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Spherically localized discrete breathers in bcc metals V and Nb

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ABSTRACT

Discrete breathers (DBs), also called intrinsic localized modes (ILMs), are spatially localized, large-amplitude vibrational modes in nonlinear lattices. Rod-like discrete breathers (DBs) have been reported in fcc Ni and bcc Nb by Haas et al. in 2011 based on molecular dynamics simulations. Here we use a general approach to find new type DBs in bcc V and Nb. In this approach, we firstly find the lattice symmetry dictated exact solutions to the equations of atomic motion in the form of delocalized nonlinear vibrational modes (DNVMs). Secondly, a localizing function with spherical symmetry is imposed over the DNVMs. Parameter of the localizing function is chosen such that the obtained DB has a long lifetime. The results presented in this work demonstrate that pure metals can support a variety of DBs. Interatomic potentials have a strong effect on the DB lifetime. Maximal DB lifetime in V is two orders of magnitude larger than that in Nb. The results of this study are interesting for the theory of DBs, and also they will help to better understand the impact of DBs on the physical properties of metals.

1. Introduction

Nonlinear vibrational modes called discrete breathers (DBs) or intrinsic localized modes (ILMs) gain significant attention during the last three decades [1–3]. According to the conventional definition, DB is periodic in time and localized in space vibrational mode in a nonlinear Hamiltonian lattice [1]. The first work on energy localization in a nonlinear chain has been done in [4], but an avalanche of works devoted to the theory of DBs was triggered by the work [5]. Since then DBs were investigated both theoretically and experimentally [1–8]. DBs are ubiquitous in a variety of physical systems [9–12] and, according to experimental studies, they exist in crystal lattices [3,13–21]. DBs in macroscopic systems are easy to observe [11,22–30]. On the other hand, direct experimental observation of DBs in crystals is impeded by nanometer size and picosecond lifetime of such vibrational modes. Today the computational methods are the main tool of the analysis of DB properties in crystals. By molecular dynamics modelling DBs were analyzed in various crystals, such as graphene and hydrocarbons [31–42], boron nitride [43], ordered alloys [44–46], alkali-halide crystals [47–49], covalent crystals [50,51], proteins [52–54], and Morse crystals [55,56].

For the first time, DBs in pure metals have been reported by Haas et al. [57]. They have successfully excited the rod-like DBs propagating along a close-packed atomic row of fcc Ni or bcc Nb. Later similar rod-like DBs were analyzed in various metals [58–60]. Interaction of moving rod-like DBs with crystal lattice defects in bcc Fe was analyzed in [61]. DBs in metal hydrides localized on hydrogen atoms were reported in [62].

Bachurina has demonstrated that fcc metals support not only zero-dimensional rod-like DBs (localized in three spatial dimensions), but also linear and planar DBs, delocalized in one and two dimensions, respectively [63,64]. In the work [56] it was shown that two-dimensional triangular Morse lattice supports not only rod-like DBs similar to those discovered in [57], but also DBs with radial symmetry. These works demonstrate that the same nonlinear lattice can support a variety of DBs and pose the problem of finding all possible DBs.

There are no general methods for finding solutions to the nonlinear equations of atomic motion. However, there is a quite general approach for finding approximate spatially localized solutions in the form of DBs. In this approach, one starts from finding the exact solutions of the equations of atomic motion in the form of delocalized nonlinear vibrational modes (DNVMs) dictated by the lattice symmetry [65–69]. The dynamics of a DNVM can be described by a few coupled equations of motion. If the minimum number of equations is k, then such a DNVM is called k-component mode. Dynamics of all possible 1- and 2-component DNVMs in graphene were studied in [70] and the only possible

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three-component DNVM in graphene was analyzed in [71]. After finding DNVMs for the studied lattice, one then calculates their frequency-amplitude dependencies. If in a certain amplitude range a DNVM has frequency outside the phonon spectrum, one can attempt to obtain a DB by applying a localizing function. The localizing function has a few parameters, typically, the degree of spatial localization, the position of the center of the function with respect to the lattice points, and the dimensionality. The parameters are chosen in a way to obtain long-lived spatially localized nonlinear vibrational modes, i.e. DBs. This approach has been successfully applied to identify the high-symmetry radial DB in triangular Morse lattice [56], two-dimensional DBs in fcc metals [64], and different DBs with transverse oscillations in graphene [39].

The final goal of the study of DBs is to understand their effect on the macroscopic properties of crystalline solids [72]. According to the experimental studies, DBs affect the physical properties of crystals, in particular, heat capacity [17] and thermal expansion [19]. The appearance of DBs in the crystal lattice can be a precursor of a phase transition [18]. DBs can affect thermal conductivity [73] since they scatter phonon waves [54,74–79], and they assist energy transport [40,80]. Prior to the discussion of the role of DBs in solid state physics, one should give an exhaustive analysis of their properties and possible types.

Present work is devoted to the study of a few DNVMs in bcc metals V and Nb and obtaining zero-dimensional DBs by imposing upon DNVMs localizing functions with spherical symmetry. New types of DBs will be found following this procedure.

2. Simulation details

Computer simulations are performed with the use of the LAMMPS molecular dynamics package [81,82]. Interatomic interactions for bcc vanadium and niobium are described by the interatomic potentials developed by Mendelev et al. [83] and Fellinger et al. [84], respectively. Equilibrium parameter of the bcc lattice at zero temperature was found as a result of structure relaxation from the potential energy minimum condition. For V it is equal to $a_V = 3.02987$ Å, while for Nb one has $a_{Nb} = 3.30790$ Å. The computational cell contains $14 \times 14 \times 14$ cubic translational cells of the bcc lattice, each of which includes 2 atoms, and thus, the total number of atoms in the cell is 5488. This size of the computational cell is sufficient for the DBs analyzed in this work because they have a sufficiently high degree of spatial localization and a DB, placed in the center of the cell subjected to periodic boundary conditions, practically does not interact with its periodic images. The simulations are carried out for the NVE ensemble (constant number of atoms, volume, and energy). Thermal fluctuations are not taken into account. Equations of motion are solved numerically using the Verlet algorithm of order 4 with the time step of 0.5 fs. Phonon spectra of the considered metals are calculated using the subroutine installed in the LAMMPS package.

Two different problems are addressed in this study. First is the construction of five one-component DNVMs in bcc lattice and calculation of frequency-amplitude dependences for them. We look for DNVMs with the translational cell that includes $2 \times 2 \times 2$ cubic translational cells of the bcc lattice. Initial conditions are set by applying initial displacements of atoms $\Delta \boldsymbol{r}_n = (\Delta x_n, \Delta y_n, \Delta z_n)$according to certain patterns, where $n = 1, \cdots, N$, with N being the number of atoms in the computational cell. For one-component DNVMs addressed in this study, the length of displacement vectors, $|\Delta \boldsymbol{r}_n|$, is equal to either 0 or A for all atoms, with A being the mode amplitude. Initial velocities of all atoms are equal to zero, $\Delta \dot{\boldsymbol{r}}_n = 0$. DNVM frequency is then calculated as the function of its amplitude A. The second task is to look for the spatially localized vibrational modes having a relatively long lifetime, i.e., quasibreathers [7], which will be called here discrete breathers. This problem will be solved by imposing upon the DNVMs the localization function of the form

$$\Delta \boldsymbol{R}_n = \frac{\Delta \boldsymbol{r}_n}{\cosh(\beta\, |\boldsymbol{r}_n - \boldsymbol{r}_0|)}, \tag{1}$$

where $\Delta \boldsymbol{R}_n$ is the initial displacement vector of the n-th atom, $\Delta \boldsymbol{r}_n$ is the initial displacement vector in the considered DNVM, $\boldsymbol{r}_n$ is the radius-vector of the n-th lattice point, $\boldsymbol{r}_0$ is the position of the center of the localizing function, parameter β defines the degree of spatial localization of the DB. We always take $\boldsymbol{r}_0 = 0$ though, in principle, other high-symmetry points of bcc lattice can be considered for the location of the center of the localizing function. Considering various values of the parameter β, we find the one which gives the maximal lifetime of the quasibreather.

3. Simulation results and discussion

Firstly, we construct five one-component DNVMs and calculate their frequency-amplitude dependencies. Secondly, DBs are obtained by imposing the localizing function (1) upon the DNVMs.

3.1. One-component DNVMs

There exists a rigorous method of finding all possible DNVMs for a lattice based on the consideration of the point symmetry transformations supported by the lattice [65,67,68]. Here we do not aim to consider all possible DNVMs whose number can be very large. We limit ourselves to only one-component DNVMs with the periodic cell that includes $2 \times 2 \times 2$ cubic translational cells of the bcc lattice. We use a heuristic approach for finding some of such DNVMs. By playing with initial displacements of 16 primitive cubic sublattices we look for the cases when periodic motion of the sublattices is observed. In this way, we were able to find five one-component DNVMs, but some other may exist.

In Fig. 1(a–e), the initial displacement patterns of the five one-component DNVMs designated as A to E, respectively, are presented. For each mode, we show at left the three-dimensional picture and at right the displacements of atoms in a representative atomic plane. The bcc lattice is presented as a union of the two simple cubic lattices shown by red and blue points. All five DNVMs are the exact solutions of the atomic equations of motion dictated by the symmetry of bcc lattice. This fact was proved by observing the dynamics of the modes. Excitation of DNVM results in periodic oscillations of atoms preserving in time the initial pattern. A few comments are in order. There are one-component DNVMs different from the five modes presented in Fig. 1, but here we do not aim to consider all possible one-component DNVMs. DNVMs typically are unstable if they have amplitudes above a threshold value [70,85–90]. The lifetime of DNVM is smaller for larger amplitude because the speed of the development of instability (critical exponent) increases with growing amplitude. We analyze the properties of DNVMs within their lifetime before they are destroyed by the instability.

Let us describe the DNVMs shown in Fig. 1 in more detail. The DNVMs shown in panels (a) to (e) will be labeled by the letters A to E, respectively. In the mode A, shown in (a), all atoms oscillate along the z axis. In the mode B, all atoms oscillate along the line $x = z$ with $\Delta y_n(t) = 0$. In the mode C, all atoms oscillate such that at any time t one has $|\Delta x_n(t)| = |\Delta y_n(t)| = |\Delta z_n(t)|$. In other words, all atoms oscillate along the [1 1 1] crystallographic directions. In the mode D, half of the atoms oscillate along the line $x = z$ and another half along $x = -z$ with $\Delta y_n(t) = 0$ in both cases. In the mode E, only atoms of one simple cubic sublattice move (red sublattice, for definiteness) and the atoms of the second sublattice are at rest. The moving atoms oscillate along [1 1 1] crystallographic directions so that at any time t one has $|\Delta x_n(t)| = |\Delta y_n(t)| = |\Delta z_n(t)|$.

For further analysis, it is important to calculate the frequency-amplitude dependencies for the studied DNVMs. This result is presented in Fig. 2 for (a) V and (b) Nb, where the abscissa stands for the initial DNVM amplitude. The horizontal dashed lines show the upper edge of

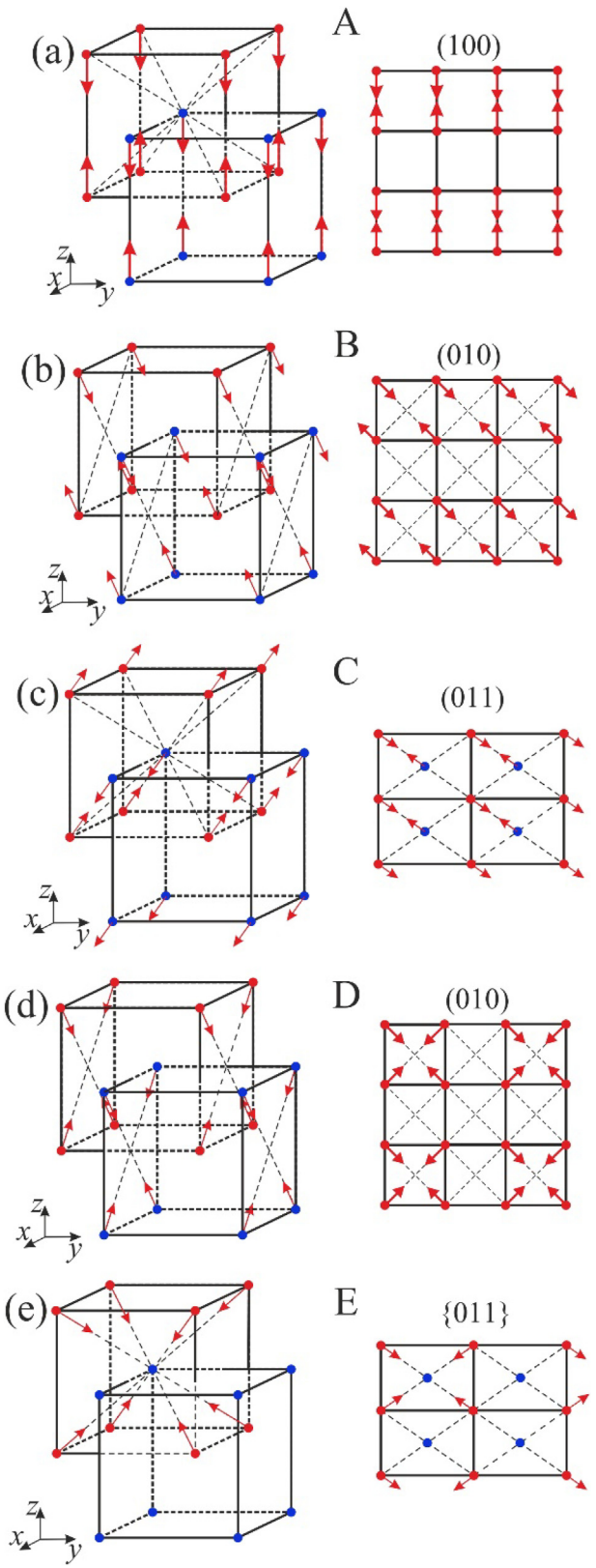

Fig. 1. (a–e) Initial displacements of atoms used for the excitation of five one-component DNVMs in bcc lattice. At left, three-dimensional plots are given, while at right, the atomic displacements of a representative plane are plotted. For clarity, the bcc lattice is decomposed into two simple cubic lattices shown by red and blue points. In the text, the modes plotted in panels from (a) to (e) are referred to as DNVMs A to E, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the phonon spectrum. It is seen that the modes A, B, and C for small amplitudes have the same frequency equal to 4 THz in V and 4.4 THz in Nb, which are within the phonon spectra. For increasing amplitudes, the frequencies of DNVMs A, B, and C increase and become different. In V the frequencies of DNVMs B and C leave the phonon spectrum at the amplitude about 0.15 Å. The DNVM A does the same for amplitudes above 0.25 Å. In Nb, DNVMs A, B, and C remain withing the phonon spectrum even for large amplitudes. Frequencies of DNVMs D and E in both metals coincide for small amplitudes and are equal to the highest phonon frequency (6.4 THz for V and 5.6 THz in Nb). Frequencies of these modes increase with the amplitude remaining above the phonon spectrum, except for the frequency of DNVM D in Nb for the amplitudes above 0.2 Å.

3.2. Discrete breathers in V and Nb

Following the procedure described in Section 2, we attempt to excite DBs by imposing the localizing function (1) upon five DNVMs described in Section 3.1. For different DNVM amplitudes, we search for the parameter β in (1) for which the lifetime of localized oscillations is maximal.

In Table 1, for the DBs having maximal lifetime $t_{\max}$, we present their parameters, namely, DB amplitude A_{DB}, localization parameter β, and DB frequency ν_{DB}. Note that DB amplitude is defined as the maximal deviation from the lattice point of the DB's central atom. In Fig. 3, DB frequency as the function of DB amplitude is plotted for the DBs based on different DNVMs in (a) V and (b) Nb. The horizontal lines show the upper edge of the phonon spectrum.

Firstly let us describe the properties of DBs in V. Very robust DBs are constructed based on DNVMs A and C with a lifetime of 235 and 270 ps, respectively. Other DNVMs in V also produce DBs with relatively long lifetime, the minimal one of 14 ps observed for DNVM B. With the oscillation frequency of about 7 THz, within this shortest lifetime, the DB makes about 100 oscillations. The DB with the longest lifetime of 270 ps makes about 1900 oscillations. Long-lived DBs have amplitudes about 0.25–0.3 Å, except for the one based on DNVM B, having an amplitude of 0.5 Å. Naturally, in all cases, long-lived DBs have frequencies above the phonon spectrum. The highest degree of spatial localization has DBs based on DNVMs A and C, for them $\beta = 1.5$, while in other cases we have $\beta = 1.2$.

The results for V are interesting in that sense that there is no clear correlation between DB frequency and its lifetime. Normally one would expect that DBs with frequencies considerably larger the maximal phonon frequency should have longer lifetime since such DBs should have weaker interaction with the phonon modes. However, from the results presented in Fig. 3(a) it is seen that the DB based on DNVM A has frequency slightly above the phonon spectrum, but its lifetime is very long, as compared to that of DNVMs D and E, having higher frequencies, see also Table 1.

Now we turn to the properties of DBs in Nb. Comparison of DB parameters in V and Nb presented in Table 1 reveals that the maximal lifetime of DBs in Nb is one to two orders of magnitude smaller than in V. This result is not surprising taking into account the fact that the frequencies of DNVMs A, B, and C in Nb are within the phonon spectrum in the whole studied range of amplitudes, see Fig. 2(b). The frequency of DNVM D is slightly higher than the phonon spectrum for amplitudes less than 0.2 Å and lies within the spectrum for larger amplitudes. Only DNVM E has frequencies lying sufficiently above the phonon spectrum and in this case, the maximal DB lifetime is longest among DBs based on different DNVMs, but still, it is just 4.1 ps (see the last line of Table 1). With the oscillation frequency of about 5 THz, the DB makes just 2 or 3 oscillations within a lifetime of 0.5 ps and about 20 oscillations within a lifetime of 4.1 ps.

A similar explanation of a very low lifetime of DBs in Nb can be deduced from the results plotted in Fig. 3(b), where DB frequency as the function of DB amplitude is shown for DBs with maximal lifetime based

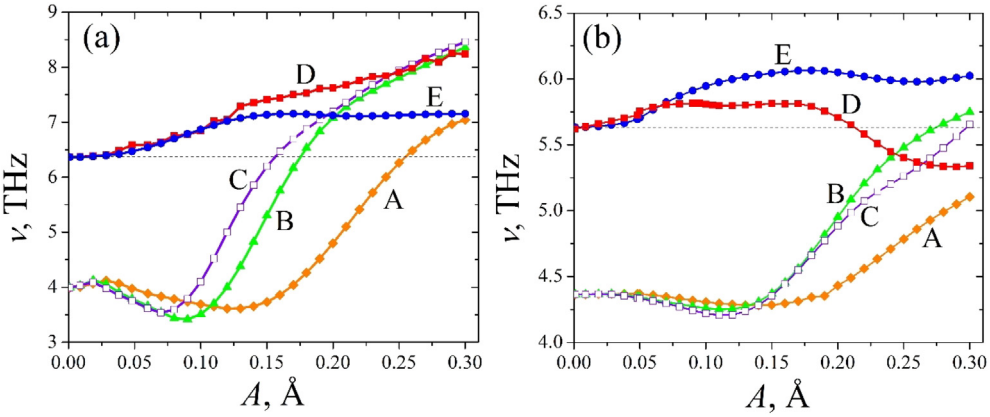

Fig. 2. Frequency as the function of the initial amplitude for the five DNVMs shown in Fig. 1 for (a) V and (b) Nb. Horizontal dashed lines show the upper edge of the phonon spectrum. Letters from A to E link the results to the modes shown in Fig. 1(a–e), respectively.

Table 1
Parameters of DBs with maximal lifetime t_{max} in V and Nb based on the five studied DNVMs: DB amplitude A_{DB}, localization parameter β, and DB frequency ν_{DB}.

DNVM	A_{DB} (Å)		β (Å^{-1})		ν_{DB} (THz)		t_{max} (ps)	
	V	Nb	V	Nb	V	Nb	V	Nb
A	0.3	0.25	1.5	0.8	6.71	5.44	235	1.5
B	0.5	0.5	1.2	1.5	6.81	5.02	14	0.5
C	0.25	0.4	1.5	1.5	7.29	5.57	270	2.5
D	0.25	0.15	1.2	1.5	8.04	5.64	58	2.5
E	0.25	0.2	1.2	1.5	7.01	5.65	26	4.1

on different DNVMs. Here the result for the DB based on DNVM B is not even presented because the maximal DB lifetime is very low, see the second line of Table 1.

All the features of the frequency-amplitude dependencies of DNVMs and DBs are related to the peculiarities of the interatomic potentials, but the relation between them remains subtle.

In some cases, DBs in V demonstrate nontrivial dynamics. For example, in Fig. 4 we plot the distance of the central atom (red line) and the next to the central atom (blue line) from their lattice positions as the functions of time for the DBs in V initially excited based on DNVM D for the three values of DB amplitude: (a) 0.2, (b) 0.25, and (c) 0.3 Å. In (a) three different regimes marked as I, II, and III can be distinguished. Initially excited DB based on DNVM D exists in the regime I and at $t = 6$ ps it spontaneously transforms into a DB based on DNVM C (regime II), which at $t = 54$ ps transforms into a DB based on DNVM A (regime III). In Fig. 4(b), the transformation from the regime I to the regime II takes place at $t = 6$ ps but the regime III is not realized. In the case presented in Fig. 4(c) the regime I is observed within the DB lifetime up to $t = 42$ ps. However, within the time interval from 10 to 16 ps the DB center moves to the neighboring atom and then back. Earlier energy exchange between DBs located at a relatively short distance has been described in diamond [51] and in a NaCl type ionic crystal [91].

4. Conclusions

With the help of molecular dynamics simulations, five one-component DNVMs were constructed for bcc lattice. Such modes are the lattice symmetry dictated exact solutions to the equations of atomic motion regardless of the type of interatomic potential and the mode amplitude. Frequency-amplitude dependences were calculated for the five DNVMs in two bcc metals, vanadium and niobium.

New types of DBs with spherical localization were obtained by imposing the localizing function (1) upon DNVMs with frequencies above the phonon spectrum. It is found that the interatomic potential has a significant effect on the DB lifetime. For instance, in V the maximal lifetime of DBs based on different DNVMs ranges from 14 to 270 ps (from 100 to 1900 oscillation periods), while in Nb the maximal DB lifetime is between 0.5 and 4.1 ps (2 and 20 oscillation periods). The reason why the DBs in the two metals studied have such a different lifetime is related to the higher degree of hard type nonlinearity in V as compared to Nb. As follows from Fig. 2(b), the highest DNVM frequency of 6.1 THz is observed in Nb for the mode E and it is just 9% above the upper edge of the phonon spectrum. In V the highest DNVM frequencies are at the level of 8.5 THz (for modes B, C, and D) which is 33% above

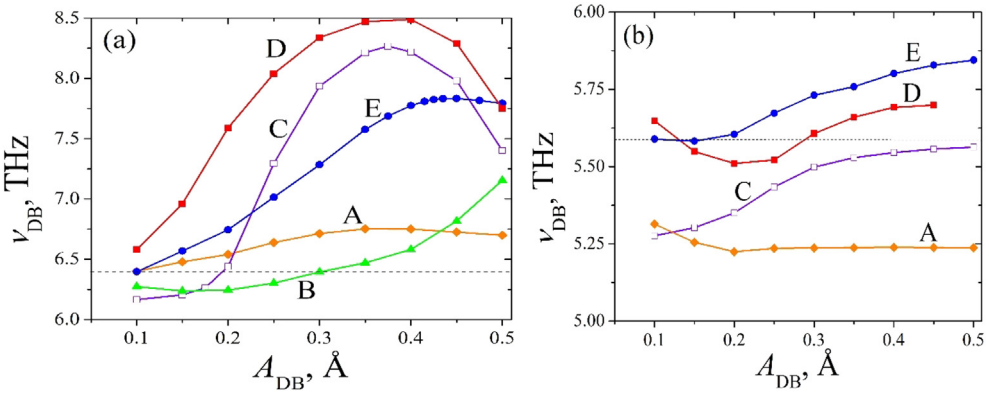

Fig. 3. DB frequency as the function of DB amplitude in (a) V and (b) Nb for DBs based on different DNVMs. The horizontal dashed line shows the upper edge of the phonon spectrum.

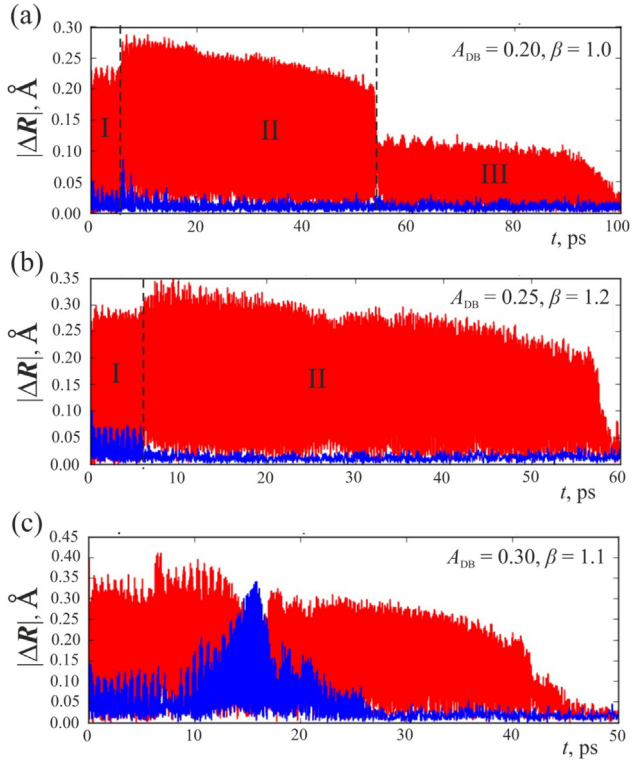

Fig. 4. Distance of the central atom (red line) and the next to the central atom (blue line) from their lattice positions as the functions of time for the DBs initially excited in V based on DNVM D for the three values of DB amplitude: (a) 0.2, (b) 0.25, and (c) 0.3 Å. In (a) three regimes marked with I, II, and III can be seen. Initially excited DB based on DNVM D exists in the regime I and then it spontaneously transforms into a DB based on DNVM C (regime II), which later transforms into a DB based on DNVM A (regime III). In (b) a spontaneous transformation from the regime I to the regime II can be seen. In (c) the regime I persist but the DB center moves to an atom next to the central one and then back. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the phonon spectrum [see Fig. 2(a)]. The same can be said about the frequencies of DBs in these two metals: in V DB frequency is further from the upper edge of the phonon band than in Nb (see Fig. 3). It is natural to expect that discrete breathers with frequencies more distant from the phonon spectrum will interact less with phonons and therefore have a longer lifetime.

It is found that DBs can spontaneously change the vibration pattern. DBs can also perform wandering movement when DB center shifts from one atom to the neighboring one and then back.

Ultimately, the results presented in this work will help to establish the role of discrete breathers in the formation of the physical properties of crystals.

As a continuation of this study, two-component DNVMs can be analyzed and, if they have frequencies above the phonon spectrum, one can attempt to obtain DBs by imposing the localizing functions. It is also interesting to study DBs of spherical symmetry in other bcc metals and try to understand why DB lifetime can differ so significantly depending on the interatomic potential. Of paramount importance is to carry out *ab initio* simulations for DNVMs, which is possible taking into account relatively small translational cell of such vibrational modes. Metals with other lattices, e.g., fcc and hcp, should also be analyzed.

CRediT authorship contribution statement

K.A. Krylova: Conceptualization, Methodology, Data curation, Investigation, Visualization, Writing - review & editing. **I.P. Lobzenko:** Conceptualization, Methodology, Software, Data curation, Writing - original draft. **A.S. Semenov:** Software, Investigation, Funding acquisition. **A.A. Kudreyko:** Supervision. **S.V. Dmitriev:** Conceptualization, Investigation, Writing - original draft, Writing - review & editing, Funding acquisition, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data Availability

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

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