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Discrete breathers in 2D and 3D crystals

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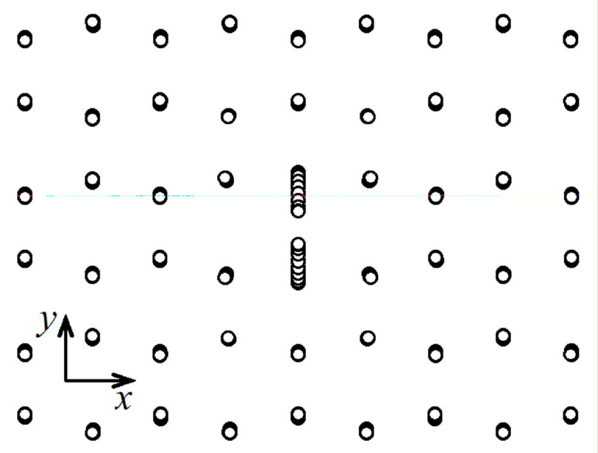
Discrete breathers (DB) are spatially localized, large-amplitude vibrational modes in defect-free nonlinear lattices. Recent numerical and experimental studies have confirmed that DB exist in crystals. In the present work, we briefly describe the well-known existence conditions of DB in crystals and present our recent results on DB in 2D crystals such as graphene and graphane and in 3D crystals such as alkali halide crystals and pure metals. The possible role of DB in solid state physics and materials science is discussed.



Stroboscopic picture of atomic motions in the vicinity of discrete breather excited in graphene homogeneously strained with $\varepsilon_{xx} = 0.3$, $\varepsilon_{yy} = -0.1$. Displacements of atoms from the equilibrium lattice positions are multiplied by the factor 4 for clarity. The discrete breather is of high spatial localization, so that only two atoms oscillate with a large amplitude.

1 Introduction Pioneering works by Dolgov [1], Sievers and Takeno [2], Page [3] and others have demonstrated that discrete nonlinear systems possessing translational symmetry can support spatially localized vibrational modes. Such modes were termed as intrinsic localized modes (ILM) or discrete breathers (DB). DB do not radiate energy in the form of small-amplitude wave packets because their frequency lies outside the linear vibration spectrum of the discrete nonlinear system. It has been established that DB may appear for both hard-type and soft-type of anharmonicity. In the former case DB frequency increases with amplitude because the effective interparticle force as the function of distance grows faster than linearly, while in the latter case the opposite is true.

Crystals are natural discrete nonlinear systems possessing translational symmetry and it is tempting to ask whether or not they support existence of DB, and if yes, then what is their role in solid state physics and materials science.

DB have been successfully observed experimentally in various settings ranging from electrical lattices [4] to optical waveguide arrays [5], Bose–Einstein condensates [6], one-dimensional micromechanical arrays of coupled cantilevers [7], and the Josephson-junction arrays [8]. There exist several reports on experimental observation of DB in crystals [9–14]. On the other hand, DB in crystals are very difficult to indicate because they are not topological defects and concentration of DB with high energy is too small in thermal equilibrium [15, 16]. Moreover, there exist experimental evidence that DB in NaI in thermal equilibrium can form ordered structures [17, 18] which also complicates their identification.

For real crystals the concept of quasibreathers introduced by Chechin et al. [19] may be useful because inherent imperfections and thermal vibrations of atoms make the search for the exact time-periodic solutions meaningless.

Computational methods play an important role in the study of DB in crystalline solids. Most of the results so far have been obtained by the molecular dynamics (MD) method based on the empirical interatomic potentials [20–38]. Very recently the density functional theory (DFT) was applied for the first time to prove the existence of DB in a crystalline solid using graphane as an example [39].

In the present work, we describe our recent results on DB in various crystals and discuss the way they can be applied to the solid state physics and materials science.

2 Gap discrete breathers

We start with the discussion of crystals having a gap in the phonon spectrum where gap DB, i.e., DB having frequency within the gap, can exist.

In the theoretical work [40] it was demonstrated that 1D chain of atoms interacting via classical potentials such as Toda, Born–Mayer, Lennard–Jones, and Morse, cannot support DB with frequencies above the phonon spectrum and only gap DB in the diatomic chains can exist, because, as a result of the anharmonic lattice dilatation, the soft tail of the potentials gives larger contribution to the atomic dynamics than the hard core of the potentials. The authors have concluded that the experimental search for anharmonic localized modes in real crystals should be directed toward those lattice systems which have a large gap between the optic and acoustic phonon branches. Later, following the work by Haas [41], it was shown that 2D Morse crystals do support DB [35, 37, 38]. Nevertheless, until recently, most of the works has been carried out for gap DB.

The first report on the gap DB in NaI crystal by Kiselev and Sievers [20] dates back to 1997. The authors have offered a special procedure to find initial conditions to excite a DB having [111] polarization. Later DB with [001], [011], and [111] polarizations were successfully excited in crystals with NaCl structure [21, 24]. The effect of elastic strain on the phonon spectrum and DB frequency in the crystal with NaCl structure was studied in [21, 24, 32].

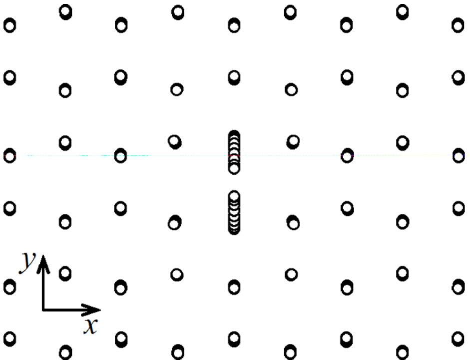


Figure 1 Stroboscopic picture of atomic motion in the vicinity of DB excited in graphene homogeneously strained with $\varepsilon_{xx} = 0.3$, $\varepsilon_{yy} = -0.1$.

The 2D graphene crystal does not have a gap in the phonon spectrum, but the gap can be induced by the elastic strain [42] and gap DB can be excited [30]. A stroboscopic picture of atomic motions in the vicinity of DB excited in graphene homogeneously strained with $\varepsilon_{xx} = 0.3$, $\varepsilon_{yy} = -0.1$ is presented in Fig. 1. Displacements of atoms from the equilibrium lattice positions are multiplied by the factor 4 for clarity. The DB is of high spatial localization, so that only two atoms oscillate with a large amplitude. Interestingly, DB in strained graphene can have frequencies within the phonon spectrum of the modes having out-of-plane displacements because the DB with in-plane displacements of atoms does not resonate with such modes [30]. Clusters of gap DB in strained graphene were investigated and the possibility of energy exchange between DB in the clusters was demonstrated [27].

The armchair edge of graphene nanoribbon under tensile strain can also support gap DB [28]. Such DB is shown in Fig. 2, where the displacements of atoms are multiplied by a factor 3 and the edge atoms are colored in light gray. Here only four atoms vibrate with a large amplitude.

Fully hydrogenated graphene, also called graphane, has a wide gap in the phonon spectrum due to the large difference in the atomic weight of C and H atoms. Consequently, it is very easy to excite a gap DB simply by initial displacement of one of the hydrogen atoms in the direction normal to the graphane plane. Such DB was studied with the use of MD [34] and DFT [39]. The latter method, which is more accurate as it takes into account the electronic structure and does not use any empirical interatomic potentials, suggests that DB frequency monotonically decreases with increase in

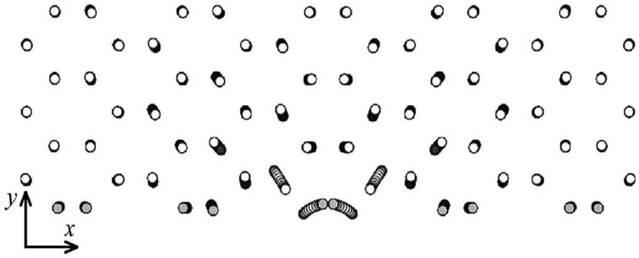


Figure 2 Stroboscopic picture of atomic motion in the vicinity of DB excited at the edge of a graphene nanoribbon strained with $\varepsilon_{xx} = 0.15$. The edge atoms are colored in light gray.

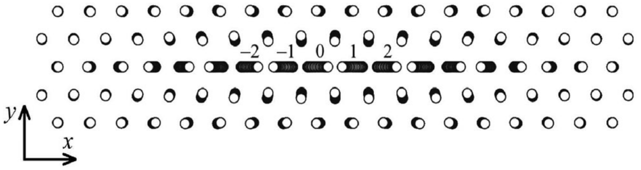


Figure 3 Stroboscopic picture of atomic motion in the vicinity of DB excited in Zr.

its amplitude. MD gives the same result only for sufficiently small DB amplitude.

3 Hard-type anharmonicity discrete breathers

Hard-type anharmonicity DB can exist in the crystals having no gaps in the phonon spectrum.

The first DB of this kind was reported in Si and Ge [22] with the help of MD simulations based on the Tersoff interatomic potential. Another successful attempt has been done by Yamayose et al. [43] for graphene. Recently the hard-type anharmonicity DB were excited in fcc Ni and bcc Nb [23]. The authors used the trial and error method for DB excitation. They applied initial displacements to eight nearest atoms located in a close-packed atomic row along this row keeping the DB symmetry (alternating sign of the displacements) but not the exact shape. The values of displacements varied from 0.09 to 0.3 Å [23]. It was shown that DB in pure metals are extended along a close-packed atomic row. Based on these results an ansatz with a few fitting parameters was offered to ease the excitation of the hard-type anharmonicity DB [35]. The ansatz was successfully used in the study of DB in 2D and 3D Morse crystals [26, 37, 38] and DB in various pure metals [44].

As an example, here we present DB in hcp Zr. The basal atomic plane of hcp lattice is shown in Fig. 3, where DB is excited in a close-packed atomic row with atoms numbered as $n = 0, \pm 1, \pm 2, \ldots$. All atoms in the row oscillate out-of-phase with their nearest neighbors. Maximal vibration amplitudes have atoms $n = 0$ and $n = 1$. In Fig. 4, for the atoms belonging to the atomic row with excited DB, the amplitudes (T_n) and displacements of the vibration centers (S_n) are shown in (a). In (b), the displacements of the 0th and 1st atoms are shown as functions of time, revealing the DB frequency of 5.19 THz, while the upper edge of the phonon spectrum is at 4.91 THz. DB frequency in Zr and other pure metals increases with the amplitude.

The stroboscopic picture in Fig. 3 suggests that DB in Zr embraces about 10 atoms. The same is true for DB in the Morse crystals and in other pure metals. This relatively low degree of localization explains why the discovery of such DB was done much later than in other materials, where typically only one or two atoms have large amplitude and hence, the excitation of DB is more evident.

Note that DB in the Morse crystal and in pure metals can move and the maximal DB velocity for different metals lies in the range from 0.1 to 0.5 of the velocity of sound. Note that the exact radiationless moving DB solutions in 1D chains can require some background oscillations [45]. In 2D and 3D crystals moving DB constantly radiate energy in the form of small-amplitude wave packets since they are not the exact solutions but rather are quasi-breathers [19].

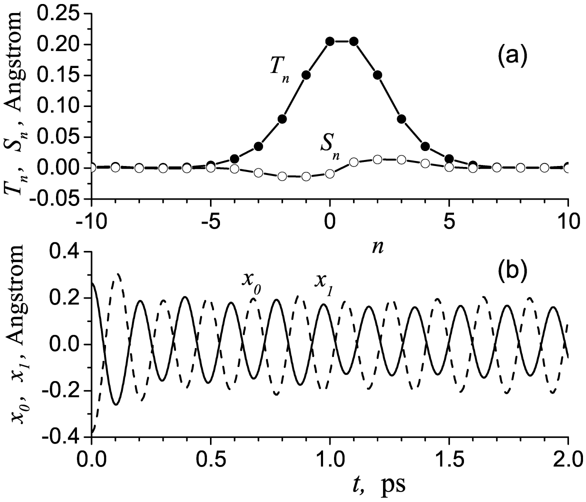


Figure 4 DB in Zr. (a) Amplitudes (T_n) and displacements of the vibration centers (S_n) of the atoms in the close-packed atomic row where DB is excited. (b) Displacements of the 0th and 1st atoms versus time.

4 Possible applications of discrete breathers

DB in crystals can localize and transport the energy of order of 1 eV. Even larger amount of energy can be localized when two or more DB collide. The localized energy can be spent on triggering a phase transition in a bistable state or on nucleation of a topological crystal lattice defect. Collisions of moving DB with each other were studied in [37]. It was demonstrated that energy exchange between colliding DB is possible, so that one of them can gain a portion of energy of the other.

In the work [26], interaction of moving DB with a vacancy was analyzed. It was found that the DB during the interaction with the vacancy reduces the potential barrier for vacancy migration [26]. In the earlier work [46] the interaction of DB with a vacancy has been analyzed in frame of the 1D Frenkel–Kontorova model with Morse nearest-neighbor interactions and sinusoidal on-site potential. It has been found that DB can be reflected, transmitted and trapped, both by the single and the double vacancy. The single vacancy can move forward, backwards and remain at rest, but the double vacancy cannot move forward, instead it can split into two single vacancies, one at rest and the other moving forward [46].

DB exist in crystals in thermal equilibrium at elevated temperatures [30, 47]. They can contribute to the thermal conductivity of crystals [48–50]. Excitation of DB may be the reason for the yield stress reduction in metals under electron irradiation [51]. The chemical reaction rate theory has been recently modified for solids to take into account the effect of DB [52–54].

A generalization of the polaron to solectron, which is the bound state of the crowdion or DB and electron has been proposed [55] to discuss the peculiarities of electron transport in crystals [56–59].

As a future challenge, it is important to search for DB in auxetics, among which are crystals and other discrete nonlinear systems [60–65].

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