REVIEWS OF TOPICAL PROBLEMS

Discrete breathers in crystals

S V Dmitriev, E A Korznikova, Yu A Baimova, M G Velarde

Contents

Abstract. It is well known that periodic discrete defect-containing systems support both traveling waves and vibrational defect-localized modes. It turns out that if a periodic discrete system is nonlinear, it can support spatially localized vibrational modes as exact solutions even in the absence of defects. Because the nodes of the system are all on equal footing, only a special choice of the initial conditions allows selecting a group of nodes on which such a mode, called a discrete breather (DB), can be excited. The DB frequency must be outside the frequency range of small-amplitude traveling waves. Not resonating with and expending no energy on the excitation of traveling waves, a DB can theoretically preserve its vibrational energy forever if no thermal vibrations or other perturbations are present. Crystals are nonlinear discrete systems, and the discovery of DBs in them was only a matter of time. Experimental studies of DBs encounter major technical difficulties, leaving atomistic computer simulations as the primary investigation tool. Despite definitive evidence for the existence of DBs in crystals, their role in solid-state physics remains unclear. This review addresses some of the problems that are specific to real crystal physics and which went undiscussed in the classical literature on DBs. In particular, the interaction of a moving DB with lattice defects is examined, the effect of elastic lattice deformations on the properties of DBs and the possibility of their existence are discussed, and recent studies of the effect of nonlinear lattice perturbations on the crystal electron subsystem are presented.

Keywords: crystal lattice, nonlinear oscillations, discrete breather, crystal lattice defect

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1. Introduction

More than four decades ago, an important discovery was made in the physics of nonlinear phenomena. It was shown that an infinite one-dimensional anharmonic chain of identical particles periodically arranged in space is capable of supporting spatially localized vibrational modes [1–4]. We can say that the precursors of this discovery were work on the vibrational energy localization in harmonic impurity and defect crystals [5–8],[1] nonlinear molecules, and molecular crystals at high vibrational excitation levels [10, 11]. It was found that the discreteness and nonlinearity of a medium were the two main conditions required for the excitation of spatially localized modes, which were called discrete breath-

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[1] Papers [5–8] and other studies by I M Lifshitz and his students on disordered crystals are included in book [9].

ers (DBs) or intrinsic localized modes. The system dimension and a particular form of the interaction potential for particles typically affect only the DB characteristics but not the possibility of their existence itself. Pioneering work on DBs was devoted to a rigorous proof of the existence and stability of DBs and most often was restricted to the analysis of one-dimensional chains of particles interacting with nearest neighbors via simple nonlinear potentials [1–4, 12–17]. Theoretical papers analyzing the integrability conditions for nonlinear chains are still of current interest [18–22].

Among popular one-dimensional models actively used for studying DBs, we refer to the Fermi–Pasta–Ulam model [23],

$$\ddot{x}_n = V'(u_{n+1}) - V'(u_n), \qquad u_n = x_n - x_{n-1}, \tag{1}$$

describing a chain of particles interacting with nearest neighbors via the polynomial potential

$$V(u_n) = \frac{1}{2} u_n^2 + \frac{\alpha}{3} u_n^3 + \frac{\beta}{4} u_n^4 \tag{2}$$

with coefficients α and β determining contributions from the quadratic and cubic nonlinearities (in the expression for the force $V'(u_n)$). Instead of polynomial expansion (2), the interaction between particles is also often described by the Toda potential

$$V(u_n) = \exp{(-u_n)} + u_n - 1, \tag{3}$$

the Lennard-Jones potential

$$V(u_n) = D\left[\left(\frac{r_0}{u_n}\right)^{12} - 2\left(\frac{r_0}{u_n}\right)^6\right], \tag{4}$$

or the Morse potential

$$V(u_n) = D\left\{1 - \exp\left[-\alpha(u_n - r_0)\right]\right\}^2. \tag{5}$$

The interaction forces determined by potentials (2) and (3) do not vanish at long distances and cannot therefore be used for describing long-range interatomic bonds in crystals. Potentials (4) and (5) are free of this disadvantage. The parameters D and r_0 in (4) and (5) respectively determine the bond energy and the equilibrium bond length. The Morse potential has a third important parameter α controlling the bond hardness and thereby the crystal hardness, which makes this potential the most attractive among other two-body potentials for describing interatomic forces in crystals. Potential (4) is often used in molecular dynamics calculations to simulate the properties of liquids whose compressibility can be ignored.

Along with interatomic interactions, one-dimensional simplified models often include local potential describing the interaction of atoms in a chain with their surroundings. One such model, which is widely used in condensed matter physics to describe the dynamics of dislocations or domain walls, is the Frenkel–Kontorova model [25]

$$\ddot{x}_n = \frac{1}{h^2}\left(u_{n-1} - 2u_n + u_{n+1}\right) - \sin u_n, \tag{6}$$

where h is the interatomic distance. In this model, the interatomic interactions are harmonic, while the nonlinear local potential is periodic. The harmonic interatomic potential in (6) can be replaced with one of the nonlinear potentials in (2)–(5).

Models leading to DBs are closely connected with the discrete nonlinear Schrödinger equation (DNSE) [26] and also with the more general Salerno model [27] interpolating between the DNSE and the Ablowitz–Ladik model [28]:

$$i\frac{d\psi_n}{dt} + \frac{1}{2h^2}\left(\psi_{n-1} - 2\psi_n + \psi_{n+1}\right) + \delta|\psi_n|^2\psi_n$$
$$+ \frac{1-\delta}{2}|\psi_n|^2(\psi_{n-1} + \psi_{n+1}) = 0. \tag{7}$$

Here, ψ_n is a complex dynamic variable for the nth site of the lattice, t is time, h is the lattice constant, and δ is a real parameter determining the crossover between the Ablowitz–Ladik model ($\delta = 0$) and the DNSE ($\delta = 1$). A review of discrete solitons in one-dimensional (1D) and two-dimensional (2D) nonlinear systems generated by the Salerno model is presented in [29].

Low-dimensional models similar to those mentioned above allowed a comprehensive investigation of the spatial localization of vibrations in nonlinear discrete systems.

The theoretical prediction of DBs set the task of finding these objects in real world, and after about a decade they were experimentally observed in various nonlinear discrete systems, for example, in optical fibers [30–32], atomic wave packets [33], superconducting Josephson junctions [34–36], periodic nonlinear electric circuits [37, 38], mechanical cantilevers and nano-electromechanical shuttles [39–43], etc. [44, 45].

Of course, crystals, which are also discrete nonlinear systems, attracted the attention of researchers as well. But the microscopic size of such localized excitations of a crystal lattice severely complicates their direct experimental observation. Nevertheless, several successful experiments confirmed the existence of DBs in crystals [46–55]. In addition, the possibility of the existence of DBs in crystals was conclusively proved by many atomistic computer simulations [56–73]. The complexity of the functional representation of realistic many-particle potentials complicates the application of analytic methods to the analysis of DBs in crystals.

Today, a new scientific avenue has opened up for researchers in the field of solid state physics and materials technology. The task is to perform detailed studies of the properties of DBs in different crystals, the mechanisms of DB excitation and pumping with energy, and the possibility of their movement in a crystal, and to describe their interaction with each other, crystal lattice defects, thermal vibrations, and external fields. The results of such studies will elucidate the role of DBs in crystal physics and mechanics, and DBs can become a part of new technologies in the future.

In this review, we present recent advances in the field of investigations of DBs in crystals and formulate unsolved problems in the conclusion.

2. Examples of discrete breathers in crystals

We consider several examples of nonlinear spatially localized vibrational modes, called discrete breathers, in different defect-free crystals based on the results of molecular dynamics simulations. In the absence of thermal lattice vibrations, these modes have a very long lifetime of several thousand or more vibration periods.

The first result was obtained for an alkali-halide NaI crystal with ionic interatomic bonds (Fig. 1) [56]. The sodium and iodine sublattices have a face-centered cubic (fcc)
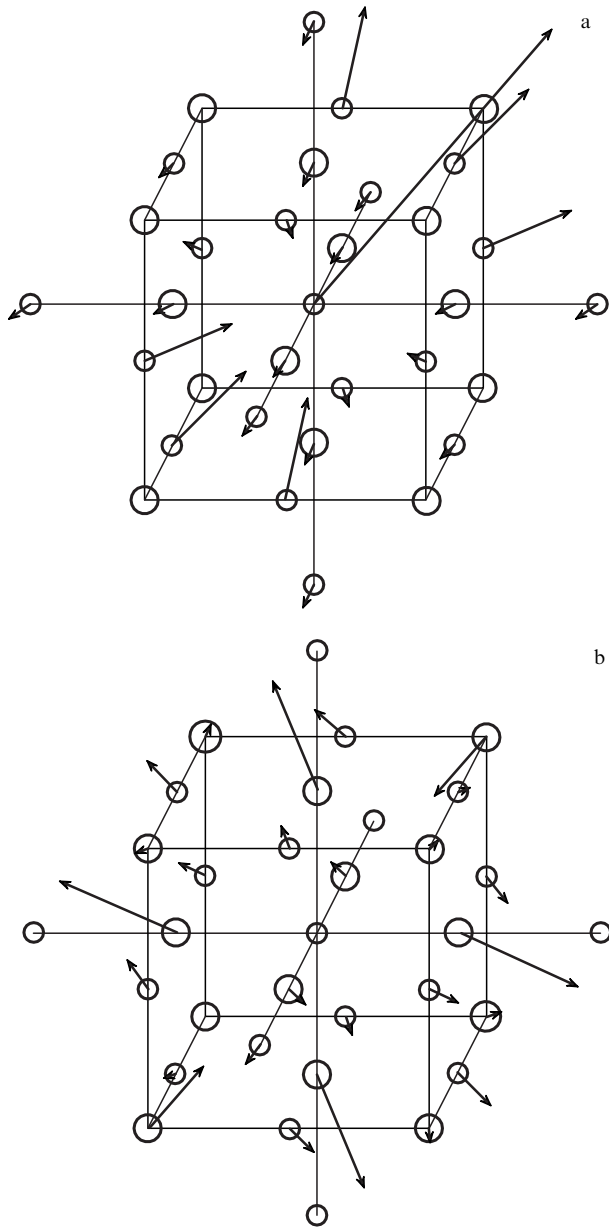
Figure 2. (Color online.) Discrete breather in an Si crystal (according to [59]). Large-amplitude out-of-phase vibrations are performed by two silicon atoms (shown in blue). This DB has frequencies lying above the gapless phonon spectrum frequencies, which first increase, reach a maximum, and then decrease with increasing the amplitude.

Figure 1. Discrete breather in an NaI crystal (according to [56]). The heavier iodine atoms are shown by larger circles. (a) The vibrational amplitudes of atoms and (b) displacements of the centers of atomic vibrations (increased ten times). We can see that vibrations are predominantly performed by light Na atoms, the Na atom vibrating in the $\langle 111 \rangle$ direction having the maximum vibrational amplitude. The DB frequency lies in the phonon spectrum gap and decreases with increasing the DB amplitude (soft nonlinearity type). The study of DBs in ionic crystals with the NaCl structure was continued in [57, 58].

structure with a lattice constant a and one of the sublattices displaced with respect to the other by the vector $(a/2, 0, 0)$, such that crystal atoms occupy the sites of a simple cubic lattice. Large-amplitude vibrations are performed by one Na atom in the $\langle 111 \rangle$ or $\langle 011 \rangle$ crystallographic directions with the frequency lying in the gap of the phonon spectrum of the crystal. Such a DB is called a gap DB. The DB frequency decreases with increasing the amplitude, reflecting the soft type of the nonlinearity of this vibrational mode. The presence of a gap in the phonon spectrum is caused by a considerable difference in the masses of crystal components (the iodine atom is 5.5 times heavier than the sodium atom). It
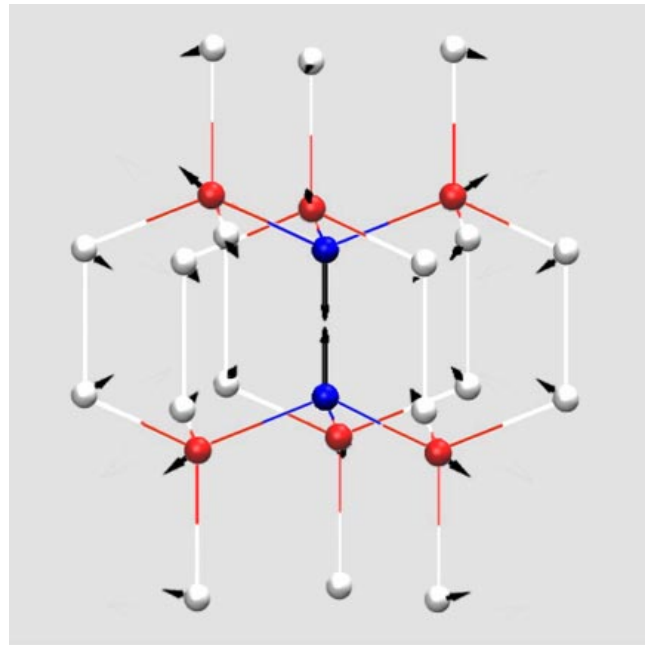
was shown later that long-lived gap DBs in ionic crystals with the NaCl structure can have the $\langle 001 \rangle$, $\langle 011 \rangle$, and $\langle 111 \rangle$ polarizations [57, 58].

Another example is a DB in covalent Si and Ge crystals obtained in [59] using the interatomic Tersoff potentials (Fig. 2). This DB has frequencies exceeding those of the gapless phonon spectrum. The DB frequency first increases, reaches its maximum, and then begins to decrease as the amplitude increases.

Gap DBs can be easily excited in models of ordered alloys with components having greatly different masses, which leads to a wide gap in the phonon spectrum, for example, in Pt$_3$Al [74–82]. These papers were based on Morse interatomic potentials [83]. We note that in Pt$_3$Al, both a gap DB and a DB with a frequency exceeding phonon-spectrum frequencies can be excited (Fig. 3) [80, 81]. The gap DB is predominantly localized on one aluminum atom and is immobile. On the contrary, a DB with a frequency exceeding the phonon-spectrum frequencies is manly localized on four to five aluminum atoms and can move along a close-packed row. Collisions of moving DBs with each other and with immobile gap DBs were investigated in [80].

Quasi-breathers in the presence of point defects in A_3B crystals were studied in [82].

Japanese researchers studied DBs in graphene and carbon nanotubes [60–64]. To launch a DB in graphene, a complex procedure for choosing the initial conditions was used [60]. The DB had frequencies higher than the gapless phonon spectrum and proved to be unstable. The gap in the phonon spectrum could be opened by applying a uniform elastic deformation, which allowed exciting a strongly localized gap DB [68], shown in Fig. 4. Clusters of such DBs were studied in [69], where the possibility of energy exchange between DBs in clusters was demonstrated.
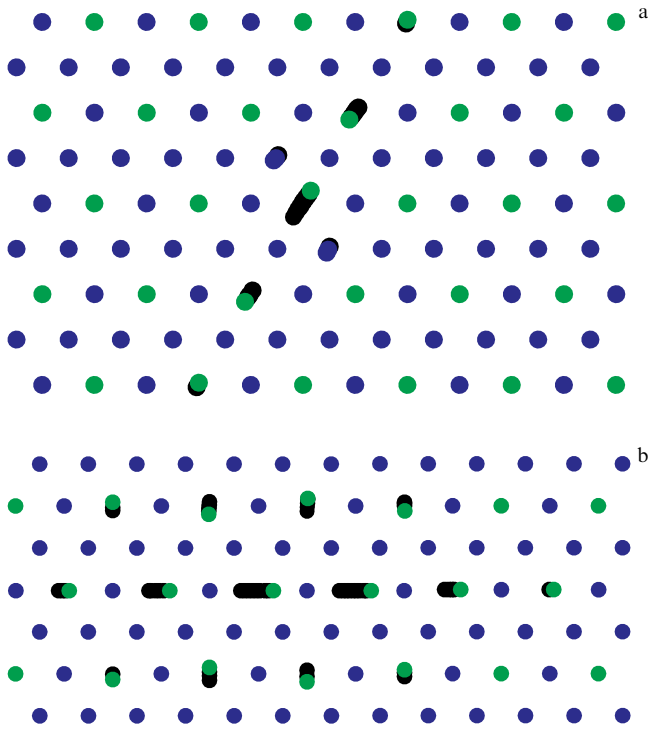
Figure 3. Stroboscopic picture of the motion of atoms near a DB in a Pt_3Al crystal (according to [80]). Heavy Pt atoms are shown by the darker color, compared to light Al atoms. (a) A gap DB mainly localized on one light atom oscillating out of phase with neighboring light atoms in a close-packed atomic row. (b) A DB with the frequency above the phonon spectrum frequencies, mainly localized on four to five Al atoms located in one close-packed row. These atoms perform in-phase oscillations. Unlike the gap DB, this DB can move along a close-packed row.
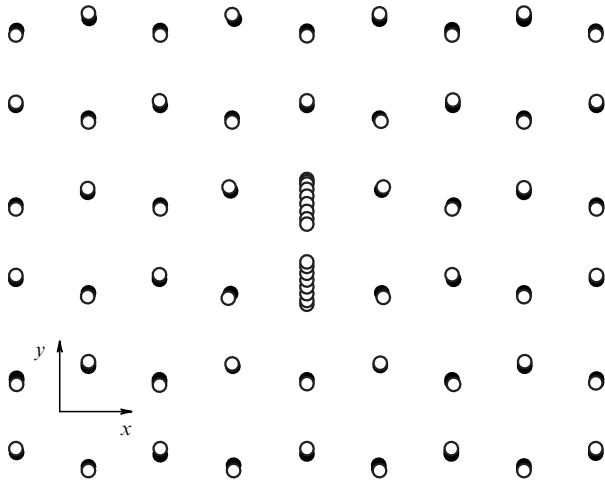

Figure 4. Stroboscopic picture of the motion of atoms near a DB in uniformly deformed graphene (according to [68]). Clusters of such DBs were studied in [69]. The DB frequency lies in the graphene phonon spectrum gap appearing due to applied uniform deformation.

Discrete breathers can also be excited at the edge of a stretched nanostrip with the 'armchair' orientation, as shown in Fig. 5 [70, 71]. The DB frequency lies in the phonon spectrum gap produced by the applied stretching deformation.

A fundamentally new type of DBs in graphene, with atoms vibrating perpendicular to the graphene sheet, is described in [84].
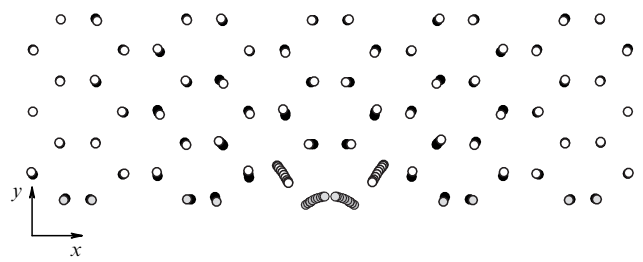

Figure 5. Stroboscopic picture of the motion of atoms representing a DB on the edge of a stretched graphene 'armchair' nanostrip [70, 71]. Atoms on the nanostrip edge are shown in grey. The DB frequency lies in the gap of the nanostrip phonon band appearing due to the nanostrip stretching.
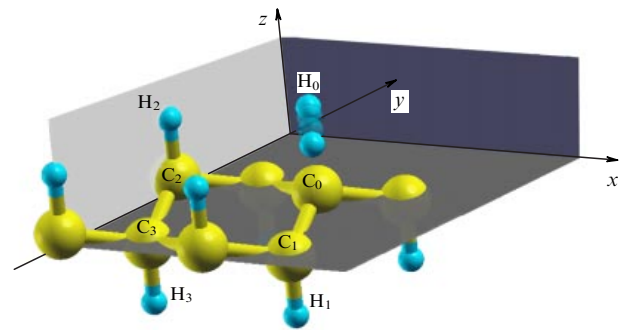

Figure 6. Discrete breather in graphene [72, 73]. The DB consists of one hydrogen atom H_0 oscillating perpendicular to the graphane sheet plane at a frequency lying in the phonon spectrum gap.

An example of a DB in a two-dimensional graphene crystal (completely hydrogenated graphene) is presented in Fig. 6 [72, 73]. The DB is given by a hydrogen atom vibrating with a large amplitude perpendicular to the graphene sheet. The DB frequency lies in the phonon spectrum gap and decreases with increasing the amplitude [73]. The energy exchange between DBs and the influence of temperature on the DB lifetime in graphene were studied in [85], where it was concluded that DBs can be involved in graphene dehydrogenation at increased temperatures.

The properties of DBs in carbon and hydrocarbon materials are reviewed in [86].

Beginning with [65], where mobile DBs were excited for the first time in an fcc Ni lattice and a body-centered cubic (bcc) Nb lattice, DBs have been extensively studied in pure metals [66, 87–90]. The DBs discovered so far in all pure metals have the same structure. Atoms located in one close-packed row vibrate out of phase with their neighbors at a frequency higher than the phonon spectrum frequencies, which increases with increasing the DB amplitude. An example of the vibration of interatomic bond lengths near a DB in fcc nickel is shown in Fig. 7 [90]. Discrete breathers in practically all pure metals can move along close-packed atomic rows, where they are excited by a few hundred or thousand interatomic distances with a speed ranging from zero to some maximal value. The maximum DB speed for different metals is 0.1–0.5 times the speed of sound [65, 66, 87–89].

With the example of a two-dimensional hexagonal lattice, the authors of [91, 92] proposed launching moving DBs in metals using an ansatz that contains a small number of parameters having a clear physical meaning. The interaction of moving DBs with each other was studied in [93, 94] and with crystal lattice defects in [95, 96].
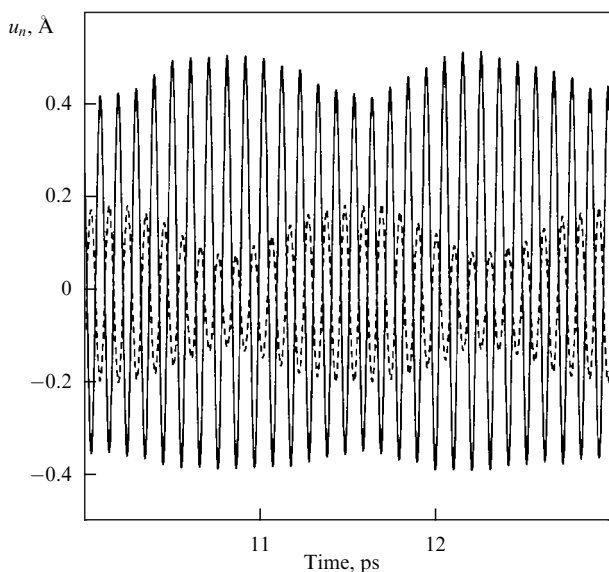
Figure 7. Discrete breather in an fcc Ni crystal [90]. Shown are oscillations of the lengths u_n of interatomic bonds: the central (solid curve) and the third from the center (dashed curve). The DB frequency lies above phonon spectrum frequencies and increases with increasing the amplitude.

3. Experimental studies of discrete breathers in crystals

Discrete breathers were experimentally observed in a strongly nonlinear and strongly anisotropic $[Pt(en)_2][Pt(en)_2Cl_2](ClO_4)_4$ crystal ('en' denotes ethylenediamine; hydrogen atoms are omitted) [46]. These localized states are determined by analyzing the crystal structure and resonance Raman spectra demonstrating a strong redshift of the higher harmonics. The authors of subsequent theoretical papers [47–49] conclusively proved that these features of Raman spectra are related to the excitation of localized vibrations of the Pt–Cl bond, accompanied by the excitation of vibrational polarons.

Inelastic X-ray and neutron scattering was used in [50, 51] to analyze the vibrational modes of an α uranium crystal lattice at the $[01\zeta]$ Brillouin zone boundary. The authors of [50, 51] observed excitation of a vibrational mode due to fluctuations of the amplitude of another mode representing its mirror image, which can suggest the excitation of a DB. The found modes are extended along the [010] direction of their polarization and are almost completely localized in the perpendicular [001] direction.

Because discrete breathers are substantially nonlinear modes, they are more actively excited at increased temperatures. At temperatures above 450 K, both experimental methods showed softening and a drastic decrease in the intensity of the longitudinal branch along the $[00\zeta]$ direction. In addition, a new dynamic mode appears along the $[01\zeta]$ Brillouin zone boundary with a frequency somewhat higher than the phonon spectrum frequencies. The authors of [51] assigned this mode to a DB appearing due to strong electron–phonon interaction.

Measurements in [52] of the high-temperature vibrational spectra of NaI crystals by inelastic scattering of neutrons revealed a weak peak in the phonon spectrum gap under thermal equilibrium conditions at 555 K, which was assigned by the authors to the excitation of gap DBs. The existence of such DBs was earlier predicted in molecular dynamics calculations [56]. Similar conclusions were made in [53]. However, it was shown in theoretical paper [54] that the probability of the thermofluctuation generation of DBs in an NaI crystal is low. Data obtained in [97, 98] demonstrate the ordered location of DBs in NaI. In [99], thermofluctuation DBs were not observed in an NaI crystal, which most likely suggests that the organization of such experiments is complex rather than the absence of DBs, because many theoretical studies predict their existence [100–109].

The anomalous (nonexponential) decay of the slow component of luminescence of a number of alkali-haloid crystals doped with lead or thallium [110] can be explained by the generation of DBs in the vicinity of an impurity atom [111, 112].

The phonon spectrum of a solid bcc ^{4}He crystal was measured by the neutron scattering method [113]. In addition to three phonon acoustic branches, a new mode with optical vibrations of atoms along the [110] direction was discovered. One of the possible interpretations of these data is the spontaneous excitation of localized vibrations [113].

The existence of moving DBs in germanium was quite convincingly proved in sophisticated experimental study [55]. The authors of [55] treated a high-purity germanium single crystal with plasma and studied the spectra, revealing five characteristic defects of the crystal structure. The action of plasma consists in the bombardment of the crystal surface by 2–8 eV ions. The bombardment resulted in the annealing of defects located deeply enough in the material, a few micrometers beneath the crystal surface. We note that simple heating does not produce a similar annealing of defects in germanium. Hence, the results obtained in [55] can be explained only by assuming that the energy in the concentrated form is transferred from the crystal surface inside the crystal with the help of DBs.

The acceleration of diffusion at the copper–nickel interface caused by the bombardment of the bimetal sample surface by 500 eV Ar^+ ions was observed in cases where the interface was at distances of 0.5, 1.0, and 1.5 mm from the surface [114]. It is known that structural changes caused by ion bombardment under these experimental conditions cannot occur at such considerable depths. Therefore, it is reasonable to assume that an effective mechanism of energy transport from the crystal surface to its depth exists, and the authors of [114] assume that this mechanism involves DBs.

It was shown in [115] that heavy ion bombardment of the surface of a common mica crystal at room temperature leads to knocking out the atoms on the opposite surface from a 7 mm thick crystal. The authors of [115] assume that DBs are responsible for the energy transfer sufficient for knocking out an atom from the opposite surface of a crystal approximately 10^7 translational cells in thickness. Interest in the study of nonlinear excitations in mica was initiated by Russell [116–118], who assumed that the dark lines seen by the naked eye in mica crystals can be the tracks of quasiparticles, which he called quodons.

Discrete breathers in ferromagnetic spin lattices were studied in theoretical papers [119–123]. The appearance of DBs in a layered quasi-one-dimensional $(C_2H_5NH_3)_2CuCl_4$ ferromagnet due to the instability of a homogeneous vibrational mode was experimentally demonstrated in [124].

Using the Kikuchi diffraction, the authors of [125] showed the presence of nonlinear vibrations in graphene with polarization properties drastically different from the polar-

ization of linear modes. They assumed that this fact can be explained by the excitation of DBs.

4. Computer simulation studies of discrete breathers in crystals

We describe some specific problems of the physics of real crystals that were not considered well enough in classical pioneering papers on DBs.

4.1 Quasi-breather nature of real discrete breathers

The introduction of the concept of a quasi-breather (QB) [126] became an important step on the way from the DB theory to the study of DBs in real crystals. The vibrations of individual QB particles are not completely synchronized, and therefore QBs have a finite but long enough lifetime. The QB degree can be estimated, for example, by the closeness of the QB to the single-frequency vibrational mode [126].

The origin of a QB can be related, first, to some inaccuracy in the initial conditions used for launching the idealized DB. Second, the crystal under study may not allow an exact solution in the form of an idealized DB at all, but can support long-lived spatially localized vibrational modes, i.e., QBs. Third, an idealized DB can transform into a QB in the presence of different types of perturbations, which inevitably exist in real physical systems. For example, a DB located near a topological defect undergoes crystal lattice distortion and its lifetime is finite.

Different mechanisms of phonon emission by a DB were studied in [127]. For each crystal, it is important to estimate the QB degree of DBs supported in the crystal. It is necessary to find the relation between the QB degree and the DB lifetime. Despite the practical importance of these problems, we are not aware of attempts to solve them for real crystals.

4.2 Lattice dimension

Solid crystals have translation symmetry in one, two, or three spatial dimensions. Examples of one-dimensional crystals are polymer chains [128], zigzag or armchair carbon nanotubes, etc. Among two-dimensional crystals, graphene (mono-atomic carbon layer) [60, 68, 69] and graphane [72, 73] have recently been attracting great interest of researchers. However, most of the crystals used in modern physics are three-dimensional. The influence of the crystal lattice dimension on the existence, stability, mobility, and DB excitation methods in real crystals is far from having been completely studied at present.

The theoretical foundations for studying the properties of DBs in model nonlinear discrete systems of different dimensions were laid in classical papers [12, 129–138]. The existence of DBs not moving in lattices of different dimensions was rigorously proved by the authors of [12] based on the anticontinuum limit, i.e., the case of noninteracting oscillators. The estimate of the upper bound on the interparticle interaction parameter providing the DB existence is given, for example, in [15, 16].

An important question is the presence or absence of the lower energy bound for DBs. It was found for a wide class of one-dimensional Hamiltonian lattices that two or three DBs can have an arbitrarily small energy [135, 136]. These papers refined the previous estimate in [133] based on more stringent assumptions according to which DBs can have an arbitrarily small energy only in one-dimensional lattices, whereas the DB energy in higher-dimensional lattices is bounded from below.

Discrete breathers in molecular dynamics calculations for three-dimensional crystals often have a distinct lower energy bound [80].

Discrete breathers in one-dimensional crystals can be polarized only along or perpendicular to the translation direction. In higher-dimensional crystals, the number of possible directions of atomic vibrations in DBs increases. For example, it was already mentioned that in a crystal with the NaCl structure, where atoms occupy the sites of a simple cubic lattice, one atom of the easy fcc sublattice at the DB center can oscillate with a large amplitude in the highly symmetric $\langle 001 \rangle$, $\langle 011 \rangle$, and $\langle 111 \rangle$ directions [56–58]. Such gap DBs have different amplitude dependences of the frequency and different minimal and maximal energies.

Discrete breathers in one-dimensional crystals can move only in one direction, whereas the question of possible directions of moving DBs in two-dimensional and three-dimensional crystals remains open. In [139–143], the DBs in two-dimensional crystals (common mica, cuprates) could move along close-packed atomic rows. The same is true for DBs in a two-dimensional Morse crystal [89, 91, 92] and pure metals [65, 66, 87, 88]. In a crystal with the NaCl structure, the energy exchange can occur between neighboring DBs, which can cause the random walk of DBs in the crystal [144, 145].

We discuss a nontrivial effect of the lattice dimension on the possibility of the existence of DBs of a certain type. It was shown in theoretical paper [146] that a one-dimensional chain of atoms interacting via any of the classic potentials such as Toda, Born–Mayer, Lennard-Jones, or Morse cannot support DBs with frequencies above the phonon spectrum frequencies; all realistic interatomic interactions are hard at small distances and soft at large distances, reflecting the structure of atoms consisting of compact nuclei and electron clouds surrounding them. For the vibrational mode frequency to increase above the phonon spectrum frequencies with increasing the amplitude, the hard core of the potential must make a greater contribution to the dynamics than its soft 'tail' does. However, because of the local rarefaction of the lattice in the vicinity of DBs (the local thermal expansion of the lattice), distances between the centers of oscillating atoms increase compared to those in the lattice, and the contribution from soft tails increases. Under these conditions, the authors of [146] could obtain only gap DBs by considering biatomic chains. The frequency of such DBs decreases with increasing the amplitude and enters the phonon spectrum gap that separates acoustic and optical phonons. Based on the results obtained, the authors of [146] concluded that the experimental search for DBs should be performed in crystals with a wide gap in the phonon spectrum.

However, based on the results obtained in [65], it was shown that unlike one-dimensional crystals, two-dimensional and three-dimensional Morse crystals without a local potential support DBs with frequencies above the phonon spectrum frequencies [91–93]. To explain this, we consider the DB structure in the two-dimensional Morse crystal in Fig. 8a. Calculations were performed with the dimensionless parameters of potential (5) $D = r_0 = 1$, $\alpha = 5$, and the atom mass equal to unity. The equilibrium interatomic distance a was 0.98813 and the truncation radius of the potential was $5.5a$. Figure 8a shows that the DB is elongated along one close-packed atomic row, but this row obviously experiences the action of a periodic local potential induced by surrounding atoms (Fig. 8d). This potential restricts the 'thermal expan-
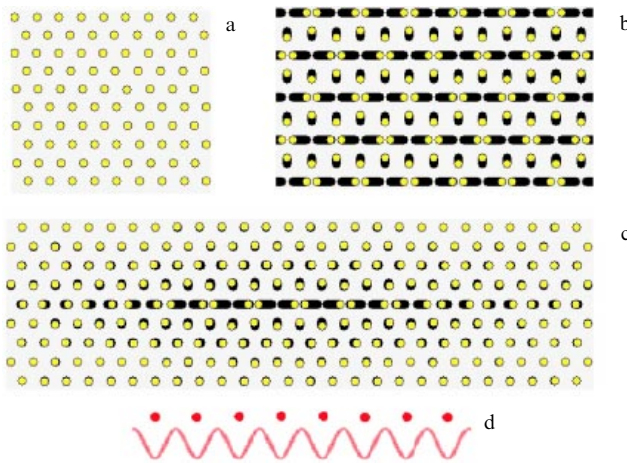
Figure 8. (a) Two-dimensional Morse crystal with atoms located at the sites of a triangular lattice. (b) Stroboscopic picture of the motion of atoms for a short-wavelength phonon mode in the nonlinear regime. (c) Stroboscopic picture of the motion of atoms near a DB obtained by the superposition of bell-shaped functions on the short-wavelength phonon mode shown in Fig 8b. The displacements of atoms in Figs 8b, c are magnified by a factor of seven for clarity. (d) Diagram of a one-dimensional model for the qualitative study of the DB shown in Fig. 8c. The atomic chain experiences the action of a periodic local potential produced by atoms surrounding the close-packed atomic row in which the DB is excited.

Figure 9. (a) Two-dimensional Morse crystal with atoms located at sites of a triangular lattice. (b) Stroboscopic picture of the motion of atoms for a highly symmetric phonon mode with the wave vector at the Brillouin zone boundary in the nonlinear regime. (c) Stroboscopic picture of the motion of atoms near the DB obtained by superimposing a bell-shaped function with the radial symmetry on the short-wavelength phonon mode in the nonlinear regime. The displacements of atoms in Figs 8b, c are magnified seven times for clarity.
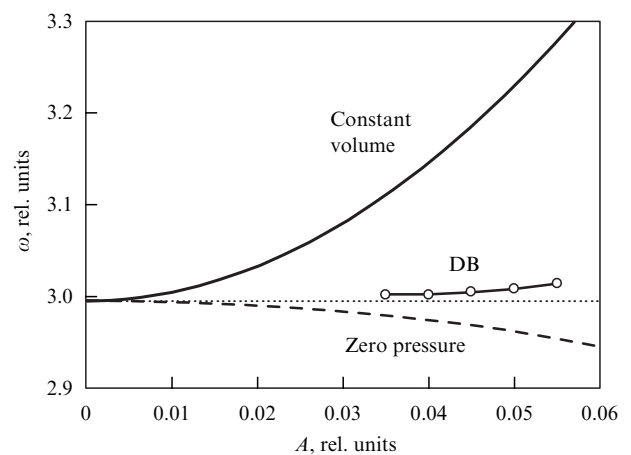
Figure 10. Dependence of the phonon mode frequency shown in Fig. 9b on the amplitude in the nonlinear regime: the solid curve corresponds to the constant size of the computation cell, and the dashed curve to zero pressure. The horizontal dotted line shows the upper boundary of the phonon spectrum $\omega_{max} = 2.995$. The circles connected by a line show the dependence of the DB frequency shown in Fig. 9c on the oscillation amplitude of its central atoms.

sion' of the atomic row in which the DB is excited, resulting in a noticeable contribution of hard potential cores to the dynamics of the vibrational mode whose frequency increases with increasing the amplitude. Because a periodic local potential was not introduced in [146], DBs with frequencies exceeding the phonon spectrum frequencies were not obtained.

To excite DBs similar to those shown in Fig. 8c, an ansatz was proposed in [91] and successfully used later in [92]. However, superimposing of bell-shaped functions on the short-wavelength phonon mode shown in Fig. 8b proved to be more efficient for the excitation of DBs in a two-dimensional Morse crystal. We note that the bell-shaped function was much more strongly localized along the vertical direction than along the horizontal direction, reflecting the structure of the DB shown in Fig. 8c.

It was recently shown in [147] that besides the DB described in [91–93] (Fig. 8c), the same two-dimensional Morse crystal (Fig. 9a) can also support the highly symmetric DB shown in Fig. 9c. This DB was obtained by superimposing a radially symmetric bell-shaped function on the short-wavelength phonon mode in a nonlinear regime (Fig. 9b).

Figure 10 shows the dependences of the short-wavelength phonon mode frequency ω on the amplitude A in two cases: for a constant size of the computation cell (solid curve) and for zero pressure (dashed curve). The zero pressure was provided by increasing the size of the computation cell, depending on the phonon mode amplitude, to take the 'thermal expansion' effect into account. We can see that the short-wavelength phonon mode demonstrates the hard type of nonlinearity in the first case and the soft type in the second case, i.e., the mode frequency increases (decreases) with increasing the amplitude in the first (second) case. This is explained by the fact that when the cell volume is constant, the dynamics of the short-wavelength mode is largely determined
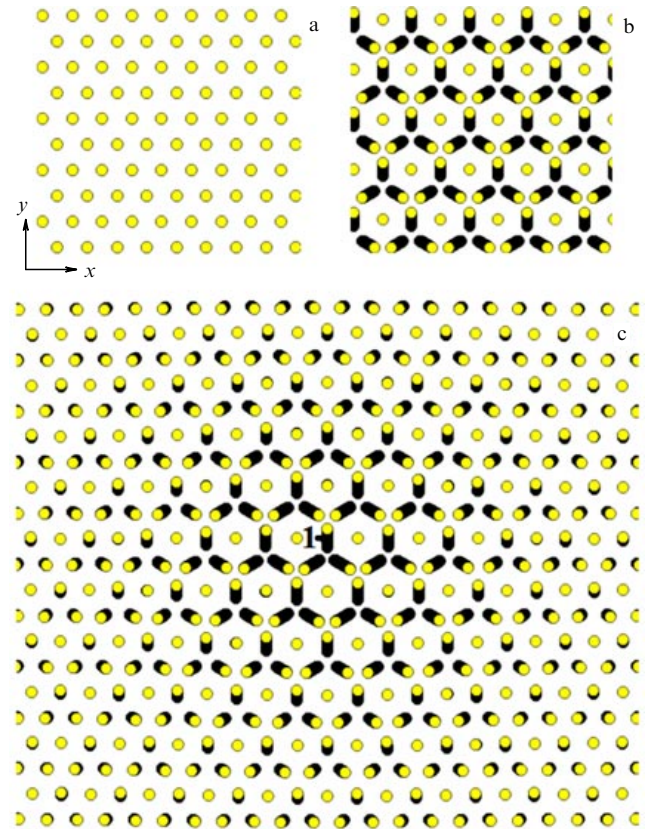
by the hard core of the Morse potential, while in the case of free thermal expansion, the dynamics is determined by the soft tail of the potential.

As regards the DB shown in Fig. 9c, its nucleus demonstrates the tendency to thermal expansion, which is restrained by the part of the crystal surrounding the DB. The suppression of the local expansion in the DB nucleus proves to be sufficient for the DB frequency to exceed phonon spectrum frequencies, increasing weakly with increasing the DB amplitude. This is seen from Fig. 10, where the horizontal dotted straight line shows the upper boundary $\omega_{max} = 2.995$ of the phonon spectrum of the crystal, and the circles connected by a solid curve represent the dependence of the DB frequency on the oscillation amplitude of its central atoms. We recall that calculations are performed for the dimensionless time normalized such that the atom mass is unity.

It can be shown that the static field of the radial displacements of atoms caused by the DB in a two-dimensional crystal decreases at large distances as $1/r$, i.e., rather slowly. This follows from the solution of the elasticity theory problem for a circular thin plate with a diameter d and a concentric circular hole with diameter c [148]. We assume that the plate is made of an isotropic elastic material with the Young modulus E and Poisson ratio v. The radial pressure p is applied to the edges of the inner cut. In polar coordinates, we have the unknown radial displacement $u(r)$, two nonzero components σ_r and σ_θ of the stress tensor, and three nonzero components ε_r, ε_θ, and ε_z of the deformation tensor. The equilibrium equation expressed in terms of displacements has the form

$$\frac{d^2 u}{dr^2} + \frac{1}{r}\frac{du}{dr} - \frac{u}{r^2} = 0, \tag{8}$$

and its general solution is

$$u = C_1 r + \frac{C_2}{r}, \tag{9}$$

where the integration constants

$$C_1 = \frac{1-v}{E}\frac{c^2 p}{d^2 - c^2}, \quad C_2 = \frac{1+v}{E}\frac{c^2 d^2 p}{d^2 - c^2} \tag{10}$$

are determined from boundary conditions, according to which $\sigma_r(c) = -p$ at the inner cut and $\sigma_r(d) = 0$ at the external edge. For an infinite plate with a circular hole, the limit $d \to \infty$ should be considered, which gives $C_1 = 0$ and $C_2 = c^2 p(1+v)/E$. From (9), we then obtain the radial displacement

$$u = c^2 p \frac{1+v}{E}\frac{1}{r}. \tag{11}$$

Expression (11) determines the long-range static field of radial movements of atoms in a two-dimensional crystal along the DB center. The factor $c^2 p$ has the dimension of force and therefore represents the effective concentrated force acting from the DB on an infinite two-dimensional crystal.

We note that in a three-dimensional crystal, the elastic displacement field produced by a DB decreases as $u(r) \sim 1/r^2$ with increasing the distance from the DB center, i.e., faster than in the two-dimensional case. This follows from the calculation of the radial displacement field for a hollow elastic sphere produced by internal pressure in the limit of the infinite external radius of the sphere. As a result, in a three-dimensional crystal, the local expansion in the DB nucleus is more efficiently suppressed by its surroundings, and DBs should be more strongly localized in space than they are in the two-dimensional case.

Another important conclusion is that DBs producing long-range elastic displacement fields should interact with each other at considerable distances, like dislocations [149].

4.3 Long-range interatomic bonds
Theoretical work typically considers chains in the approximation of taking the interaction only between nearest particles into account [44, 45]. However, interatomic forces in crystals can be long-range (for example, the Coulomb interaction in ionic crystals or metallic bonds). Polynomial potentials of the α and β Fermi–Pasta–Ulam type and the Toda potential cannot be used to describe long-range forces in real crystals, because they do not vanish at large distances, which is nonphysical for interatomic interactions. As mentioned in Section 4.2, realistic interatomic potentials are hard at small interatomic distances and become soft with increasing distance, reflecting the structure of atoms consisting of nuclei and electron shells.

The molecular dynamics method, which is widely used for studying DBs in crystals, is based on the interatomic interaction potentials with the parameters chosen to reproduce the experimental data as much as possible, first of all, the crystal structure, the lattice parameter, the sublimation energy, and elastic constants.

Two-body interatomic potentials, for example, the Lennard-Jones and Morse potentials, are the simplest. The use of such potentials is based on the assumption that the presence of other atoms does not affect the interaction of the pair of atoms under study. This assumption is not always justified; for example, the unpaired component of interactions for many metals and alloys can be significant. Classical (single-wall) two-body potentials can reproduce only the closest packings, for example, a two-dimensional triangle lattice or a three-dimensional fcc lattice, but loose packings, for example, a two-dimensional square lattice or a three-dimensional bcc lattice, are always unstable for a single-component material. In addition, when pair potentials are used for crystals with the cubic symmetry, the Cauchy relation $C_{12} = C_{44}$ is always satisfied for elasticity constants [150, 151]. However, it is known, for example, from experiments with many fcc and bcc metals that a noticeable deviation from the Cauchy relation is possible, and the magnitude of this deviation characterizes how much the interatomic interaction differs from a two-body one. These difficulties can be eliminated by using many-particle potentials constructed, for example, using the embedded atom model [152].

4.4 Interaction of discrete breathers with crystal lattice defects
According to its classical definition, a discrete breather is a spatially localized vibrational mode in a *defect-free* nonlinear lattice. However, crystal lattice defects play a very important role in condensed matter physics and materials technology. Discrete breathers can interact with defects, which causes distortions of the crystal lattice and local changes in the mass and hardness of bonds, both directly and by exciting vibrational modes localized on a defect or by acquiring energy from such modes.

The first studies on the interaction of a DB with a vacancy were performed using the one-dimensional Frenkel–Kontorova model with nonlinearly interacting particles [153, 154]. It was shown that a moving DB interacting with a vacancy can cause vacancy migration. Moreover, a nonlinear vibrational mode localized on an atom near the vacancy can play an

important role in this process [154]. The interaction of moving DBs with an interstitial atom was studied using the same model in [155]. The scattering of a DB on an interstitial atom leads to migration of the latter, the interstitial atom being more mobile than the vacancy, as follows from experiments. Thus, it was found that DBs can increase the mobility of point defects, which is in turn related to diffusion (mass transfer). It is known that the mobility of point defects favors the 'creeping over' of dislocations [149].

A two-dimensional Morse crystal supports moving DBs [91], allowing the study of their interaction with crystal lattice defects, for example, vacancies [95]. Figure 11 presents the results of such a study. The stroboscopic picture of the motion of atoms in a two-dimensional Morse crystal, where the DB moves along a close-packed atomic row in the vacancy direction, is shown in Fig. 11a. The atoms of the close-packed row, along which the DB is moving, are numbered with an index n. To estimate the potential barrier of the migration of atom I to a vacant lattice site, the time evolution of the distance $2Y$ between atoms II and III is investigated. Figures 11b, c show examples of the interaction of a DB with a vacancy at the position indicated by a vertical dashed straight line. The DB velocity in Fig. 11b is half the velocity in Fig. 11c. In Fig. 11b, elastic repulsion of the DB from the vacancy is observed, while in Fig. 11c, the DB is scattered by the vacancy. The deviation of the distance Y from its equilibrium value Y_0 as a function of time measured in the DB vibration periods θ is shown for two cases: the DB is elastically reflected from the vacancy (Fig. 11d) and scattered from it (Fig. 11e). The increase in the distance Y means a decrease in the potential migration barrier for atom I to the vacancy. Based on these results, we can conclude that the DB in a two-dimensional Morse crystal does not cause vacancy displacement, but reduces its migration barrier in the course of approximately 10^2 atomic oscillations for as long as the vacancy interacts with the DB [79].

The interaction of the DB with a vacancy, dislocation, and surface was studied by the molecular dynamics method for the bcc of iron [96]. It was found in all cases that the interaction of the DB with defects results in the vibrational excitation of atoms near the defect, which can cause structural transformations in the crystal.

The interaction of DBs with a substitution defect was studied in [156] for a one-dimensional chain with the nearest-neighbor interaction taking the linear component and the cubic anharmonicity into account. A few scenarios of the interaction of the DB with a defect were found, depending on the substitution atom mass, the interatomic interaction parameters, the degree of localization, and the DB velocity. The trapping of one or several DBs by an impurity was studied in the one-dimensional DNA model [157]. It was shown that the impurity can favor the merging of two DBs into one, resulting in a greater spatial energy localization [158]. The interaction of moving DBs with several impurities was studied theoretically and experimentally in a one-dimensional non-linear chain to find different mechanisms of their interaction and thereby to characterize the impurity type [159].

The existence of localized vibrational modes in a mono-atomic chain on a heavy impurity atom was shown in [138].

4.5 Discrete breathers on the surface of crystals
The atomically smooth surface of a three-dimensional crystal can be treated as a two-dimensional periodic system that can support localized nonlinear vibrations, i.e., DBs. Steps on a
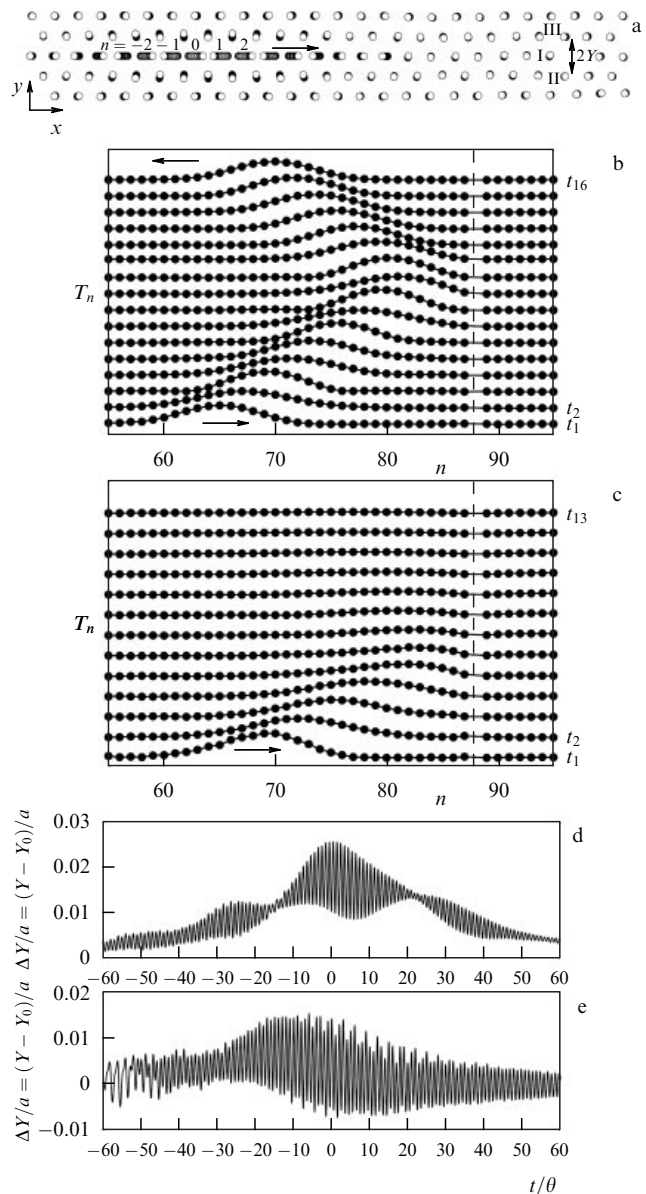

Figure 11. (a) Motion of a DB to a vacancy. The potential barrier for migration of atom I to the vacant site is estimated from the time dependence of the distance $2Y$ between atoms II and III. T_n is the dimensionless oscillation amplitude of the nth atom of a close-packed row along the x axis calculated as $T_n = (u_n^{\max} - u_n^{\min})/(2a)$, where $u_n^{\max}$ and $u_n^{\min}$ are the successive maximum and minimum of the function $u_n(t)$ describing the time dependence of the oscillation of the nth atom along the x axis, and a is the interatomic distance. (b, c) Examples of the DB interaction with a vacancy whose position corresponding to $n = 88$ is indicated by the vertical dashed line. The deviation of Y/a from the equilibrium value Y_0/a as a function of time: (d) A DB is elastically reflected from the vacancy and is scattered from the vacancy [95].

vicinal surface of a three-dimensional crystal have a quasi-one-dimensional periodic structure, and DBs can also exist on them (Fig. 12). In addition, DBs can exist on the edge of two-dimensional crystals. An example is presented in Fig. 5 for a graphene nanostrip [70, 71]. Such DBs can make their contribution to the physics of solid surfaces.

Discrete breathers were identified by the molecular dynamics method on a large step of an NaI crystal and in a monoatomic hydrogen layer on the (111) surface of silicon [160]. The authors of [160] assert that DBs can be more easily
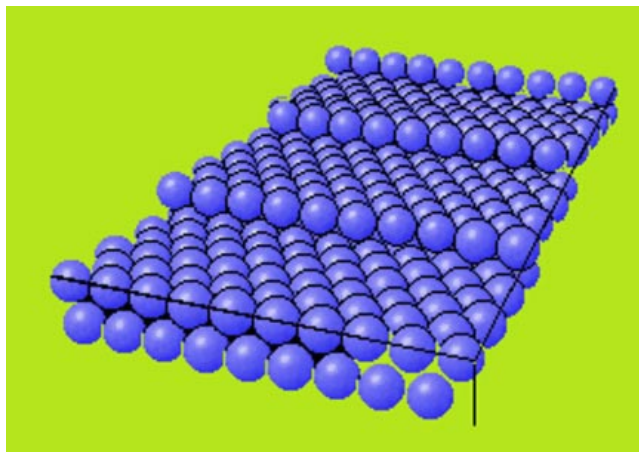
Figure 12. Vicinal surface of a crystal. The edge of a terrace is a one-dimensional periodic structure on which DBs can exist. The atom-smooth surface is a two-dimensional periodic structure that can also support DBs.

studied experimentally on the surface of crystals than in the bulk of a crystal lattice.

A one-dimensional model of the adsorbed layer gives three types of DBs, two of which turned out to be stable [161].

A number of papers have been devoted to the analysis of linear and nonlinear vibrational modes localized on the ends of one-dimensional chains [162–165] and on the edge of a graphene nanostrip [166]. They develop the idea expressed in pioneering work by Tamm [167] and Shockley [168] that provided the basis for physics of surfaces. Modes localized on the edge of one-dimensional chains cannot be classified as DBs because the translation symmetry of the system is broken in this case.

4.6 Influence of elastic lattice deformation on the properties of discrete breathers

Homogeneous elastic deformation of a crystal can noticeably affect its properties due to a change in the crystal symmetry and interatomic interactions depending on the distance between atoms at the lattice sites [169]. This method for controlling crystal properties can be most efficiently applied to nanomaterials that can withstand strong elastic deformations without structural changes and damage (graphene, nanofibers, etc. [64, 169–171]).

It was shown in [172] that the elastic deformation of a one-dimensional chain with the third- and fourth-order anharmonicities leads to a redistribution of the contributions from these anharmonicities, thereby changing the properties of DBs in the chain.

The elastic deformation of graphene and a graphene nanostrip induces a gap in the phonon spectrum, allowing gap DBs to exist in these materials [68–71]. An elastic deformation on the order of 0.01 noticeably affects the phonon spectra and frequencies of gap DBs in crystals with the NaCl structure [173].

4.7 Interaction of discrete breathers with the electronic and magnetic subsystems of a crystal

Recently, Velarde [174] proposed a new concept of a solectron, which extended the notion of a polaron, i.e., a coupled electron–phonon state, by considering nonlinear localized excitations of the lattice (solitons, DBs, etc.) instead of a small-amplitude phonon wave. It was shown that

solectrons can be involved in electron transport [174–183]. Based on the fact that the number of anharmonic excitations in crystals increases with temperature [184, 185] and on the recent electron transport theory [178], the authors of [186] obtained a power-law dependence of the electric resistance on the temperature for the general one-dimensional model of a crystal.

Figure 13 shows the results of numerical calculations in a one-dimensional model described by a system of two equations, one of which determines the lattice dynamics (the Toda lattice) and the other the density of electronic states (the Schrödinger equation) [174]. In the cases in Figs 13a, b, the interaction between the lattice and the electron subsystem is absent. At the initial moment, a perturbation is applied to both subsystems, resulting in a soliton excitation propagating in the lattice and in complete delocalization of the electron density. In the presence of interaction between the subsystems (Figs 13c, d), a lattice soliton was launched, with electrons completely delocalized at the zero moment of time. With time, electron trapping by the soliton and its transport were observed.

Large-amplitude lattice vibrations near a DB result in lattice dilation [187], which can affect the local magnetic properties due to magnetoelastic effects [188].

Discrete breathers in ferromagnets have been studied theoretically [119–123] and experimentally [124].

4.8 Excitation mechanisms of discrete breathers in crystals

The most natural excitation mechanism of DBs in crystals is their spontaneous thermofluctuation generation in thermodynamic equilibrium [52, 100–106]. Thermal vibrations of the lattice, on the one hand, reduce the DB lifetime [79], and on the other hand, the probability of the thermofluctuation excitation of a DB increases with temperature [100–105]. As a result, the DB concentration increases with the temperature [105].

A rather interesting DB generation mechanism discovered in [189, 190] was then discussed for one-dimensional [122, 191–194] and two-dimensional [195] models and also for a three-dimensional crystal with the NaCl structure [57]. According to this mechanism, DBs appear spontaneously due to the modulation instability [196, 197] of a short-wavelength phonon vibrational mode whose amplitude is not too small. The development of the instability leads to spatial energy localization in the form of large-amplitude DBs, which then slowly emit energy in the form of small-amplitude waves. As a result, the system comes into thermal equilibrium with the equal energy distribution over all vibrational modes. An example of such dynamics for a chain of magnetic spins is presented in Fig. 14.

The modulation instability of different phonon modes in a two-dimensional nonlinear lattice was rigorously analyzed in [198].

It is known that if a nonlinear discrete system is subjected to a periodic force at a frequency outside the spectrum of its small-amplitude vibrations, the energy is not transferred into the system if the force amplitude is smaller than a certain value, because traveling phonon waves are not excited. But in the nonlinear regime, when the force amplitude exceeds the threshold, nonlinear vibrational modes (for example, DBs) can be excited that can transfer energy over the system. This mechanism of excitation of nonlinear modes by an external periodic force with a frequency outside the small-amplitude spectrum of the system, which is called nonlinear supratrans-
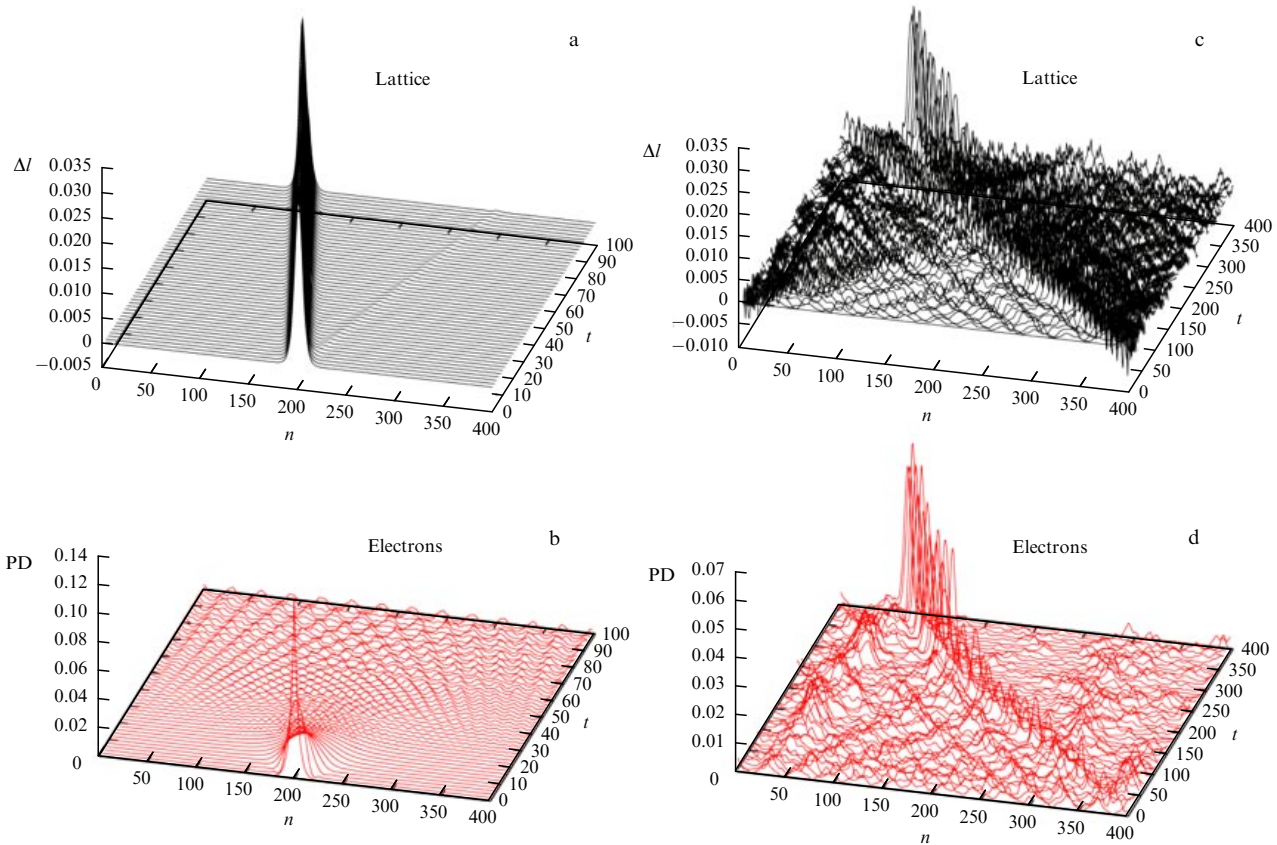
Figure 13. (Color online). Dynamics of a one-dimensional discrete system described by two equations, one of which determines the lattice dynamics (the Toda lattice) and other the density of electronic states (the Schrödinger equation) [174]. Δl is the relative displacement of Toda lattice sites and PD is the probability density of electronic states. The lattice and electronic subsystems in Figs 13a, b do not interact with each other. The initial perturbation introduced into both subsystems gives rise to a soliton propagating in the lattice and to complete delocalization of the electron density. The lattice and electronic subsystems in Figs 13c, d interact with each other. The electronic subsystem is not excited at zero time. A lattice soliton captures and transfers an electron.
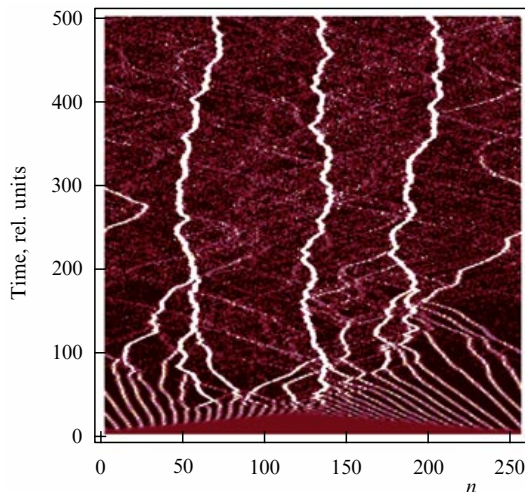

Figure 14. (Color online). Evolution of the energy density in a magnetic spin chain [122]. The lighter regions correspond to a higher energy density. Due to the modulation instability, the homogeneous energy distribution in the chain disappears. Discrete breathers produced in this case collide with each other and exchange their energy such that the amplitude of high-energy DBs increases. As a result, three slow-moving DBs with large amplitudes appear in the system, which slowly emit energy, and finally the system comes to thermal equilibrium with the equal energy distribution over all vibrational modes (this regime is not shown in the figure).

mission [199], was later studied for different nonlinear systems [200, 201].

In [202], gap DBs were generated in a Pt_3Al crystal subjected to the action at a frequency close to the DB frequency.

The possibility of exciting DBs in crystals irradiated by particles with different energies was discussed in [66].

Theoretical foundations for the observation of DBs in crystals generated by external action are developed in [203–205].

4.9 Moving discrete breathers in crystals and their collisions

The rigorous definition of a moving DB in a one-dimensional chain assumes the exact repetition of its profile after a time t displaced by some number k of lattice sites. The possibility of the existence of such solutions in nonlinear chains has been actively discussed and algorithms for constructing numerically accurate moving DBs have been proposed [44, 45, 193, 206–210]. Recently, a method for constructing DBs moving in a chain was proposed in [211] using a nonlinear local potential due to the compensation of one type of nonlinearity of interatomic bonds by the opposite type of the local potential nonlinearity.

For quasi-breathers [126] in real crystals, the concept of moving DBs should be changed to require slow enough energy emission by a spatially localized mode moving in the lattice.

Moving DBs in two-dimensional crystal models with a local potential were studied in [139–142]. It is known that at least in pure metals, DBs can move at the speed of 0.2–0.5 of the speed of sound [65, 87, 212]. In addition, it is known that strongly localized DBs in deformed graphene can exchange their energy [69]. Thus, DBs can be involved in energy transfer in a crystal. Collisions between DBs result in even stronger spatial energy localization at the collision point [93]. Colliding DBs can exchange their energy and momentum [93, 94].

Discrete solitons in a quadratically nonlinear 2D lattice can move in arbitrary directions [213].

For a system of parallel weakly coupled fields with the Fermi–Pasta–Ulam potential, the authors of [214] showed the existence of a delocalization transition, when a breather initially excited on a specified chain suddenly distributes its vibrational energy over the entire two-dimensional system of chains upon decreasing its amplitude (or frequency) below a threshold. The authors of [214] also showed the existence of two regimes: tunneling between chains and self-trapping on one chain for stationary or moving breathers in a system of two weakly coupled Fermi–Pasta–Ulam chains. These regimes are separated by a separatrix on which the rate of energy exchange between the two chains tends to zero. The same two regimes were observed for linear Josephson plasma oscillations and for a linear self-trapping in a tunneling contact of two weakly coupled Bose–Einstein condensates [215], which is not surprising because both physical systems are described by similar pairs of equations.

Discrete breathers travel over the lattice relatively slowly, moving by one lattice period in a time of ten oscillation periods [65, 139–142, 144, 145]. Supersonic motion is demonstrated by ultradiscrete kinks, whose profile is related to the 'magic' wavenumber $q = 2\pi/(3a)$, where a is the crystal lattice parameter [216]. This wavenumber appeared earlier in the analysis of standing or traveling sinusoidal waves that are exact solutions of the Fermi–Pasta–Ulam model [193, 217, 218].

4.10 *Ab initio* calculations

Molecular dynamics is based on empirical interatomic potentials, which should be verified by more accurate methods such as the quantum mechanical density functional method, which takes the quantum nature of the electron subsystem of the crystal into account. The importance of such calculations is clearly demonstrated in the *ab initio* study of DBs in graphane [73]. The dependence of the DB frequency on its amplitude found previously with the help of molecular dynamics [72] agrees qualitatively with the *ab initio* calculations [73] only for relatively small amplitudes. The use of the steepest descent method allowed refining the initial conditions for launching DBs in graphene [219].

An *ab initio* simulation of a gap DB in uniformly deformed graphene was recently performed in [219]. In the computation cell with periodic boundary conditions including 18 carbon atoms, the DB was excited by specifying the initial displacements of atoms with the numbers 10 and 15 along the Y axis in Fig. 15a. The dependence of the DB frequency on its amplitude is shown in Fig. 15b. The DB frequency lies in the phonon spectrum gap and decreases with increasing the amplitude, which is in qualitative agreement with the results obtained earlier by the molecular dynamics method [68, 70]. The distributions of the electron density in the vicinity of the DB nucleus in graphene at the moments of maximum separation, passing through the equilibrium
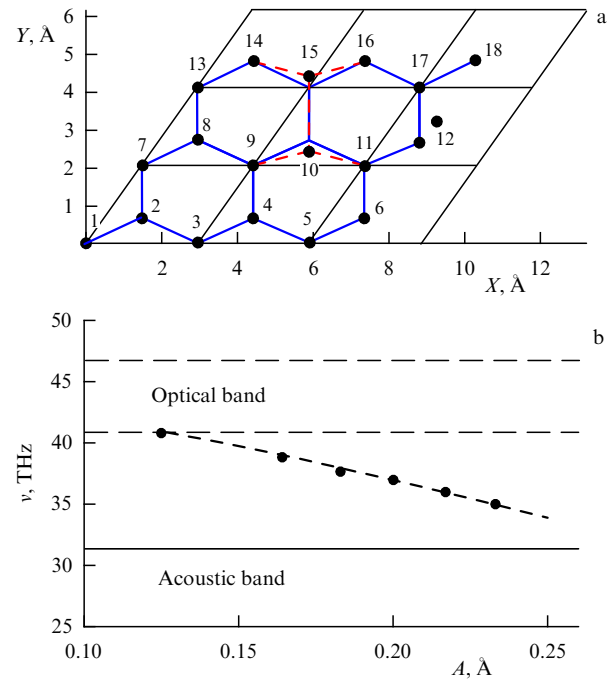

Figure 15. (a) Computation cell with periodic boundary conditions for the *ab initio* simulation of a DB in graphene subjected to uniaxial stretching along the X axis [220]. The DB was excited by displacing atoms 10 and 15 along the Y axis in opposite directions. (b) Dependence of the DB frequency v in graphene on its amplitude A.
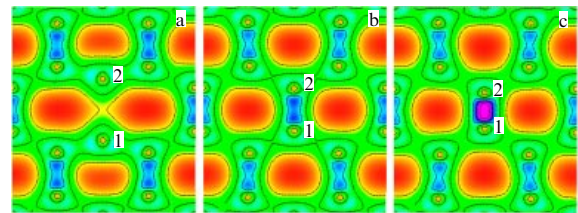

Figure 16. (Color online). Electron density distribution in the vicinity of the nucleus of a gap DB in deformed graphene at the moments of (a) maximal distance, (b) passage through equilibrium positions, and (c) minimal distance between carbon atoms 1 and 2, corresponding to atoms 10 and 15 in Fig. 15a.

position, and maximum approach of carbon atoms 1 and 2 (corresponding to atoms 10 and 15 in Fig. 15a) are shown in Figs 16a–c.

Nonlinear vibrational modes in graphene were studied in [221] using *ab initio* calculations. Some of the described modes can be treated as periodically arranged DBs.

A quantum mechanical description of DBs is available in the Bose–Hubbard model (see recent review [29]).

4.11 Group theory studies of discrete breathers in crystals with different types of spatial symmetry

In one-dimensional chains, two types of DBs with different symmetries are usually distinguished: the symmetric Sievers–Takeno mode and the antisymmetric Page mode. In [222], in the example of a planar quadratic lattice, group theory methods were used for the first time to determine all possible invariant varieties of a crystal lattice on which DBs can be localized. The stability of DBs was studied in that paper using the theorem on the possibility of decomposing multidimensional variational systems (obtained within the Floquet
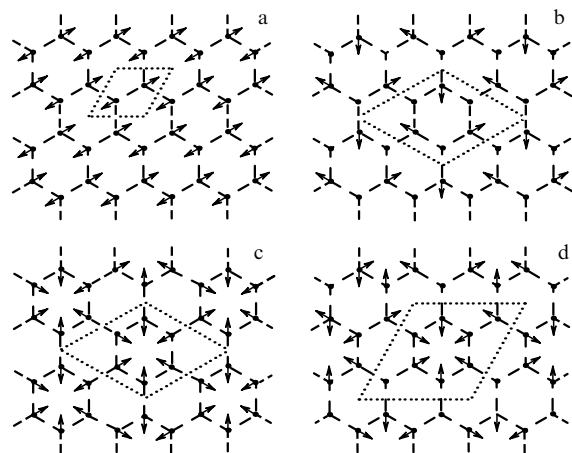
Figure 17. One-dimensional mode bushes in graphene with spatial symmetry groups (a) Cmm2, (b) P31m, and (c, d) P6mm [224].

theory) into independent low-dimensional systems [223]. The decomposition method, based on the use of irreducible representations of symmetry groups, is general and can be applied for studying the stability of DBs of different symmetry types in different two-dimensional and three-dimensional crystal structures, irrespective of the type of interatomic interactions.

It was recently shown in [224] that nondeformed graphene allows 4 one-dimensional (Fig. 17), 14 two-dimensional, one three-dimensional, and 6 four-dimensional vibrational bushes representing exact solutions of the dynamic equations of motion. If the frequency of these bushes increases with increasing the amplitude, they can be used to obtain spatially localized vibrational modes by superimposing bell-shaped functions.

5. Contribution of discrete breathers to the physical properties of crystals

If the properties of DBs are known, we can talk about their influence on the properties of crystals. Discrete breathers can contribute to the heat capacity of crystals [50], while mobile DBs can also contribute to heat conduction. Discrete breathers can transfer not only energy but also electric charge [174–183, 186]. Large-amplitude oscillations in the DB nucleus lead to a local dilatation of the crystal lattice, which should be reflected in the thermal expansion of the crystal [187]. The excitation of DBs in relaxor ferroelectrics allows explaining many phenomena observed in experiments with these materials [225, 226]. By transferring energy over considerable distances, DBs excited by plasma processing of the surface of a germanium single crystal are capable of transforming crystal structure defects at a large depth [55]. Nonlinear vibrations also play an important role in the formation of vacancies [227].

The contribution of DBs to the kinetics of thermo-activated reactions in crystals is quite large. Although the DB concentration is low, the rate of chemical reactions and phase transformations in the vicinity of DBs depends on their energy exponentially. This energy can be lower than the activation barrier height of the reaction, but higher than the mean thermal vibrational energy of atoms, which results in a huge acceleration of the reaction in the vicinity of the DB [228]. For example, for the typical DB energy of the order of 0.5 eV, the reaction rate in the DB vicinity at 300 K

increases by eight orders of magnitude [229]. In this case, the observed rate of phase transitions depends on the DB concentration and increases by 4 to 5 orders of magnitude, in accordance with experimental data [228–230].

The contribution of DBs to the kinetics of radiation-induced reactions is especially large [231]. This is explained by the fact that radiation efficiently excites DBs due to localized displacements of atoms from the equilibrium positions. If the displacement is large, a Frenkel pair containing a vacancy and an interstitial atom appears or a cascade of initially knocked-out atoms is observed, whose evolution is studied in the physics of radiation damage to crystals. The threshold energy of the Frenkel pair formation is about 10 eV. There-fore, the greater part of the energy of incident particles is spent to excite vibrational displacements of atoms, i.e., to the formation of DBs. As a result, not only does the radiation-induced acceleration of chemical reactions occurs but qualitatively new reactions and phase transformations appear that are not related to crystal heating.

For example, the interaction of mobile DBs with vacancy pores results in knocking out the vacancies from them, i.e., in dissolving the pores, called radiative annealing [232] because its rate is determined by the radiation intensity rather than the crystal temperature. Moreover, the natural anisotropy of the propagation of quodons in a crystal (along close-packed crystallographic directions) leads to a selective dissolving of pores, resulting in the formation of a superlattice of pores copying the crystal lattice (the bcc lattice of pores in bcc metals, the fcc lattice in fcc metals, and a planar ordering of pores in HCP crystals, where DBs propagate in basis planes) [232, 233].

Another example of the qualitative difference of phenom-ena related to the radiation-induced formation of DBs from known phenomena caused by radiation damage is the radiation-induced plastification (RIP) of metals [234, 235]. Radiation defects lead to the well-known radiation hardening (and thereby brittleness) of materials of atomic reactors, which occurs due to the stopping of dislocations on structural defects. Such a radiation hardening accumulates for many years and represents a severe technological problem.

At the same time, irradiation leads to the instant weakening of a material (RIP) due to the alleviation of the detachment of dislocations from stoppers caused by interac-tion with DBs [234, 235]. This effect is reversible, disappear-ing outside the reactor. For this reason, RIP was ignored by the radiative scientific community despite direct experimental observations of this phenomenon in reactors [236]. Recently, due to understanding the physics of this phenomenon and its relation to DBs, interest in it was rekindled and a number of experimental studies of RIP were performed in laboratories [235].

The list of new studies of the role of DBs in radiation physics is increasing. For example, phase transformations were investigated in [237] and the radiation growth of HCP metals was studied in [238], where old problems were analyzed using a new approach.

6. Conclusions

In this review, we presented the main advances in the study of DBs in crystals and considered classic work performed over the last three decades, which has laid the theoretical foundation for studying DBs in crystals. Most of these studies were performed for model low-dimensional discrete

nonlinear systems with greatly simplified potentials, which allowed the use of mathematical methods for the analysis. The main goal of these studies was to prove the existence of DBs in a variety of nonlinear discrete systems.

Passing to the study of DBs in real crystals involves the development of experimental work and increasing the role of numerical methods, because the possibilities of analytic methods with the use of realistic interatomic potentials or in quantum mechanical calculations are scarce. The focus of studies is shifting from the search for general laws governing various nonlinear discrete systems to the analysis of the specific features of DBs in particular crystals. It is this problem that should be solved in order to explain the role of DBs in the formation of the properties of real crystals and the development of applications of DBs in new technologies.

We outline the scope of further possible investigations aimed at elucidating some problems concerning DBs, which have been poorly studied so far.

(1) The development of methods for exciting DBs in crystals and molecular dynamics calculations. There are a number of approaches for searching for the initial conditions generating long-lived localized vibrations, for example, by using the rotation wave approximation [60], the gradient descent method [219], the spontaneous excitation of chaotic DBs due to the modulation instability of certain vibrational modes [57, 60, 122, 189–195], and by the rapid removal of thermal vibrations from the computation cell [107] or superposition of bell-shaped functions on certain short-wavelength phonon modes in the nonlinear regime [46, 239–241]. The complexity of this problem is that the same crystal can support DBs of different types (see Figs 8 and 9) [80].

(2) The determination of the main properties of DBs in crystals with different types of coupling at zero temperature: their minimal and maximal energies, the frequency and vibrational amplitude ranges, spatial localization degrees, the ability or inability of the elastic strain fields produced by them to move in crystals, etc. The main tool for solving these problems can be the molecular dynamics method.

(3) *Ab initio* calculations for refining data obtained by the molecular dynamics method. To date, only a few calculations have been performed for DBs in low-dimensional crystals using the density functional theory [73, 219, 220], which is explained by time-consuming computations. Nevertheless, computations with the use of the density functional theory are more convincing than molecular dynamics calculations because, unlike the latter, they are independent of empirical interatomic potentials.

(4) The estimate of the probability of the thermofluctuation generation of DBs in crystals, the determination of the concentration and lifetime of DBs under thermal equilibrium conditions, the development of numerical methods for DB identification on the background of thermal vibrations of the lattice in molecular dynamics computations.

(5) The study of the DB contribution to the physics of crystals far from equilibrium under strong external actions. Because DBs are nonlinear vibrational modes, they are most likely generated under strong external actions (irradiation, rapid heating, the flow of a high-density electric current, plastic deformation, phase transitions, etc.) when the crystal receives energy in large portions [55, 229, 231, 242]. Therefore, it is reasonable to assume that the role of DBs considerably increases in processes far from thermodynamic equilibrium.

(6) The estimate of the DB contribution to the electric charge [174–183, 186] and magnetic moment [122] transfer, heat capacity and heat conductivity [106–109], thermal expansion [187], and other properties of crystals.

(7) The study of the DB involvement in the generation of defects and the interaction of DBs with crystal defects [95, 96, 153–155].

(8) Experimental studies of DBs in crystals, which remain especially important. The most direct investigation method of DBs is the analysis of spectra of different waves interacting with a crystal (see Section 3). As the amount of information on the influence of DBs on the properties of crystals increases, it will be possible to indirectly identify DBs by measuring physical properties sensitive to the presence of DBs.

The solution of these problems will draw us closer to the elucidation of the role of DBs in solid state physics.

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