Invited Paper

Discrete breathers in metals and ordered alloys

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Abstract: It has been rigorously proved that nonlinear lattices can support spatially localized and periodic in time vibrational modes called either discrete breathers (DBs) or intrinsic localized modes (ILMs). DB does not radiate its energy because its frequency does not belong to the spectrum of small-amplitude running waves (phonons). Discreteness and nonlinearity are often said to be the two major necessary conditions for the existence of DBs. Interatomic interactions are nonlinear and the discovery of DBs in crystals, which are nonlinear lattices at the atomic scale, was just a question of time. The first successful attempt to excite DB in alkali-halide NaI crystal in molecular dynamics simulations dates back to 1997. However, the first report on DBs in pure metals was delayed till 2011. In this review we discuss the reason of this delay, describe the latest results on DBs in pure metals and ordered alloys, and outline the open problems in this area.

Key Words: discrete breather, intrinsic localized mode, metal, ordered alloy, nonlinear lattice dynamics, molecular dynamics

1. Introduction

Discrete breather (DB) is a spatially localized and time-periodic vibrational mode in a defect-free nonlinear lattice [1–3], e.g., in a crystal lattice. In a number of studies it has been shown that DBs are ubiquitous in crystals [4–8] and nowadays the focus of studies shifts to the analysis of the specific features of DBs in particular crystals. This problem should be solved in order to explain the role of DBs in the formation of the properties of real crystals and to possibly develop new DB-based technologies.

DB does not radiate its energy because its frequency is outside the spectrum of small-amplitude running waves (phonons) of the crystal. Thus, in the discussion of DBs in crystals there are two important issues, firstly, what is the structure of the phonon spectrum of the crystal and secondly, how DB frequency can leave the spectrum. Phonon spectra of crystals with simple structure, e.g., pure metals, do not possess gaps, meaning that such crystals can support only DBs with frequencies above the phonon spectrum. On the other hand, crystals with complex structures can have gaps in...
the phonon spectrum, allowing the existence of DBs with frequencies within the gaps, so called gap DBs. DB frequency leaves the phonon spectrum due to nonlinearities in the interatomic interactions, owing to the fact that in nonlinear systems vibration frequency is amplitude dependent. It is said that DB demonstrates a hard (soft) type of nonlinearity when its frequency increases (decreases) with the amplitude. Obviously, soft nonlinearity type DBs are possible only in the crystals having a gap in the phonon spectrum. Typically, frequency of a soft nonlinearity DB splits out from the upper edge of the gap and, with growing amplitude, goes deeper inside the gap. Gap DB can also have hard type nonlinearity, with frequency splitting out from the lower edge of the gap and growing inside the gap with increasing amplitude. In crystals with gapless spectrum only hard type nonlinearity DBs can exist.

A natural question arises: what type of nonlinearity, hard or soft, is typical for interatomic bonds in crystal lattices? The starting point in this discussion is the observation made by Kiselev et al. [9], where the one-dimensional (1D) monatomic and biatomic crystals were considered [see Fig. 1(a,b)] with the atoms interacting via one of the five pairwise interatomic potentials: polynomial $K_2 - K_3 - K_4$, Toda, Born-Mayer, Lennard-Jones and Morse. Note that the polynomial and Toda potentials produce interatomic forces not vanishing with increasing interatomic distance and thus, they cannot be used for modelling long-range interactions. On the other hand, three other tested potentials are widely used for this purpose. The main result of [9] is that the Born-Mayer, Lennard-Jones and Morse realistic potentials produce soft type of nonlinearity and do not support localized modes with frequencies growing above the phonon spectrum. Considering biatomic crystal with a gap in the phonon spectrum [see Fig. 1(c)] the authors were able to excite gap DBs with the soft nonlinearity type. The conclusion has been made that typical interatomic potentials produce soft type nonlinearity modes and it is unlikely to find DBs in crystals with gapless spectra [9] (e.g., in pure metals). The attention of researchers turned to the crystals possessing gap in the phonon spectrum. The first successful attempt to simulate DB was devoted to the NaI alkali halide crystal with ionic interactions [10]. For the same crystal, a series of experiments attempting to find DBs in thermal equilibrium at elevated temperatures has been done [11].

However, it should be pointed out that all realistic potentials have an inflection point where second derivative with respect to interatomic distance changes sign from positive to negative, so that the rigidity of the potential is hard at small distances and soft at large. The fact that the realistic interatomic potentials have a hard core and a soft tail is related to the structure of atoms having a compact nucleus and soft electron clouds. At large distances the atoms interact mostly via electrons, while at small distances their nuclei play a more significant role. One can expect that if the soft tail contributes more to the dynamics of a particular vibrational mode than the mode frequency will decrease with amplitude and the opposite will happen if the hard core is more involved.

To demonstrate this let us consider the 1D chain of identical atoms of unit mass where each particle interacts with the nearest neighbors via potential $U(r)$, where $U$ is the potential energy and $r$ is the distance between two atoms. Let $x_n(t)$ be the coordinate of the $n$th particle which is an unknown
Fig. 2. (a) Staggered vibrational mode in 1D monatomic crystal. All atoms oscillate with the same amplitude, $A$, each out-of-phase with the nearest neighbors. (b) Frequency (left ordinate) and distance between vibration centers of neighboring atoms (right ordinate) as the functions of $A$ in the case of zero external pressure. (c) Frequency (left ordinate) and pressure (right ordinate) as the functions of $A$ in the case of constant volume ($h = 1$).

function of time $t$. Dynamics of the chain is described by the following equations of motion

$$
\frac{d^2 x_n}{dt^2} = U' (x_{n+1} - x_n) - U' (x_n - x_{n-1}).
$$

(1)

Interatomic interactions are described by the Morse potential, which is the softest potential among those considered in the work [10],

$$
U(r) = D(e^{-2\alpha(r-r_m)} - 2e^{-\alpha(r-r_m)}),
$$

(2)

where $D$, $\alpha$, and $r_m$ are the potential parameters. The function $U(r)$ has a minimum at $r = r_m$, the binding energy (the depth of the potential) is equal to $D$ and $\alpha$ defines the stiffness of the bond. We take $D = 1$, $r_m = 1$, and $\alpha = 5$.

In the frames of this model the dynamics of the staggered mode shown in Fig. 2(a) (all particles oscillate with the same amplitude $A$, each out-of-phase with the nearest neighbors) is studied for the two cases. In the first case the interatomic distance $h$ is the function of the mode amplitude $A$, so that the chain is under zero external pressure. In the second case distance between vibration centers of the atoms is fixed, $h = 1$, and then for $A > 0$ one has positive pressure $p$. In Fig. 2(b), the mode frequency $\omega$ and the interatomic distance $h$ are shown as the functions of amplitude for the first case. It can be seen that $\omega$ decreases with growing $A$ so that the staggered mode demonstrates the soft type nonlinearity. However, in the second case [see Fig. 2(c)], frequency $\omega$ (and pressure $p$) increase with $A$. This happens because under the constant volume condition the hard core of the Morse potential contributes more to the dynamics of the mode, while in the case of zero pressure, when distance between vibration centers of the atoms increases, one has a larger contribution from the soft tail.

It is clear why a DB cannot be excited in monatomic 1D Morse lattice. Any spatially localized vibrational mode of large amplitude would cause local “thermal expansion” with increasing distance between vibrational centers of atoms. Then the soft tail of the potential would play a more important role than the hard core and the frequency of such mode would not grow with amplitude and would not leave the gapless phonon spectrum.

It turned out that this result is strictly one-dimensional. Already in 2D Morse lattice there are different possibilities to suppress “thermal expansion” in the core of the DB and its frequency can grow with amplitude above the phonon spectrum, making DB robust and long-lived.

One such possibility to excite a DB in 2D Morse lattice is presented in Fig. 3. A rod-like DB is excited in a close-packed atomic row, as shown in Fig. 3(a). Obviously, the atoms in the core of the DB cannot expand freely because the atomic row where DB is excited experiences the action of the periodic on-site potential induced by the surrounding atoms. In Fig. 3(b) a schematic picture of the
atomic chain in the periodic on-site potential is shown. Due to the action of the on-site potential the core of the Morse potential contributes more to the dynamics and frequency of this DB is above the gapless phonon spectrum [12, 13].

In fact, it is possible to obtain another, high-symmetry DB in 2D monatomic Morse lattice [14], as it is shown in Fig. 4(a). This DB also has frequency above the phonon spectrum because the “thermal expansion” of its core is suppressed by the surrounding part of the crystal.

Let us calculate the pressure on the DB core from the surrounding media. Note that far from DB center displacements of atoms are small and one can apply linear elasticity theory to calculate the radial displacement $u(R)$ and the radial $\sigma_{RR}(R)$ and circumferential $\sigma_{\theta\theta}(R)$ stress components as the functions of the distance from the DB center, $R$ [see Fig. 4(b)]. Considering the plane-stress problem for the elastic media having the Young modulus $E$ and the Poisson’s ratio $\nu$, and taking into account the radial symmetry of the problem, one can write the equilibrium equation in terms of the radial displacement as follows [15]

$$\frac{d^2 u}{dR^2} + \frac{1}{R} \frac{du}{dR} - \frac{u}{R^2} = 0.$$  \hfill (3)

Suppose the DB core has radius $a$ and it creates pressure $p$ on the outer elastic media. The calculations are done for the elastic ring of outer diameter $b$. General solution to (3) is

$$u = C_1 R + \frac{C_2}{R},$$  \hfill (4)

where the integration constants

$$C_1 = \frac{1 - \nu}{E} \frac{a^2 p}{b^2 - a^2}, \quad C_2 = \frac{1 + \nu}{E} \frac{a^2 b^2 p}{b^2 - a^2},$$  \hfill (5)

were chosen to satisfy the boundary conditions for the radial stress at the inner and outer radii of the ring, $\sigma_{RR}(a) = -p$, $\sigma_{RR}(b) = 0$, respectively. In the limit $b \to \infty$ one has $C_1 = 0$, $C_2 = a^2 p (1 + \nu) / E$. Taking this and (4) into account the solution of the problem reads
\[ u = a^2 p \left( 1 + \nu \right) \frac{1}{E} \frac{1}{R^1}, \quad \sigma_{RR} = -\sigma_{\theta \theta} = -p \frac{a^2}{R^2}, \]  

(6)

where stress components were found from the relation between displacement and strains and the Hooke law [15].

It can be seen from (6) that the DB creates long-range radial displacements that decrease rather slowly with the distance from DB center, as \( R^{-1} \). Stresses decrease as \( R^{-2} \). Radial compressive stress \( \sigma_{RR} \) does not allow the free expansion of the DB core, making the contribution of the hard core of the Morse potential sufficient for the hard type nonlinearity DB to exist [12, 14].

Note that in 3D crystal similar consideration of a DB with spherical symmetry and under assumption of isotropic elastic media (though in 3D case all crystals are anisotropic) the equilibrium equation in terms of the radial displacement obtains the form

\[ R \frac{d^2 u}{dR^2} + 2 \frac{du}{dR} - \frac{2}{R} u = 0. \]  

(7)

The solution reads

\[ u = a^3 p \left( 1 + \nu \right) \frac{1}{2E} \frac{1}{R^2}, \quad \sigma_{rr} = -2\sigma_{\theta \theta} = -p \frac{a^3}{R^3}. \]  

(8)

In 3D case the radial displacements decrease as \( R^{-2} \) and stresses as \( R^{-3} \), which is faster than in the 2D case. From this result one can conclude that in 3D Morse crystals it is even easier to obtain DBs with frequencies above the phonon spectrum because the suppression of “thermal expansion” by the surrounding elastic media is more efficient than in two dimensions.

We thus conclude that in 2D and 3D crystals, described by realistic interatomic potentials with a hard core and soft tail, hard-type nonlinearity DBs can exist because “thermal expansion” of the DB core is suppressed by the surrounding part of the crystal and the hard core of the interatomic potential contributes more to the DB dynamics than the soft tail.

In Sec. 2 and Sec. 3 the review of the results on DBs in pure metals and in ordered alloys, respectively, is given. Finally, Sec. 4 contains concluding remarks and poses some open problems.

2. DBs in pure metals

Haas et al. were the first who have succeeded in excitation of DBs in pure metals, particularly, in fcc Ni and bcc Nb [16]. DBs they have excited had rod-like structure similar to that shown in Fig. 3(a), and they were able to move along the close packed atomic row. This revolutionary result has demonstrated for the first time that realistic interatomic potentials can produce localized vibrational modes with hard type nonlinearity in non-covalent crystals. They have legitimized the research on DBs in a very broad class of practically important materials, namely, in pure metals. The authors explained the existence of hard type nonlinearity DBs in metals noting that the odd anharmonicity is strongly reduced due to the screening of the ion-ion interaction by the conducting electrons [17]. This is additional source of bond hardening but, as it was shown in Sec. 1, even classical Morse potential is sufficiently hard if its core contributes to the dynamics more than tail.

2.1 How to excite a DB?

DBs can be highly localized, e.g., gap DBs are localized practically on a single atom in graphane and in the NaCl family ionic crystals with considerable difference in atomic masses of anions and cations [18–20]; in strained graphene DB is localized on a pair of carbon atoms vibrating out-of-phase [21–23]. Such DBs are very easy to excite, e.g., by initial displacement of one or two atoms that have large vibration amplitudes. However, DBs in metals are much less localized [images can be seen in Fig. 3(a) and Fig. 4(a)] and excitation of such collective vibrational modes in molecular dynamics simulations is a challenge. Particularly, in the pioneering work, to excite a rod-like DB in Ni, initial displacements were given to eight atoms in a close-packed atomic row [16]. In order to boost the DB, an asymmetry was introduced in the initial displacements.

One consistent way to find proper initial conditions to excite a DB is to start from the analysis of zone-boundary phonon modes in nonlinear regime. For those extended modes whose frequency leaves
Fig. 5. (a,b) Standing DB in bcc vanadium presented by the amplitudes $T_n$ and displacements of vibration centers $S_n$ of the atoms of the close-packed atomic row where DB is excited, see (11). (c) Moving DB in vanadium presented by the functions $\Delta x_n(t)$. The DBs were excited with the following parameters of the ansatz (9), (10): (a,b) $A = 0.45\text{Å}$, $B = 0.14\text{Å}$, $\beta = 0.7$, $\gamma = 0.9$, $\phi_0 = 0$, $x_0 = 1/2$, $\delta = 0$; (c) same but $\delta = 0.3\pi$.

phonon spectrum at large vibration amplitudes, a bell-shaped function can be used to cut a localized mode. This approach was shown to be very efficient to excite DBs in 2D Morse crystal [24].

For the excitation of standing and moving rod-like DBs, an ansatz (physically motivated assumption about the form of the solution) with a few physically meaningful parameters was offered [12]. Atoms in a close-packed atomic row are numbered by the index $n$. In fcc, bcc, and hcp crystals such rows have [011], [111], and [11¯20] crystallographic directions, respectively. It is convenient to choose $x$ axis of the Cartesian coordinate system along a close-packed direction. To excite a moving rod-like DB the initial displacements and velocities can be set for the atoms of a close-packed atomic row as follows

$$x_n(t) = \cos[\omega t + \phi_0 + \delta n]T_0^n + S_0^n, \quad \dot{x}_n(t) = -\omega \sin[\omega t + \phi_0 + \delta n]T_0^n,$$

$$y_n(0) = 0, \quad \dot{y}_n(0) = 0, \quad z_n(0) = 0, \quad \dot{z}_n(0) = 0,$$

while all other atoms in the computational cell are in their equilibrium positions and have zero initial velocities. The atoms are excited with the vibration amplitudes $T_0^n$ and initial static displacements $S_0^n$, the latter is to take into account the effect of “thermal expansion” in the DB core. Vibrations are initiated with the frequency $\omega$ lying above the phonon band, the initial phase $\phi_0$, and the phase difference for neighboring atoms $\delta$. Both $T_0^n$ and $S_0^n$ are exponentially localized

$$T_0^n = \frac{(-1)^n A}{\cosh[\beta(n - x_0)]}, \quad S_0^n = \frac{-B(n - x_0)}{\cosh[\gamma(n - x_0)]},$$

where $A$ is the DB amplitude, $B$ defines the amplitude of displacements of the vibration centers of the atoms, $\beta$ and $\gamma$ define the degree of spatial localization of DB, $x_0$ is the DB initial position. For $x_0 = 0$ the DB is centered on a lattice site, while for $x_0 = 1/2$ in the middle between two neighboring lattice sites. The DB velocity depends on $\delta$, and for $\delta = 0$ it is equal to zero. Sign of $\delta$ defines the direction of DB motion.

DB amplitude $A$ is a free parameter whose maximal possible value is typically of order of 10% of the interatomic distance. $\delta$ is also a free parameter with a typical maximal value of order of 0.01$\pi$. For chosen $A$ and $\delta$ proper values of $B$, $\beta$, and $\gamma$ should be found. Very often $\beta \approx \gamma$.

It should be noted that the ansatz (9), (10) is not an exact solution to the equations of atomic motion. That is why, a part of energy given to the system at $t = 0$ is radiated in the form of small-amplitude extended waves and then a stable and robust moving DB emerges, if the parameters in (9), (10) are properly chosen.

The functions $T_0^n$ and $S_0^n$ in (10) describe the initial amplitudes and displacements of the vibration centers of the atoms. These quantities can be calculated for each period of DB oscillation as

$$T_n = \frac{x_{n,\text{max}} - x_{n,\text{min}}}{2}, \quad S_n = \frac{x_{n,\text{max}} + x_{n,\text{min}}}{2},$$
where \( x_{n,\text{max}} \) and \( x_{n,\text{min}} \) are the maximal and minimal values of the (quasi)periodic function \( x_n(t) \) that describes the motion of \( n \)th atom of the close-packed atomic row.

### 2.2 Examples of rod-like DBs

The ansatz (9), (10) was successfully used to excite DBs in pure metals such as bcc V, Fe and W [25], hcp Be, Zr, Co, and Mg [26–28].

As an example, in Fig. 5 standing DB in vanadium is presented by the functions (a) \( T_n \) and (b) \( S_n \) (11) showing for the close-packed atomic row the vibration amplitudes and the shifts of the vibration centers of the atoms, respectively. Parameters of the ansatz (9), (10) are \( A = 0.45\text{Å}, B = 0.14\text{Å}, \beta = 0.7, \gamma = 0.9, \phi_0 = 0, x_0 = 1/2, \delta = 0. \) The inter-site DB is localized on six atoms. Its frequency lies above the phonon spectrum, increasing with the DB amplitude. Maximal \( S_n \) is about four times smaller than maximal \( T_n \). If in (9) instead of \( \delta = 0 \) one sets \( \delta = 0.3\pi \), then moving DB is excited, as shown in Fig. 5(c) by the functions \( \Delta x_n(t) \). DB velocity increases nearly linearly with \( \delta \) and reaches a maximal possible value at \( \delta = 0.3\pi \) equal to 14 Å/ps, which is 0.31 of the speed of sound. DBs in vanadium are very mobile, while in other metals maximal DB velocity is about 0.1 of the sound velocity [25].

Next example is the rod-like DB in \( \alpha \)-uranium [29]. This metal has unique orthorhombic structure presented in Fig. 6(a). In Fig. 6(b) phonon density of states (DOS) separated into \( x, y \), and \( z \) components are presented. Straight atomic rows in \( \alpha \)-uranium are oriented along \( x \) direction, however, the shortest interatomic distance is between the atoms \( A \) and \( B \) (or \( A' \) and \( B' \)). The shorter is the interatomic bond the higher is its stiffness. That is why, DOS for the \( x \)-component has maximal frequency of 4.8 THz, while that for \( y \) and \( z \) have higher maximal frequency of 5.0 THz. In the rod-like DB atoms of a straight atomic row oscillate along \( x \) axis out-of-phase with the nearest neighbors, and this short-wavelength mode interacts with the phonons in the \((x, y)\)-plane very weakly. This is the reason for the existence of DBs in \( \alpha \)-uranium [29]. In Fig. 6(c) standing DB is shown excited with the help of the ansatz (9), (10) with parameters \( A = 0.55\text{Å}, B = 0.38\text{Å}, \beta = 0.67, \gamma = 0.75, \phi_0 = 0, x_0 = 1/2, \delta = 0. \) For small amplitudes DB frequency is above the \( x \)-component phonon DOS but within the \( y \)- and \( z \)-component DOS. DB frequency increases with the amplitude and at larger amplitudes it is above the cumulative phonon spectrum. Mobility of DBs in \( \alpha \)-uranium is very low [29].

More examples of moving rod-like DBs in fcc Ni and Cu as well as in bcc Fe can be found in [7, 17].

### 2.3 DBs and crystal lattice defects

Crystal lattice defects to a large extent define mechanical and physical properties of metals. The first studies of the DB interaction with the vacancy were carried out in the framework of a 1D
Fig. 7. (a) Phonon DOF of Pt₃Al. (b) Schematic picture of the initial shifts applied to two nearest Al atoms to excite moving DB with frequency above the phonon spectrum shown in (c). Pt (Al) atoms are shown by dark (light) dots [39].

Fig. 8. Collision of moving DBs in Pt₃Al. DBs bounce off nearly elastically [39].

Frenkel-Kontorova model [30, 31]. It has been shown that a moving DB can cause vacancy migration. Moreover, a significant role in this process is played by a nonlinear vibrational mode localized on the atom adjacent to the vacancy [31]. In frame of the same model migration of interstitial atom due to the interaction with moving DB has been studied [32]. Later the collision of a rod-like moving DB with a vacancy was addressed in 2D Morse crystal to demonstrate that the DB reduces the energy barrier for vacancy migration [33].

MD simulations of recoil processes following the scattering of x-rays or neutrons have been performed for metals (Ni, Nb and Fe) [17, 34]. It has been shown that if the recoil energy exceeds tens of eVs, vacancies and interstitials can be formed, which are strongly dependent on the direction of the recoil momentum.

Interaction of moving rod-like DBs with vacancy, dislocation, and free surface in Fe has been addressed in [35]. In all cases DBs reduce the energy barriers for defect migrations promoting transformation of the defect structure in the crystal lattice.

3. DBs in ordered alloys

Before it was realized that hard type nonlinearity DBs can exist in pure metals, the gap, soft non-linearity DBs were studied in ordered alloys with a large difference in the atomic masses of the components [36–39]. The most studied is the Pt₃Al intermetallic compound having L₁₂ superstructure based on fcc lattice. In L₁₂ superstructure one of the four sublattices of cubic fcc translational cell has atoms of different type than the three others.
Fig. 9. Collision of moving and standing DBs in Pt$_3$Al. As a result of collision moving DB looses some energy to radiation and to amplify the standing DB [39].

Morse potentials written in the form

$$\phi_{PQ}(r_{ij}) = D_{PQ} \beta_{PQ} \exp(-\alpha_{PQ} r_{ij})[\beta_{PQ} \exp(-\alpha_{PQ} r_{ij}) - 2],$$

were employed. Parameters of the potentials were fitted to reproduce the lattice parameter, sublimation energy, and the bulk elastic modulus of the alloy. The following values were obtained: $\alpha_{PtPt} = 1.638 \text{ Å}^{-1}, \beta_{PtPt} = 118.83$, $D_{PtPt} = 0.685$ eV, $\alpha_{AlAl} = 1.287 \text{ Å}^{-1}, \beta_{AlAl} = 57.932$, $D_{AlAl} = 0.247$ eV, $\alpha_{PtAl} = 1.138 \text{ Å}^{-1}, \beta_{PtAl} = 39.085$, $D_{PtAl} = 0.481$ eV.

A wide gap in the phonon spectrum of the alloy [see Fig. 7(a)] appears due to the large difference in the atomic masses of the components: $M_{Pt} = 195.23$ a.m.u. and $M_{Al} = 26.97$ a.m.u. Equilibrium interatomic distance is 2.83 Å, fcc lattice parameter is 3.99 Å.

In the work [39] two types of DBs were analyzed, the standing gap DB and the moving DB with frequency above the phonon spectrum. Standing DB is localized on single Al atom vibrating along a close-packed direction. It was excited simply by applying initial shift to this atom along close-packed direction. Standing DB has soft type nonlinearity with frequencies in the phonon gap. Moving DBs were excited by initial displacements applied to two nearest Al atoms located in one close-packed atomic row in the opposite directions, as schematically shown in Fig. 7(b). The absolute values of the displacements must be different to boost the DB. Due to inaccuracy of the initial conditions, a part of the energy initially given to the system was radiated and a robust moving DB was formed. The DB is localized on about four or five Al atoms in one close-packed atomic row, as schematically depicted in Fig. 7(c). These atoms oscillate nearly in phase with the frequencies above the phonon spectrum. Remarkably, one crystal is able to support both soft and hard type nonlinearity DBs.

Collisions between moving and moving and standing DBs were analyzed, see Fig. 8 and Fig. 9, respectively. Moving DBs collide nearly elastically bouncing off each other. When moving DB hits the standing DB, a part of energy is radiated and some portion of energy is given to the standing DB, so that its amplitude after the collision is somewhat larger than before the collision.

In the work [38] three different types of initial atomic displacements were analyzed to obtain different spatially localized vibrational modes in Pt$_3$Al ordered alloy (see Fig. 10, where heavy Pt atoms are shown darker than light Al atoms). The authors have succeeded in excitation of (a) rod-like DB where Al atoms in a close-packed atomic row move out-of-phase with nearest neighbors; (b) rod-like DB with the Al atoms vibrating in-phase; and (c) all Al atoms in the atomic row vibrate with equal amplitudes out-of-phase with the nearest neighbors. Frequency of the mode shown in Fig. 10(c) as the function of amplitude is shown in Fig. 11 by the line 1 connecting the numerical data points. The modes shown in Figs. 10(a) and (b) have very close frequency-amplitude dependencies shown by the curve 2 in Fig. 11. Thus, all three vibrational modes demonstrate hard type nonlinearity with frequencies above 93.
the optic phonon band. Recall that the Pt$_3$Al crystal supports soft type nonlinearity DB localized on a single Al atom. Its frequency-amplitude relation is plotted by the line 3 in Fig. 11.

An interesting phenomenon was observed in [38]. As the result of modulational instability of the vibrational mode shown in Fig. 10(c), the formation of soft type nonlinearity DBs was observed. This is illustrated in Fig. 12 where the kinetic energy of one vibrating Al atom is shown as the function of time by gray line. Black line shows kinetic energy of a Pt atom belonging to the row. The instability of mode shown in Fig. 10(c) develops within about 13 ps and after that the transformation of the vibrational mode takes place, which takes about 1 ps. As a result, a chain of gap DBs is formed vibrating at frequencies lower than the initial mode frequency.

The results of work [38] suggest that in ordered alloys with a gap in the phonon spectrum it is possible to excite many different types of nonlinear vibrational modes.
4. Conclusions

The results presented in this review can be summarized as follows.

1. Realistic interatomic potentials have a hard core and a soft tail reflecting the structure of atoms that have compact nuclei and soft electron clouds. Because of the asymmetry of the nonlinear potentials, at large vibration amplitudes the average distance between atoms tends to increase. However, in 2D and 3D crystals “thermal expansion” of the DB core is suppressed to some extent by the surrounding media. Since free expansion of the DB core is not possible, the hard core of the interatomic potential contributes to the DB dynamics more than the soft tail. As a result, DB frequency can grow with amplitude above the phonon spectrum.

2. Even simple 2D Morse lattice can support at least two different types of DBs, as shown in Fig. 3(a) and Fig. 4(a). 3D fcc metals can support at least three types of DBs. In ordered alloys with a gap in the phonon spectrum the variety of possible DBs should be even greater. Thus we come to the problem of a systematic search for the DBs of different type in pure metals and ordered alloys. Properties of various DBs (mobility, degree of spatial localization, lifetime, range of possible frequencies, amplitudes, and energies, etc.) should be described and analyzed.

3. The results of MD simulations of DBs are very sensitive to the interatomic potentials. It is thus of crucial importance to use \textit{ab initio} simulations to verify the accuracy of the MD results.

4. Crystal lattice defects play a very important role in the physics of metals. The possible role of DBs in the nucleation or motion of defects should be uncovered. For this, the interaction of DBs with lattice defects and DB collisions with each other should be studied in detail for various metals.

5. Effect of temperature on DB properties and spontaneous excitation of DBs in thermal equilibrium at elevated temperatures are the issues of great importance for the physics of metals.

Overall, it is important to find the similarities and the differences between DBs in different metals and alloys. This will help to find technological applications for DBs.

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