," *Physica D* vol. 239, pp. 407, 2010.

[21] Y. Doi, A. Nakatani, "Structure and stability of nonlinear vibration mode in graphene sheet," *Proc. Eng*. vol. 10, pp. 3393, 2011.

[22] Y. Doi, A. Nakatani, "Structure and stability of discrete breather in zigzag and armchair carbon nanotubes," *Letters on Materials* vol. 6, pp. 49, 2016.

[23] L. Z. Khadeeva, S. V. Dmitriev, Y. S. Kivshar, "Discrete breathers in deformed graphene," *JETP Lett*. vol. 94, pp. 539, 2011.

[24] E. Korznikova, A. Savin, Y. Baimova, S. Dmitriev, R. Mulyukov, "Discrete breather on the edge of the graphene sheet with the armchair orientation," *JETP Lett*. vol. 96, pp. 222, 2012.

[25] E. Korznikova, J. Baimova, S. Dmitriev, "Effect of strain on gap discrete breathers at the edge of armchair graphene nanoribbons," *Europhys. Lett*. vol. 102, pp. 60004, 2013.

[26] I. P. Lobzenko, G. M. Chechin, G. S. Bezuglova, Y. A. Baimova, E. A. Korznikova, S. V. Dmitriev, "Ab initio simulation of gap discrete breathers in strained graphene," *Phys. Solid State* vol. 58, pp. 633, 2016.

[27] V. Hizhnyakov, M. Klopov, A. Shelkan, "Transverse intrinsic localized modes in monatomic chain and in graphene," *Phys. Lett. A* vol. 380, pp. 1075, 2016.

[28] E. Barani, I.P. Lobzenko, E.A. Korznikova, E.G. Soboleva, S.V. Dmitriev, K. Zhou, A.M. Marjaneh, "Transverse discrete breathers in unstrained graphene," *Eur. Phys. J. B* vol. 90, pp. 38, 2017.

[29] A. Fraile, E. Koukaras, K. Papagelis, N. Lazarides, G. Tsironis, "Long-lived discrete breathers in free-standing graphene," *Chaos Solitons Fractals* vol. 87, pp. 262, 2016.

[30] A. V. Savin, Y. S. Kivshar, B. Hu, "Suppression of thermal conductivity in graphene nanoribbons with rough edges," *Phys. Rev. B* vol. 82, pp. 195422, 2010.