

Surface discrete breathers in Pt₃Al intermetallic alloy

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ABSTRACT

It is known that defect-free crystals can support spatially localized, large amplitude vibrational modes with frequencies outside the linear phonon spectrum. Such excitations are called discrete breathers (DB) or intrinsic localized modes. So far, for 3D crystals DB were considered only in the bulk. In the present molecular dynamics study, for the first time, we demonstrate that DB can be excited at the low Miller indices surfaces of the Pt₃Al intermetallic alloy. It is shown that properties of the DB depend essentially on the surface orientation and termination, as well as on DB polarization. The study of DB at crystal surfaces is important because they can localize energy of order of 1 eV, which can reduce the potential barrier for local structure transformation or a chemical reaction.

1. Introduction

Discrete breathers (DB) are high amplitude localized vibrational modes in perfect nonlinear lattices. They have been analyzed in the pioneering studies [1,2] that have initiated a great research activity summarized in the reviews [3,4]. Since the last decade, DB have been actively investigated in solid state physics and material science [5–28]. In experimental works DB are detected in crystals by measuring their vibrational spectra [6], but these results are still debated [7]. Experimental detection of DB in crystals is a challenging task because of their sub-nanometer size and short lifetime in presence of thermal fluctuations. That is why atomistic simulations are very useful in the study of DB properties in crystals [5]. With the help of molecular dynamics DB have been analyzed in pure metals [8–12], in model crystals with Morse interactions [13,14], in diamond [15], in graphene [16–20] and boron nitride [21]. First-principle simulations for DB in graphene confirm the molecular dynamics results [22]. A number of studies have been devoted to the crystals with A₃B composition with a big difference in the atomic masses of the components [23–28]. Such crystals possess a gap in the phonon spectrum and support DB with frequencies within the gap. Such DB is easy to excite since it is highly localized on a light atom.

It should be pointed out that DB are traditionally investigated in the bulk of crystals [5–18,21–28]. In some studies, vibrational modes localized at the end of a 1D chain are called DB [29–33], but rather they should be called localized surface modes or Tamm states [34–36], since DB by definition is a vibrational mode localized in a perfect lattice with translational symmetry. DB at the edge of a homogeneously stretched

graphene nanoribbon were studied in [19,20] and it was shown that the configuration of such DB differs strongly from DB inside the graphene sheet [17,22]. Note that the DB at the edge of graphene sheet exists in a one-dimensional discrete medium, with the direction of translation along the edge of the sheet. By analogy, one can search for DB close to an atomically flat (singular) surface of a three-dimensional crystal. To the best of our knowledge, so far no attempts have been made to find near-surface DB for a 3D crystal.

Near-surface DB can contribute to the physics and chemistry of surface. They localize some energy which can reduce the potential barriers for structure transformations at the surface, for creation of surface crowdions [37,38] or voidions [39] contributing to surface diffusion [40–42]. DB can accelerate chemical reactions [43]. DB at crystal surface can be excited by external driving [44–48].

In the present work molecular-dynamic study of near-surface DB is carried out for Pt₃Al crystal.

2. Simulation details

We consider the model of Pt₃Al intermetallic alloy with L1₂ superstructure based on fcc lattice. Primitive translational cell of this crystal is shown in Fig. 1a. One of the four cubic sublattices is occupied by Al atoms (blue balls) and the other three by Pt atoms (brown balls).

Three surface orientations are considered with all possible terminations, as shown in Fig. 1b–f. Here large (small) balls show the atoms of the first (second) atomic plane. Surface translational cells are indicated. In Fig. 1b and Fig. 1c the surface is parallel to (100)

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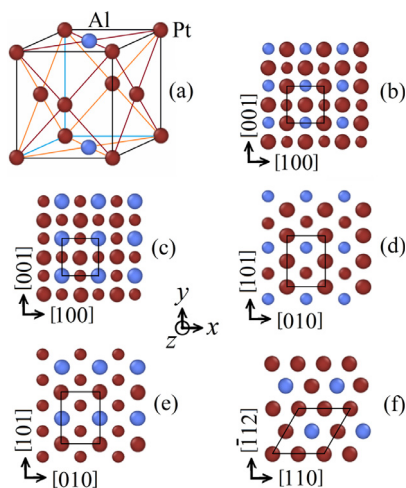


Fig. 1. (a) Primitive translational cell of Pt_3Al intermetallic alloy based on fcc lattice. One of four cubic sublattices is occupied by Al atoms (blue balls), while the other three by Pt atoms (brown balls). (b–f) Top views of the studied surfaces. Larger and smaller balls show the atoms in the first and second atomic planes, respectively. Surface translational cells are specified. Cartesian coordinate system used in the simulations is shown. (b,c) Surface parallel to (100) crystallographic plane terminated by Pt atoms and by atomic plane with composition PtAl , respectively. (d,e) Surface parallel to (110) crystallographic plane terminated by Pt atoms and by atomic plane with composition PtAl , respectively. (f) Surface parallel to (111) crystallographic plane. All (111) atomic planes have composition Pt_3Al . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

crystallographic plane. In the former case it is terminated by Pt atoms, while in the latter case the first atomic plane has composition PtAl . In Fig. 1d and Fig. 1e the surface is parallel to (110) crystallographic plane and it is terminated by Pt atoms and by the atomic plane with composition PtAl , respectively. In Fig. 1f the surface is parallel to (111) crystallographic plane and the surface atomic plane has composition Pt_3Al .

The number of atoms in the system varied from about 10^5 to 2×10^5 , depending on the surface crystallographic orientation. Relatively small computational cells are sufficient for the present study since DB is highly localized on single Al atom with neighboring atoms having much smaller oscillation amplitudes.

Periodic boundary conditions are applied in x and y directions and free surfaces parallel to xy -plane are modeled on both sides of the computational cell.

The interatomic potentials for the Pt_3Al intermetallic alloy were generated by the use of the method proposed by Zhou [49], which is based on the embedded atom method (EAM) [50]. Potentials used in this study are fitted to reproduce basic properties of the alloy such as lattice constant, elastic moduli, sublimation and defects formation energies, demonstrating satisfactory agreement with the experimental values. Details of the interatomic potential development and testing are given in [24].

Homemade software is used for simulations. The equations of atomic motion are integrated with the use of the Störmer method of order six with the time step of 0.5 fs. This symplectic method belongs to a wider family of integrators, as described in [51]. For a typical numerical run relative reduction of total energy of the system was not greater than 10^{-8} .

Before excitation of DB the crystal structure with free surfaces is relaxed with the use of the steepest descent method to obtain equilibrium surface structure.

All simulations are done at 0 K, i.e., the effect of thermal fluctuations is not taken into account.

An important problem is to find initial conditions that result in excitation of a DB. Pt_3Al intermetallic alloy supports several types of DB

in the bulk [26,27]. In this study we consider the simplest one, which is localized on single Al atom and shows the soft type anharmonicity, i.e., its frequency decreases with the amplitude, being within the gap of phonon spectrum (from 5.82 to 8.45 THz). Such highly localized DB can be easily excited in the bulk by initial displacement of one Al atom with initial zero velocities for all atoms in the computational cell. The magnitude and direction of the initial displacement define the amplitude and polarization of the DB, respectively. Pt_3Al crystal supports gap DB in the bulk polarized along $\langle 100 \rangle$ crystallographic direction [25–27]. An attempt to excite a DB in the bulk with another polarization results in a very rapid decay of the vibrational mode or in a spontaneous change of oscillations to $\langle 100 \rangle$ polarization.

Note that in the present study we always choose Cartesian coordinate system with xy plane parallel to the surface and z axis normal to the surface, as shown in Fig. 1. Attempting to excite a DB near crystal surface, we apply initial displacement of different magnitude to one Al atom closest to the surface in x or y direction parallel to the surface or in the direction normal to the surface (along z axis). The direction of initial displacement defines DB polarization. All other atoms have zero initial displacements and all atoms have zero initial velocities. If the amplitude and direction of the initial displacement are chosen properly, a long-lived vibrational mode is established after a short transient period. We then measure the frequency and energy of the DB.

3. Results and discussion

3.1. (100) surface orientation

For the surface parallel to (100) plane two surface terminations are possible: the first atomic plane has (i) only Pt atoms (Fig. 1b) and (ii) equal amount of Pt and Al atoms (Fig. 1c). In the relaxed crystal, the interplanar spacing for the near-surface planes is different from the value in the bulk, as shown in Fig. 2a by triangles for Pt termination and by circles for PtAl termination. In the former (latter) case the interplanar distance near the surface is smaller (larger) than in the bulk.

Firstly we consider the case of Pt-terminated surface. If an initial displacement along x or y direction is given to a Al atom closest to the surface, a long-lived DB is excited. Lifetime of such DB can reach up to a few ns, which is above 10^4 oscillation periods. DB lifetime is defined as the time when its energy becomes 1/3 of the energy given to the system at $t = 0$. In our simulations there are two major reasons limiting DB lifetime. First is the use of very simple and thus rather poor initial conditions that produce not a DB but a quasi-DB [52]. Second reason is the initial energy burst produced by the poor initial conditions and constant energy radiation from quasi-DB. This emitted energy plays a role of thermal fluctuations that affect DB dynamics. Frequency and total (kinetic plus potential) energy of the DB as the functions of DB amplitude are shown by triangles in Fig. 2b and c, respectively. Horizontal dashed lines in Fig. 2b show the lower and the upper edges of the gap in the phonon spectrum of the crystal, 5.82 and 8.45 THz, respectively. The spectrum was calculated for the bulk crystal and it does not take into account the effect of the surface. DB amplitude can exceed 0.8 Å. DB frequency reduces with its amplitude revealing the soft type anharmonicity of this vibrational mode, and it lies within the gap of the phonon spectrum. DB energy can reach up to 2 eV. It turns out that the near-surface DB polarized along x or y direction has properties close to the DB in the bulk.

An interesting phenomenon was observed when Al atom closest to the surface was excited by initial displacement along z axis (normal to the surface). In a few picoseconds the vibrational energy of this atom was given to the Al atom just below the excited Al atom. This process is shown in Fig. 3, where displacements Δz as the functions of time are presented for the initially excited Al atom (dashed line) and for the Al atom below the excited atom (solid line). This process can be regarded as DB migration from the surface deeper into the bulk. After the DB vibrating along z axis moves deeper into the crystal, its properties

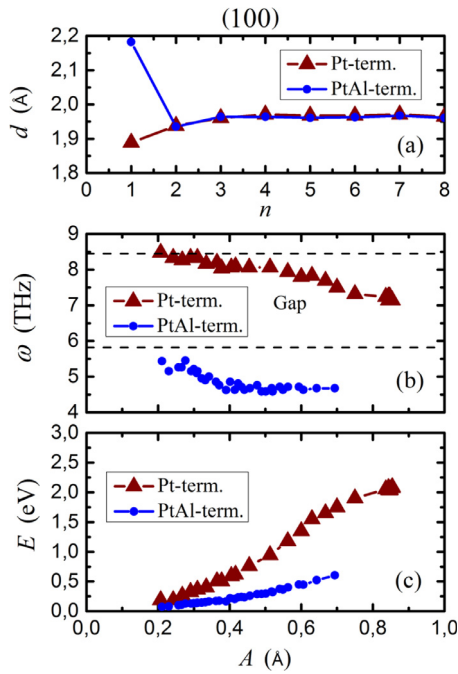


Fig. 2. Results for the surface parallel to (100) crystallographic plane. (a) Interplanar distance as the function of plane number away from the surface. (b) DB frequency as the function of its amplitude for Pt-terminated surface (triangles) and surface terminated by atomic plane with composition PtAl (circles). Horizontal dashed lines show the lower and the upper edges of the phonon spectrum gap. (c) DB energy as the function of its amplitude for Pt-terminated surface (triangles) and surface terminated by atomic plane with composition PtAl (circles).

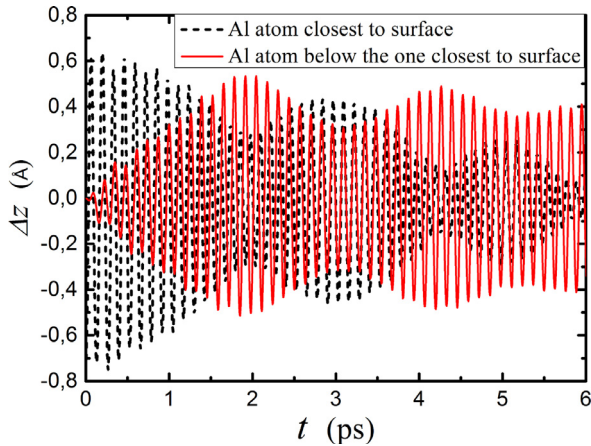


Fig. 3. Result for Pt-terminated (100) surface. Displacements Δz as the functions of time are presented for the initially excited Al atom (dashed line) and for the Al atom below the excited atom (solid line). In a few picoseconds the DB excited at the surface moves inside the crystal by one interplanar distance.

become very close to the DB in the bulk and to the DB near surface vibrating along x or y direction.

As for the PtAl-terminated surface, only DB polarized along z axis are possible, while initial displacements parallel to the xy -plane result in a fast decay of the vibrational mode and energy delocalization. Properties of the DB oscillating along z axis are shown by circles in Fig. 2b and c, respectively. Maximal DB amplitude is about 0.7 Å. As follows from Fig. 2b, DB frequency decreases with DB amplitude being within the bulk phonon spectrum. The reduction of the DB frequency can be explained by the large interplanar distance close to the PtAl surface (see Fig. 2a). Interatomic bond stiffness decreases with increase

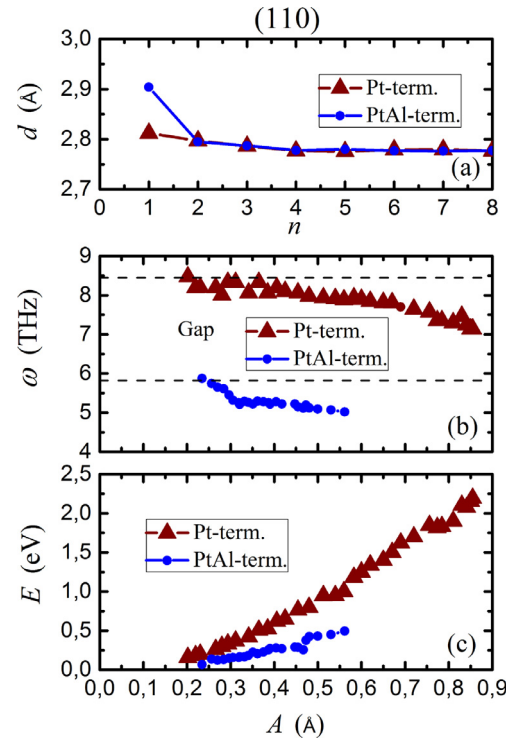


Fig. 4. Same as in Fig. 2 but for the surface parallel to (110) crystallographic plane.

in interatomic distance, resulting in softening of the DB oscillations. Maximal DB energy is about 0.6 eV.

3.2. (110) surface orientation

In this case as well, Pt-termination (Fig. 1d) and PtAl-termination (Fig. 1e) are possible. Interplanar distance close to the surface is greater than in the bulk for both terminations and this effect is more pronounced for PtAl-termination (see Fig. 4a).

For Pt-terminated surface only x -polarized DB can have very long lifetime of order of 1 ns. Properties of such DB are close to that for the DB in the bulk, as it can be seen from the data shown by triangles in Fig. 4b and c. Excitation of z -polarized DB, similar to the case of (100) Pt-terminated surface, results in DB motion inside the crystal by one interplanar distance. However the lifetime of the DB after moving inside the crystal is relatively short, about 10 ps or 10^2 oscillation periods.

For PtAl-terminated surface only z -polarized DB is long-lived. Properties of such DB are presented by circles in Fig. 4b and c. This DB also has frequencies decreasing with DB amplitude and lying within the phonon spectrum. The reason is the same as for the PtAl-terminated DB at the (100) surface. Softening occurs due to the increase in the interplanar distance close to the surface.

3.3. (111) surface orientation

For this close-packed surface only Pt₃Al-termination is possible (see Fig. 1f). In Fig. 5a the interplanar distance is shown as the function of plane number away from the surface. Close to the surface the interplanar distance is greater than in the bulk. We could not excite a DB with oscillations along z axis. Initial displacement of a surface Al atom along z axis results in a fast energy delocalization. Both x -polarized and y -polarized DB are long-lived and they have similar properties, as can be seen from Fig. 5b and c. DB can have amplitude greater than 0.6 Å and maximal energy about 0.7 eV. Frequency of small-amplitude DB lies in the gap of phonon spectrum. With growing amplitude DB frequency decreases and enters the phonon band. Again, DB softening is

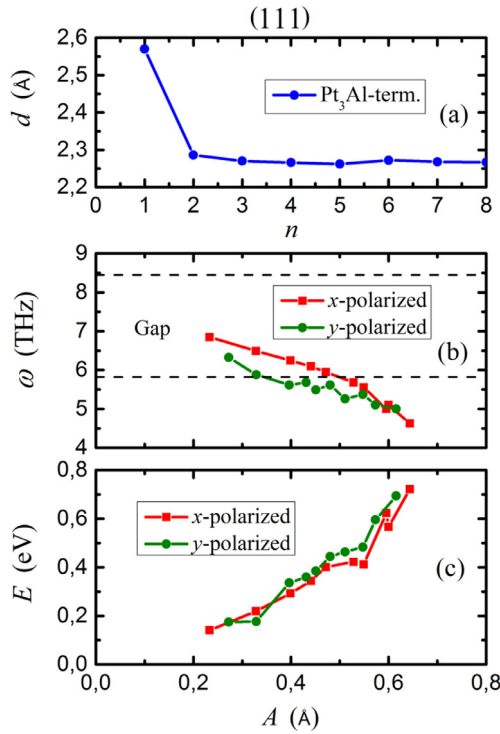


Fig. 5. Results for the surface parallel to (111) crystallographic plane. (a) Interplanar distance as the function of plane number away from the surface. (b) DB frequency as the function of its amplitude for oscillations along x axis (squares) and along y axis (circles). Horizontal dashed lines show the lower and the upper edges of the phonon spectrum gap. (c) Energy of x -polarized DB (squares) and y -polarized DB (circles) as the functions of DB amplitude.

explained by the fact that the interplanar distance close to the surface is larger than in the bulk.

It is important to provide a direct comparison of DB in the bulk with surface DB. In Fig. 6 results are presented for DB in the 1st, 2nd, and 3rd closest to the surface atomic planes with (111) orientation. Notation of the curves is given in (a). In (a) and (b) DB frequency as the function of its amplitude is given for DB polarized along x and y directions,

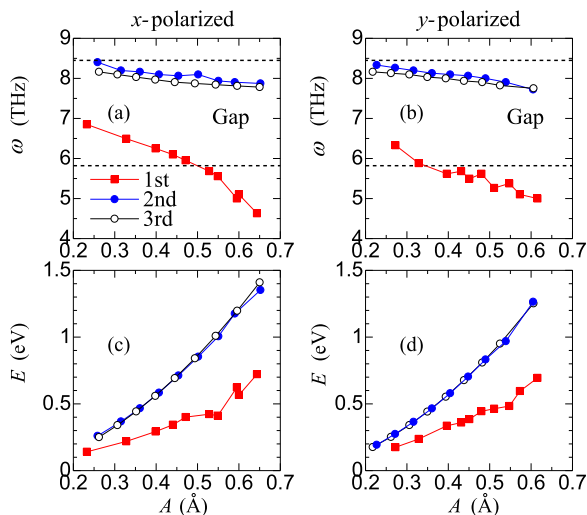


Fig. 6. Results for DB in the 1st, 2nd, and 3rd closest to the surface atomic planes with (111) orientation [see (a) for the notations of the curves]. (a,b) DB frequency as the function of its amplitude for oscillations along x and y axes, respectively. Horizontal dashed lines show the lower and the upper edges of the phonon spectrum gap. (c,d) Energy of x -polarized and y -polarized DB, respectively, as the functions of DB amplitude.

respectively. In (c) and (d), energy of DB polarized along x and y directions, respectively, is presented. It can be seen that DB in the 1st plane have properties considerably different from the DB in the 2nd and the 3rd planes. In the 1st plane DB frequency and DB energy are lower than that of DB in the 2nd and 3rd planes. Actually, DB in the 2nd and especially in the 3rd plane have properties very close to the bulk DB. This can be explained by the fact that interplanar distances very quickly approach the bulk value with increasing depth [see panels (a) in Figs. 3–5] and also by very high degree of spatial localization of the DB considered in the present study. For DB in pure metals, which have much smaller degree of spatial localization [8–12], this conclusion may be altered.

4. Conclusions

With the help of molecular dynamics, for the first time, the possibility of DB excitation close to low Miller indices surfaces of 3D crystal was demonstrated. For this first study the Pt₃Al intermetallic alloy was chosen because DB in the bulk of this crystal have been thoroughly studied.

Our main results can be listed as follows.

Properties of near-surface DB naturally depend on surface orientation and termination.

For Pt-terminated (100) and (110) surfaces only DB vibrating parallel to the surface are long-lived. Such DB have properties similar to the DB in the bulk, i.e., they have frequencies within the gap of phonon spectrum, decreasing with increase in DB amplitude. If a closest to the surface Al atom is excited along z axis (normal to the surface), in a few picoseconds its oscillation energy is given to Al atom deeper in the crystal. After moving inside the crystal by one interplanar distance DB demonstrates properties close to DB in the bulk.

For PtAl-terminated (100) and (110) surfaces, near-surface DB can oscillate only along z axis and such DB have properties different from the bulk DB. Interestingly, z -polarized DB have frequencies within the bulk phonon spectrum. This can be explained by the fact that interplanar distance close to the surface is larger than in the bulk and at larger distances interatomic bonds become softer.

For Pt₃Al-terminated (111) surface only DB polarized along x or y axis have long lifetime. They also can have frequencies within the phonon band for the same reason – the interplanar distance close to the surface is larger than in the bulk.

Near-surface DB in the absence of thermal fluctuations can have very long lifetime, about 10^4 oscillation periods. Near-surface DB with properties close to the bulk DB have maximal amplitudes about 0.8–0.9 Å and maximal energies about 2.0–2.2 eV. Near-surface DB oscillating along z axis have maximal amplitudes about 0.6–0.7 Å and maximal energies about 0.5–0.6 eV.

All near-surface DB localized on Al atoms demonstrate soft type nonlinearity, i.e., their frequency decreases with the amplitude.

Highly localized DB considered in the present study have properties considerably different from bulk DB only in the plane closest to the surface. This is because the interplanar distances very quickly approach the bulk value with increasing depth [see panels (a) in Figs. 3–5]. For less localized DB in pure metals [8–12] this conclusion may be altered.

The results reported in the present study are important for a number of reasons. DB can have relatively large oscillation amplitudes and energies. This energy can be spent to overcome potential barrier of evaporation, migration, point defect nucleation, chemical reaction acceleration, etc. It is well-known that experimental observation of DB in the bulk of crystals is a challenge. Probably it would be easier to identify them on the crystal surfaces.

The following directions for the future studies can be mentioned: (i) search for near-surface DB of different types in Pt₃Al alloy; (ii) study of the effect of temperature on near-surface DB; (iii) search for near-surface DB in other crystals, such as pure metals, ionic crystals, covalent crystals.

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Conflict of interest

None.

References

- [1] A.J. Sievers, S. Takeno, Intrinsic localized modes in anharmonic crystals, *Phys. Rev. Lett.* 61 (1988) 970.
- [2] J.B. Page, Asymptotic solutions for localized vibrational modes in strongly anharmonic periodic systems, *Phys. Rev. B* 41 (1990) 7835.
- [3] S. Flach, A.V. Gorbach, Discrete breathers, *Phys. Rep.* 467 (2008) 1–116.
- [4] S. Flach, C.R. Willis, Discrete breathers, *Phys. Rep.* 295 (1998) 181–264.
- [5] S.V. Dmitriev, E.A. Korznikova, J.A. Baimova, M.G. Velarde, Discrete breathers in crystals, *Phys. Uspekhi* 59 (2016) 446.
- [6] M.E. Manley, A.J. Sievers, J.W. Lynn, S.A. Kiselev, N.I. Agladze, Y. Chen, A. Llobet, A. Alatas, Intrinsic localized modes observed in the high-temperature vibrational spectrum of NaI, *Phys. Rev. B* 79 (2009) 134304.
- [7] A.J. Sievers, M. Sato, J.B. Page, T. Rossler, Thermally populated intrinsic localized modes in pure alkali halide crystals, *Phys. Rev. B* 88 (2013) 104305.
- [8] M. Haas, V. Hizhnyakov, A. Shelkan, M. Klopov, A.J. Sievers, Prediction of high-frequency intrinsic localized modes in Ni and Nb, *Phys. Rev. B* 84 (2011) 144303.
- [9] V. Hizhnyakov, M. Haas, A. Shelkan, M. Klopov, Theory and molecular dynamics simulations of intrinsic localized modes and defect formation in solids, *Phys. Scripta* 89 (2014) 044003.
- [10] D.A. Terentyev, A.V. Dubinko, V.I. Dubinko, S.V. Dmitriev, E.E. Zhurkin, M.V. Sorokin, Interaction of discrete breathers with primary lattice defects in bcc Fe, *Model. Simul. Mater. Sci.* 23 (2015) 085007.
- [11] R.T. Murzaev, A.A. Kistanov, V.I. Dubinko, D.A. Terentyev, S.V. Dmitriev, Moving discrete breathers in bcc metals V, Fe and W, *Comput. Mater. Sci.* 98 (2015) 88–92.
- [12] R.T. Murzaev, R.I. Babicheva, K. Zhou, E.A. Korznikova, S.Y. Fomin, V.I. Dubinko, S.V. Dmitriev, Discrete breathers in alpha-uranium, *Eur. Phys. J. B* 89 (2016) 168.
- [13] L.Z. Khadeeva, S.V. Dmitriev, Lifetime of gap discrete breathers in diatomic crystals at thermal equilibrium, *Phys. Rev. B* 84 (2011) 144304.
- [14] S.V. Dmitriev, N.N. Medvedev, R.R. Mulyukov, O.V. Pozhidaeva, A.I. Potekaev, M.D. Starostenkov, Localized vibrational modes in an A3B two-dimensional perfect crystal, *Russ. Phys. J.* 51 (2008) 858–865.
- [15] R.T. Murzaev, D.V. Bachurin, E.A. Korznikova, S.V. Dmitriev, Localized vibrational modes in diamond, *Phys. Lett. A* 381 (2017) 1003.
- [16] E. Barani, I.P. Lobzenko, E.A. Korznikova, E.G. Soboleva, S.V. Dmitriev, K. Zhou, A.M. Marjanek, Transverse discrete breathers in unstrained graphene, *Eur. Phys. J. B* 90 (2017) 38.
- [17] J.A. Baimova, E.A. Korznikova, I.P. Lobzenko, S.V. Dmitriev, Discrete breathers in carbon and hydrocarbon nanostructures, *Rev. Adv. Mater. Sci.* 42 (2015) 68–82.
- [18] I. Evazzade, I.P. Lobzenko, E.A. Korznikova, I.A. Ovid'ko, M.R. Roknabadi, S.V. Dmitriev, Energy transfer in strained graphene assisted by discrete breathers excited by external ac driving, *Phys. Rev. B* 95 (2017) 035423.
- [19] E.A. Korznikova, J.A. Baimova, S.V. Dmitriev, Effect of strain on gap discrete breathers at the edge of armchair graphene nanoribbons, *Europhys. Lett.* 102 (2013) 60004.
- [20] E.A. Korznikova, A.V. Savin, Y.A. Baimova, S.V. Dmitriev, R.R. Mulyukov, Discrete breather on the edge of the graphene sheet with the armchair orientation, *JETP Lett.* 96 (2012) 222–226.
- [21] E. Barani, E.A. Korznikova, A.P. Chetverikov, K. Zhou, S.V. Dmitriev, Gap discrete breathers in strained boron nitride, *Phys. Lett. A* 381 (2017) 3553–3557.
- [22] I.P. Lobzenko, G.M. Chechin, G.S. Bezuglova, Y.A. Baimova, E.A. Korznikova, S.V. Dmitriev, Ab initio simulation of gap discrete breathers in strained graphene, *Phys. Solid State* 58 (2016) 633–639.
- [23] P.V. Zakharov, M.D. Starostenkov, A.M. Eremin, E.A. Korznikova, S.V. Dmitriev, Excitation of gap discrete breathers in an A3B crystal with a flux of particles, *Phys. Solid State* 59 (2017) 223–228.
- [24] P.V. Zakharov, A.M. Eremin, M.D. Starostenkov, I.S. Lucenko, Analysis of statistical characteristics of quasi-breather with soft-type of nonlinearity in the crystals of A₃B stoichiometry, *Key Eng. Mater.* 743 (2017) 86.
- [25] M.D. Starostenkov, A.I. Potekaev, S.V. Dmitriev, P.V. Zakharov, A.M. Eremin, V.V. Kulagina, Dynamics of discrete breathers in a Pt3Al crystal, *Russ. Phys. J.* 58 (2016) 1353–1357.
- [26] N.N. Medvedev, M.D. Starostenkov, P.V. Zakharov, S.V. Dmitriev, Exciting discrete breathers of two types in a computer 3D model of Pt3Al crystal, *Tech. Phys. Lett.* 41 (2015) 994–997.
- [27] P.V. Zakharov, M.D. Starostenkov, S.V. Dmitriev, N.N. Medvedev, A.M. Eremin, Simulation of the interaction between discrete breathers of various types in a Pt3Al crystal nanofiber, *J. Exp. Theor. Phys.* 121 (2015) 217–221.
- [28] N.N. Medvedev, M.D. Starostenkov, A.I. Potekaev, P.V. Zakharov, A.V. Markidonov, A.M. Eremin, Energy localization in the ordered condensed systems: A3B alloys with L12 superstructure, *Russ. Phys. J.* 57 (2014) 387–395.
- [29] A. Franchini, V. Bortolani, R.F. Wallis, Surface localized modes in anharmonic systems at low dimensionality, *Surf. Sci.* 377–379 (1997) 301–303.
- [30] A. Franchini, V. Bortolani, R.F. Wallis, Surface and gap intrinsic localized modes in one-dimensional III–V semiconductors, *J. Phys.* 12 (2000) 1–11.
- [31] A. Franchini, V. Bortolani, R.F. Wallis, Surface and gap intrinsic localized modes in one-dimensional lattices, *Surf. Sci.* 502–503 (2002) 458–462.
- [32] A. Franchini, V. Bortolani, R.F. Wallis, Intrinsic localized modes and their interaction with the plasmon electric field in one-dimensional zinc-blende lattice, *Surf. Sci.* 566–568 (2004) 926–930.
- [33] A. Franchini, V. Bortolani, R.F. Wallis, Interaction of an external impurity with the surface intrinsic mode in a Heisenberg chain, *Phys. Rev. B* 73 (2006) 054412.
- [34] I.E. Tamm, A possible kind of electron binding on crystal surfaces, *Phys. Z. Sowjetunion* 1 (1932) 733–735.
- [35] A.V. Savin, Y.S. Kivshar, Vibrational Tamm states at the edges of graphene nanoribbons, *Phys. Rev. B* 81 (2010) 165418.
- [36] A.V. Savin, Edge vibrations of graphene nanoribbons, *Phys. Solid State* 60 (2018) 1046–1053.
- [37] W. Xiao, P.A. Greaney, D.C. Chrzan, Adatom transport on strained Cu(001): surface crowdions, *Phys. Rev. Lett.* 90 (2003) 156102.
- [38] Z. Chen, N. Ghoniem, Biaxial strain effects on adatom surface diffusion on tungsten from first principles, *Phys. Rev. B* 88 (2013) 035415.
- [39] T.I. Mazilova, E.V. Sadanov, V.N. Voyevodin, V.A. Ksenofontov, I.M. Mikhailovskij, Impact-induced concerted mass transport on W surfaces by a voidion mechanism, *Surf. Sci.* 669 (2018) 10–15.
- [40] G. Antczak, G. Ehrlich, Jump processes in surface diffusion, *Surf. Sci. Rep.* 62 (2007) 39–61.
- [41] Z. Duan, W. Xiao, Cu dimer diffusion on strained Cu(001), *Surf. Sci.* 604 (2010) 337–345.
- [42] Y.N. Wen, J.M. Zhang, K.W. Xu, Diffusion of single adatom Cu on Cu (001) and (110) surfaces, *Appl. Surf. Sci.* 256 (2009) 1521–1525.
- [43] V.I. Dubinko, P.A. Selyshchev, J.F.R. Archilla, Reaction-rate theory with account of the crystal anharmonicity, *Phys. Rev. E* 83 (2011) 041124.
- [44] T. Rossler, J.B. Page, Intrinsic localized modes in driven anharmonic lattices with realistic potentials, *Phys. Lett. A* 204 (1995) 418–426.
- [45] T. Rossler, J.B. Page, Driven intrinsic localized modes and their stability in anharmonic lattices with realistic potentials, *Physica B* 219–220 (1996) 387–389.
- [46] T. Rossler, J.B. Page, Optical creation of vibrational intrinsic localized modes in anharmonic lattices with realistic interatomic potentials, *Phys. Rev. B* 62 (2000) 11460.
- [47] V.L. Levshunova, G.P. Pokhil, D.I. Tetelbaum, Oscillations of the charge in oxide at silicon surface as an origin of the process leading to the long-range effect, *J. Surf. Invest. X-Ray* 5 (2011) 276–278.
- [48] D. Saadatmand, D. Xiong, V.A. Kuzkin, A.M. Krivtsov, A.V. Savin, S.V. Dmitriev, Discrete breathers assist energy transfer to ac-driven nonlinear chains, *Phys. Rev. E* 97 (2018) 022217.
- [49] X.W. Zhou, R.A. Johnson, H.N.G. Wadley, Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers, *Phys. Rev. B* 69 (2004) 144113.
- [50] S.M. Foiles, M.I. Baskes, M.S. Daw, Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys, *Phys. Rev. B* 33 (1986) 7983.
- [51] R.D. Skeel, G. Zhang, T. Schlick, A family of symplectic integrators: stability, accuracy, and molecular dynamics applications, *SIAM J. Sci. Comput.* 18 (1997) 203–222.
- [52] G.M. Chechin, G.S. Dzheleuhova, E.A. Mehonoshina, Quasibreathers as a generalization of the concept of discrete breathers, *Phys. Rev. E* 74 (2006) 036608.