



Two-component localized vibrational modes in fcc metals

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Abstract. Discrete breathers (DB) are spatially localized vibrational modes of large amplitude in a defect-free crystal lattice. In this work, for the first time, two-dimensional DBs based on a two-component delocalized nonlinear vibrational mode (DNVM) are excited in a single (111) close-packed atomic plane in fcc metals (Al, Cu, and Ni). DNVM provides a pattern according to which the initial displacements of atoms from their equilibrium lattice positions are set. Classical molecular dynamics simulations have demonstrated the possibility to excite a long-lived two-dimensional DB with the energy of the order of 0.5–1.0 eV per oscillating atom. The two-dimensional DBs have a hard-type of nonlinearity and a lifetime of 12–24 ps, after which they decay into one-dimensional DBs, which, in turn, decay into zero-dimensional DBs, which also have a sufficiently long lifetime. A new class of two-dimensional DBs expands our understanding of the variety of spatially localized vibrational modes in nonlinear fcc lattices.

1 Introduction

At elevated temperatures, during plastic deformation, etc., it is particularly important to take into account anharmonicity of interatomic interactions. Analysis of atomic oscillations allows determining such important characteristics of crystals as heat capacity, thermal expansion, and changes in elastic constants. About 3 decades ago, it has been revealed that in addition to phonon wave packets and vibrational modes localized on defects, nonlinear lattices are able to support oscillatory modes of a fundamentally new type—discrete breathers (DBs) (or intrinsic localized modes), whose contribution to crystal physics has yet to be described.

The possibility of the existence of discrete breathers in a one-dimensional chain of atoms was first demonstrated theoretically in Refs. [1–3]. Properties of DBs have been extensively studied in a number of nonlinear lattices of different physical nature [4, 5] including crystal lattices [6]. DB is a time-periodic and spatially localized vibrational mode in a defect-free nonlinear lattice. For a time being, it has been established that the same crystal lattice can support a variety of DBs of different type [7].

It is convenient to classify DBs based on their spatial dimension. Thus, zero-dimensional DB is localized in all three dimensions in a three-dimensional lattice. One-dimensional DBs are localized in two dimensions and delocalized in one dimension, that is, atoms in one close-packed atomic row vibrate with a large amplitude, and the vibration amplitude of other atoms decreases

exponentially with distance from the excited row. Two-dimensional DB is localized in one dimension and delocalized in the other two dimensions. In this case, a close-packed atomic plane is excited, and the atomic vibration amplitude decreases exponentially with distance from this plane. Zero-dimensional [7–11, 13–19, 21] and one-dimensional [7, 20] DBs have already been extensively studied via classical molecular dynamics methods in various materials with different crystal lattices, e.g., in model lattices [7–9], graphene [10], graphane [11], ionic [12] and covalent [13] crystals, in metals [14–17, 20] and ordered alloys [18, 19]. However, two-dimensional DBs in three-dimensional lattices remain poorly investigated [21–23].

Setting the initial conditions for the DB excitation is not a trivial task. In many cases, it can be solved using a delocalized nonlinear vibrational mode (DNVM). DNVMs are exact solutions of nonlinear dynamic equations that are completely determined by the lattice symmetry and exist for any type of interatomic potentials used in the modeling [24, 25]. Modulation instability of these short-wavelength vibrational modes is one of the widely used methods of DB excitation. This method works if the DNVM frequency is above the spectrum of small-amplitude oscillations of the lattice and increases with the amplitude. The mechanism of energy localization is as follows [26–28]. DNVM energy is homogeneously distributed in space. As a result of modulational instability, the inhomogeneity of energy distribution appears. The amplitudes of vibrations of atoms with higher energy increase, which leads to an increase in their frequency and further localization of energy, and, as a result, to the appearance of large-amplitude

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DBs with a long lifetime [26,27]. DBs can also be obtained by superimposing a localization function on a DNVM having frequency outside the phonon spectrum. This approach was successfully used for excitation of DBs in various crystals of different spatial dimensions [22,23,29,30]. According to their type, there are one-, two- and multi-component DNVMs. A one-component DNVM is characterized by a single parameter (oscillation amplitude of atomic displacements from their equilibrium lattice sites), while a two-component DNVM is characterized by two different oscillation amplitudes in the same vibrational mode. Due to their complexity, at present only limited attempts were made to analyze three-component vibrational modes [31].

Modulational instability of four DNVMs was studied in a two-dimensional hexagonal lattice using the polynomial β -FPU (Fermi, Pasta and Ulam) pair potential with a hard-type quartic nonlinearity [29]. For the two studied modes, development of the modulational instability resulted in a formation of long-lived zero-dimensional DBs. The DB frequency (above the phonon spectrum) were found to be increased with the increasing amplitude.

Two-dimensional DBs excited based on eight one-component DNVMs were recently investigated in fcc metals [23]. In particular, it was shown that stable DBs can be excited based on only four out of eight DNVMs, whose lifetimes are found to be in the range of 24–47 ps. At that, all the studied DBs in fcc metals are characterized by a hard-type of nonlinearity, and vibrational energy, which can be accumulated by DBs, is of the order of 0.6–1.5 eV per atom.

According to our knowledge, thorough investigations of two-dimensional DBs excited by means of two-component DNVMs have not yet been carried out. Therefore, the goal of the present work is molecular dynamics study of two-dimensional DBs in a three-dimensional fcc single crystals (Al, Cu, and Ni). We were not aimed to investigate all the two-component DNVMs in fcc lattice, but to show the possibility of excitation of a long-lived two-dimensional DB based on one selected two-component DNVM.

2 Model and computational details

Excitation of two-dimensional DBs is performed based on the two-component DNVM (see Fig. 1) derived by Chechin and Ryabov for two-dimensional triangular lattice [25,32]. A close-packed (111) atomic plane in fcc crystal precisely represents two-dimensional triangular lattice, and therefore this DNVM can be applied to excite two-dimensional DB in fcc lattice. In contrast to the previous studies [20,22,29,30], DNVM shown in Fig. 1 is a two-component one, i.e., it is characterized by two different initial amplitudes of atomic displacements A_x and A_y along the x - and y -axes, respectively [33]. Only atoms in the selected (111) plane are displaced according to the given pattern, while all other atoms in the computational cell have zero initial displacements.

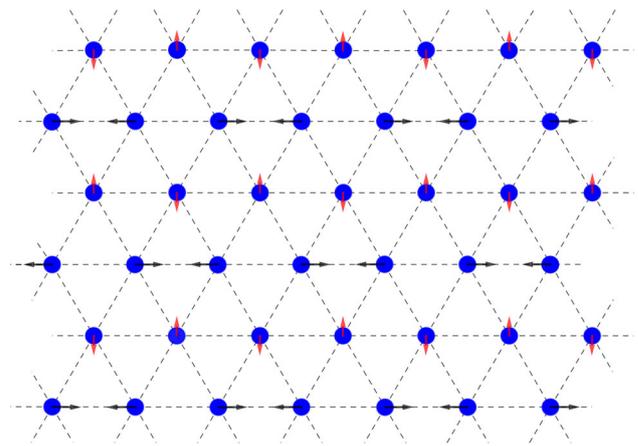


Fig. 1 Two-component DNVM used for excitation of two-dimensional DB in a close-packed (111) atomic plane in Al, Cu, and Ni. The blue atoms represent the equilibrium lattice sites. The black and red arrows indicate schematically atomic displacements along the x - and y -axes, respectively. The amplitudes of the initial atomic displacements along the x - and y -axes, A_x and A_y , are different. Only the part of a (111) plane located inside the three-dimensional computational cell is shown

At the initial moment of time, the velocities of all atoms are equal to zero.

Molecular dynamics simulations are performed with the help of the LAMMPS software package [34,35]. The atomic interactions are modeled with the standard embedded atom method potentials for fcc metals (Al, Cu, and Ni), which take into account many body interactions [36,37]. Periodic boundary conditions are applied along all three spatial directions, so the modeled single crystals do not contain free surfaces.

All the simulations are carried out at an absolute zero temperature using a thermodynamic NVE ensemble (constant number of atoms, volume and energy). The time step is chosen to be 1 fs. The simulation time is restricted to 30 ps (totally 3×10^4 time steps), which is found to be generally sufficient for this type of simulation. All the parameters related to the equilibrium lattice constants, sizes of the computational cells and number of atoms in them, the upper edges of the phonon spectrum for Al, Cu, and Ni are summarized in Table 1. For other details related to calculation of the phonon density of states via standard method implemented in the LAMMPS, the reader is referred to our previous publication [23].

Since it is unknown a priori at which values of A_x and A_y the excitation of long-lived two-dimensional DB in fcc lattice and the minimal energy dissipation onto neighboring atomic planes occurs, the variation of these parameters is used. A proper choice of initial amplitudes A_x and A_y , after a certain short transient stage, results in an excitation of a two-dimensional DB.

DBs have a finite lifetime, and therefore, it is necessary to establish a threshold for which DBs are considered as long-lived ones. From Table 1, it can be seen

Table 1 The lattice constants a_0 at $T = 0$ K, the sizes of the computational cells along the three mutually perpendicular x -, y -, and z -axes, the number of atoms (N) in them, and the upper edge of the phonon spectrum (ν) for the studied fcc metals (Al, Cu, and Ni)

Metal	a_0 (Å)	N	Computational cell (Å)	ν (THz)
Al	4.05	25344	68.2 × 78.8 × 76.6	10.0
Cu	3.62	25344	61.3 × 70.8 × 68.9	7.9
Ni	3.54	25344	59.7 × 69.0 × 67.1	10.3

that the maximal phonon frequency in the studied fcc metals is of order of 10 THz. The same applies for DBs with frequencies above the phonon band. Then, the period of DB oscillations is of the order of 0.1 ps. Thermal fluctuations have a lifetime of about one oscillation period. On this basis, vibrational modes with a lifetime of the order of ten oscillation periods can be considered as long-lived ones. Let us agree that if the DB lifetime exceeds 5 ps (50 oscillation periods), then, it will be called long-lived (or stable) DB. In this steady-state stage, the oscillation amplitudes a_x and a_y along the x - and y -axes, respectively, are measured. The steady-state amplitudes a_x and a_y are defined as half the difference between the maximum and minimum displacements compared to A_x and A_y , which are varied in the range of 0.05–0.5 Å. This interval was chosen due to the fact that at higher initial amplitudes, almost instantaneous destruction of two-dimensional DB accompanied by energy dissipation throughout the crystal takes place.

3 Simulation results and discussion

Figure 2 (upper row) shows amplitude of atomic oscillations in the steady state, a_x , as a function of initial amplitude A_x for different values of A_y in the range of 0.05–0.20 Å. This range was chosen in view of the fact that a further increase in A_y results in a decrease of DB lifetime and/or a qualitative transformation of its initial structure. Only atoms of the excited atomic plane oscillate with large amplitudes, which exponentially decrease with the distance away from the plane. Therefore, this oscillation mode excited based on the two-component DNVM can be called as two-dimensional DB. As for the case of recently studied single-component DNVMs [23], the values of a_x/a_y are always lower than A_x/A_y due to energy dissipation which always takes place in a crystal. There is a deviation from the linear dependence $a_x(A_x)$ in the range of $A_x = 0.10 - 0.30$ Å for all three metals. At $A_x > 0.3$ Å, the dependence $a_x(A_x)$ for Al and Cu is very close to linear one regardless of the values of A_y . In Ni, this occurs at $A_x = 0.25$ Å and $A_y = 0.08 - 0.18$ Å. A linear dependence $a_x(A_x)$ is established in view of the fact that two-dimensional DBs reach the stationary oscillation stage, in which the vibrational energy is maximally preserved at the sites of a crystal lattice.

An analysis of atomic structures reveals that two-dimensional DB at the end of its lifetime is lined up along the close-packed atomic rows and is of a one-dimensional character, via complete damping of oscillations along the y -axis. Further, such one-dimensional DBs after a short time also decompose into a number of zero-dimensional DBs, whose energy is concentrated on 6–8 neighboring atoms. These zero-dimensional DBs live for a while, then the oscillation frequencies are lowered into the phonon spectrum, and a transition to thermal oscillations of atoms occurs.

Figure 2 (middle row) demonstrates the dependence of oscillation frequency ν in the steady state on initial amplitude A_x for different values of A_y . In general, the behavior of all the curves for Al, Cu, and Ni are similar. Two-dimensional DBs demonstrate a rigid type of nonlinearity, namely an increase in oscillation frequency with an increase in amplitude. This is explained by the pattern of the atomic oscillation in DNVM (see Fig. 1). In the investigated two-component DNVM, atoms in groups of four move towards each other. In this case, hard cores of interatomic potentials make a greater contribution to the mode dynamics in contrast to soft tails, providing an increase in the mode frequency with increasing amplitude. Here, it is taken into account that all interatomic potentials have a soft tail and a hard core. This is due to the structure of the atom, which includes electron clouds and a nucleus. The oscillation frequencies of atoms at $A_x > 0.2$ Å are higher than the upper edges of the phonon spectrum, which are 10.0 THz for Al, 7.9 THz for Cu, and 10.3 THz for Ni (for details see Ref. [23]). At $A_x < 0.2$ Å, the atomic frequencies are within the phonon spectra, and consequently, the lifetimes of 2D DBs are very short (about 10–15 oscillations), since their vibrational energy is spent on excitation of lattice phonons. In addition, it is worth noting that variation of A_y does not lead to a significant change in $\nu(A_x)$ dependence. All the corresponding curves are almost on top of each other.

The maximal kinetic energy per oscillating atom as a function of initial amplitude A_x is also presented in Fig. 2 (lower row). The vibrational energies per atom, which can be accumulated by long-lived two-dimensional DBs are 0.5 eV for Al, 1.3 eV for Cu and 1.1 eV for Ni. Note that two-dimensional DBs can accumulate even higher vibrational energies (up to 3.5 eV); however, these DBs have short lifetimes. The accumulated energy is sufficient to overcome local

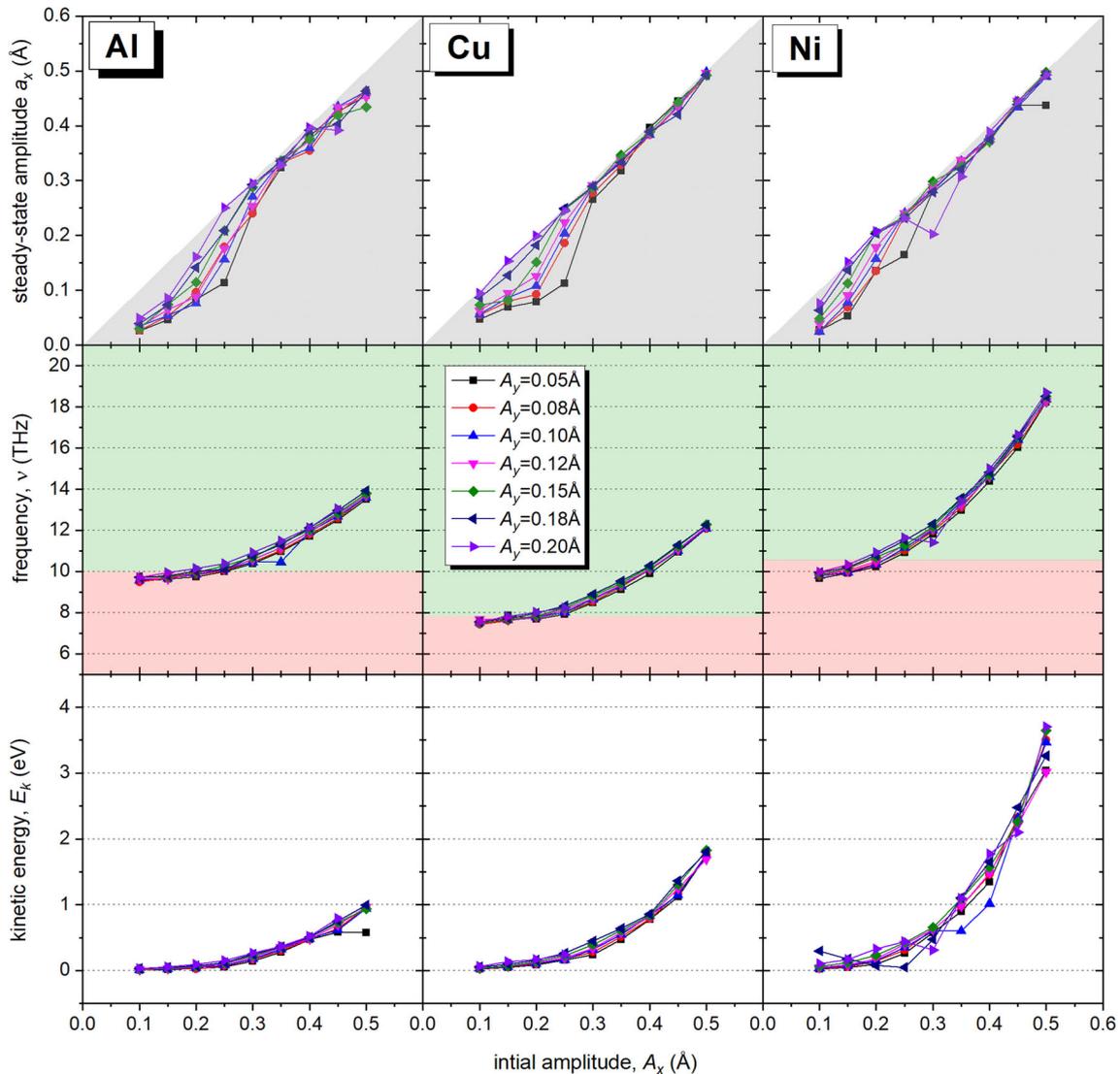


Fig. 2 Dependence of steady-state amplitude (upper row), oscillation frequency (middle row), and maximal kinetic energy per oscillating atom (lower row) for two-dimensional DBs excited via the two-component DNVM on initial amplitude A_x calculated for various values of A_y . The gray areas in the upper row illustrate the regions, where $a_x < A_x$. The solid lines interpolating the data points are guides to the eye. The regions located above/below the upper edge of the phonon spectra are shown in green/red (middle row)

potential barriers and therefore can contribute to an increase in the diffusivity of oscillating atoms. The fact that the 2D DB analyzed in the present work cannot have a long lifetime at relatively small and relatively large amplitudes can be explained as follows. In a stationary DB, the amplitudes of atomic vibrations decrease exponentially with distance from the excited atomic plane. However, in this work, rather trivial initial conditions are used. Initially, only one atomic plane is excited, and part of the energy of this excitation is spent on excitation of neighboring planes during the formation of a stationary DB. At relatively low excitation energy, the formation of a stationary DB becomes impossible due to a lack of energy. On the other hand, high-energy DBs have a

short lifetime, since the rate of development of modulation instability increases with increasing mode amplitude [28].

Figure 3 presents the dependence of the lifetime of two-dimensional DBs on initial amplitudes A_x and A_y . The lifetimes in Al are less than 7 ps for all values of A_x except $A_x = 0.20 \text{ \AA}$ at $A_y = 0.15 - 0.20 \text{ \AA}$, and $A_x = 0.25 \text{ \AA}$ at $A_y = 0.05 - 0.20 \text{ \AA}$. For Cu, the DB lifetime does not exceed 7 ps at $A_x = 0.10 \text{ \AA}$, $A_x = 0.45 - 0.50 \text{ \AA}$ and $A_y = 0.05 - 0.20 \text{ \AA}$. Similar results are obtained for Ni. At the average amplitudes, i.e., $A_x = 0.30 - 0.40 \text{ \AA}$, there are no sharp jumps. The latter means that the transition of a two-dimensional DB to the stationary oscillation stage occurs, at which the dependence $a_x(A_x)$ acquires a linear character for

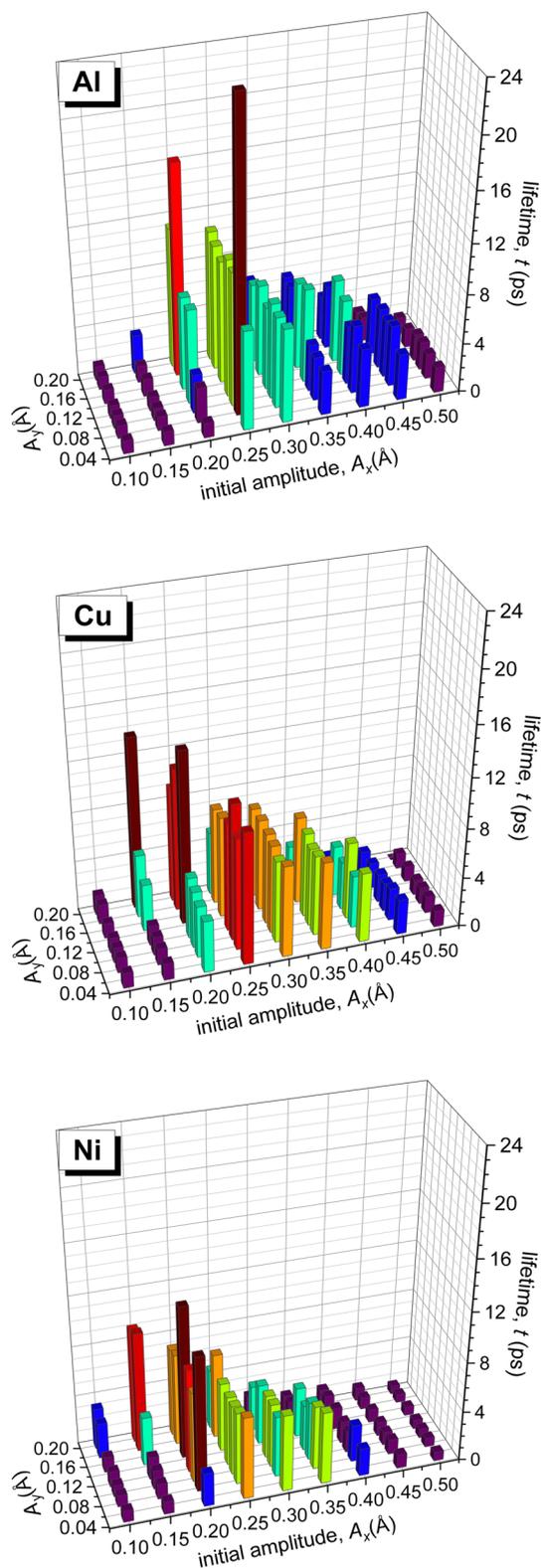


Fig. 3 Dependence of lifetime of two-dimensional DBs excited via the two-component DNVM on initial amplitudes A_x and A_y calculated for Al, Cu, and Ni. The bins in plots are colored according to their height

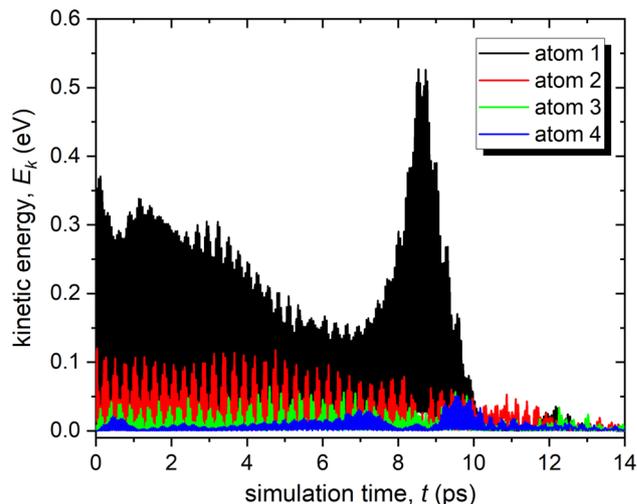


Fig. 4 Time evolution of the kinetic energy calculated for the four selected atoms. Atoms 1 and 2 are located in the plane, where the two-component DNVM was initially excited, and oscillate along the x - and y -axes, respectively. Atoms 3 and 4 are located on the first and the second adjacent atomic planes. For this particular case, DB is excited in Al at the initial amplitudes of $A_x = 0.25 \text{ \AA}$ and $A_y = 0.18 \text{ \AA}$ and has the lifetime of 10.3 ps

all metals. Thus, only at certain values of A_x and A_y , the maximum lifetimes of two-dimensional DBs in Al (24.4 ps), Cu (13.9 ps), and Ni (12.2 ps) are reached. These are: $A_x = 0.25 \text{ \AA}$ and $A_y = 0.08 \text{ \AA}$, for Al; $A_x = 0.20 \text{ \AA}$ and $A_y = 0.15 \text{ \AA}$ for Cu; $A_x = 0.20 \text{ \AA}$ and $A_y = 0.15 \text{ \AA}$ for Ni.

A separate study has shown that a smaller size of the computational cell has a negligible effect on the lifetime of a two-dimensional DB, the frequency of atomic oscillations, and the kinetic energy per oscillating atom. Note that similar fact has been established for a one-dimensional DB in fcc metals in our previous publication [20].

To demonstrate high localization of vibrational energy within the two-dimensional DB, a time evolution of the kinetic energy of the four selected atoms was computed (see Fig. 4). Atoms 1 and 2 are chosen to be located in the same plane where the two-component DNVM was excited and oscillate along the x - and y -axes, respectively (see Fig. 1 for details). Atom 3 is located on the first adjacent to the DNVM plane, while atom 4 is on the second adjacent plane, i.e., at two interplanar distances from the excited vibrational mode. In this case, the results are given for Al; however, the similar findings are obtained for both Cu and Ni. As seen in Fig. 4, the kinetic energy of atoms 1 and 2 oscillates with the amplitudes significantly higher as compared to atoms 3 and 4. The oscillations of the kinetic energy for atom 4 are at least one order of magnitude less than those for atom 2. The latter fact suggests that oscillation energy is localized within the plane and drastically decrease with distance from it. This exponential decay of the vibration amplitude away from the DB core is typical

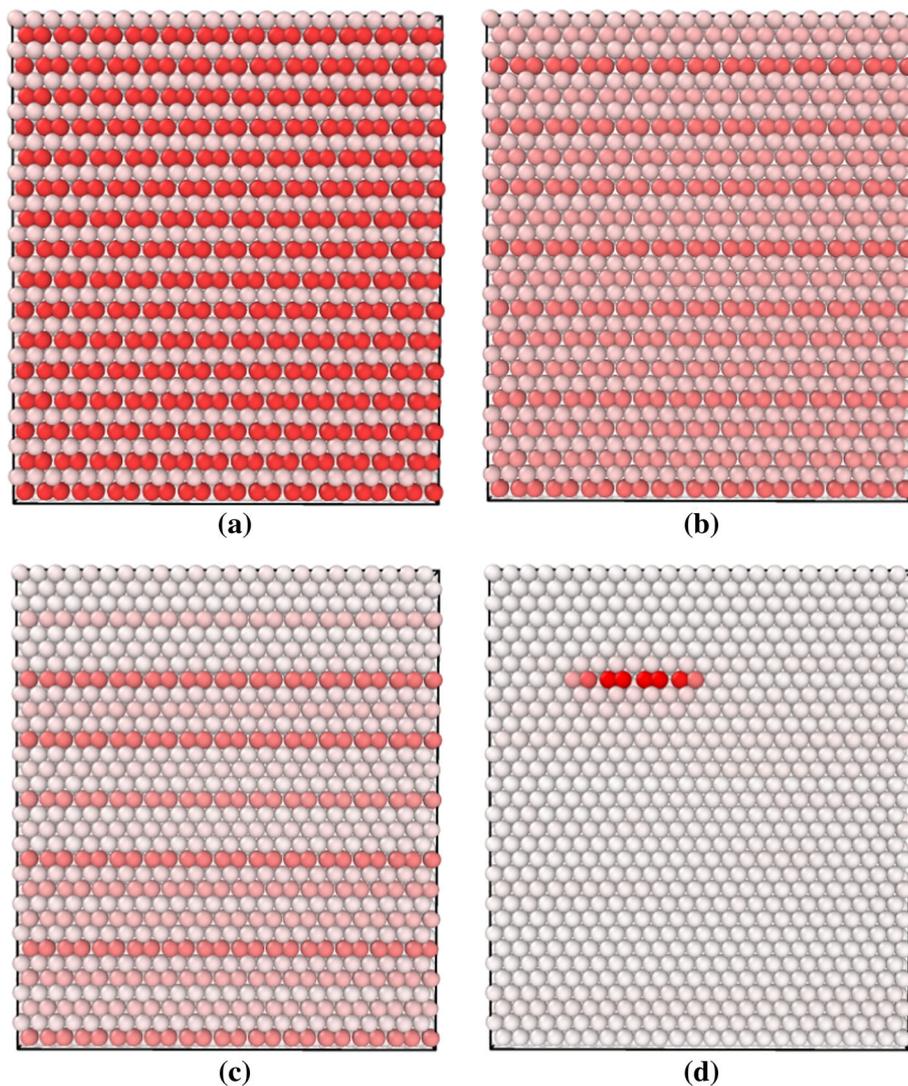


Fig. 5 Energy distribution in the initially excited atomic plane in Ni for $A_x = 0.20 \text{ \AA}$ and $A_y = 0.15 \text{ \AA}$. Red (white) atoms have high (low) energy. Snapshots are for **a** $t = 2$ ps, **b** $t = 8$ ps, **c** $t = 8.5$ ps and **d** $t = 12.5$ ps

due to the fact that the small-amplitude tails of DBs are described by the linear theory [28]. The rate of the exponential decay depends on the interatomic potentials. Thus, the studied two-component DNVM can be considered as a two-dimensional DB, where atomic oscillations are localized in one direction (z -axis) and delocalized along the other two (x - and y -axes). It is interesting to note that a decrease in the kinetic energy of atoms 1 and 2 in the time range of 4–7 ps is accompanied by a simultaneous but much less pronounced increase in the energy of atoms 3 and 4. The same applies for the range of 9–10 ps as clearly displayed in Fig. 4. The burst of the kinetic energy of atom 1 in the range of 8.5–9 ps occurs due to the fact that a part of the kinetic energy is transferred to it from neighboring atoms oscillating along the y -axis. As a result, the oscillation amplitudes along the y -axis decrease noticeably, while an increase in the amplitude of atomic oscillations along the x -axis occurs. After 10 ps of simulation, the amplitudes of the

energy oscillations of the selected atoms 1–4 are quite small, which indicates that the two-dimensional DB has dissipated its energy on lattice phonons and ceased to exist.

Time evolution of the spatial distribution of total (kinetic plus potential) energy in the initially excited atomic plane in Ni representing the development of the modulational instability is demonstrated in Fig. 5. Red (white) color is used for the atoms having high (low) energy. In (a), the energy is distributed according to the initial pattern. The atomic rows with horizontal atomic vibrations have a larger energy as compared to the rows with vertical vibrations, since $A_x > A_y$. At $t = 8$ ps, as shown in (b), the modulational instability starts to develop and the homogeneous distribution of energy is destroyed. One-dimensional DBs are formed in (c). The one-dimensional DBs are also modulationally unstable and they split into zero-dimensional DBs, as shown in

(d). Thus, the two-dimensional DB first splits into one-dimensional and then into zero-dimensional DBs.

Stability map indicating the steady-state amplitudes, a_x and a_y , for all found in this study long-lived two-dimensional DBs is displayed in Fig. 6. Recall that, as agreed above, long-lived DBs are those, whose lifetime exceeds 5 ps. First of all, it turns out that for all three fcc metals, long-lived two-dimensional DBs are distributed in a certain order on the plane of steady amplitudes a_x and a_y . The regions of steady-state amplitudes, in which long-lived two-dimensional DBs can be excited, are as follows: $a_x = 0.09 - 0.39\text{\AA}$ and $a_y = 0.07 - 0.13\text{\AA}$ for Al; $a_x = 0.08 - 0.44\text{\AA}$ and $a_y = 0.07 - 0.11\text{\AA}$ for Cu; $a_x = 0.14 - 0.33\text{\AA}$ and $a_y = 0.07 - 0.10\text{\AA}$ for Ni. Thus, the stability regions, i.e., the sets of optimal parameters a_x and a_y , in all studied metals are of approximately the same width and height. Only in Ni these regions are somewhat narrower than for the other two metals, which is related to the rigidity of interatomic bonds.

The long lifetime of two-dimensional DBs in these regions is associated with a minimal dissipation of vibrational energy into neighboring atoms. Setting the amplitudes outside the indicated range can lead to the following two possible scenarios: (1) more intensive energy dissipation and fast decay of DBs (the lifetime does not exceed 5 ps); (2) partial dissipation of energy in such a way that the oscillation amplitudes fall into the above-mentioned range of optimal parameters a_x and a_y .

A comparison of the maximal lifetime and maximal vibrational energy that can be accumulated by long-lived DBs of different spatial dimensions in fcc metals is presented in Table 2. In our previous studies, these characteristics have been established for one-dimensional DB [20] and two-dimensional DBs excited on the basis of eight one-component DNVMs [23]. The maximum lifetimes for one-dimensional DB and two-dimensional DB studied in the present work are comparable, while two-dimensional DBs excited based on one-component DNVMs live for a much longer time in Cu and Ni. The vibrational energy that can be accumulated on the oscillating atoms of DBs of different spatial dimensions is approximately the same for Al and Cu, and differs by more than two times for Ni (see Table 2). One-component two-dimensional DBs live longer than two-component two-dimensional DBs, but the latter can accumulate more vibrational energy per atom.

4 Conclusions

For the first time, it was demonstrated that two-dimensional DBs can be excited based on the two-component DNVM in a (111) close-packed atomic plane in fcc metals (Al, Cu, and Ni). Molecular dynamics simulations at a zero temperature have shown that the atomic oscillations are localized in one direction and delocalized in the other two directions, and therefore,

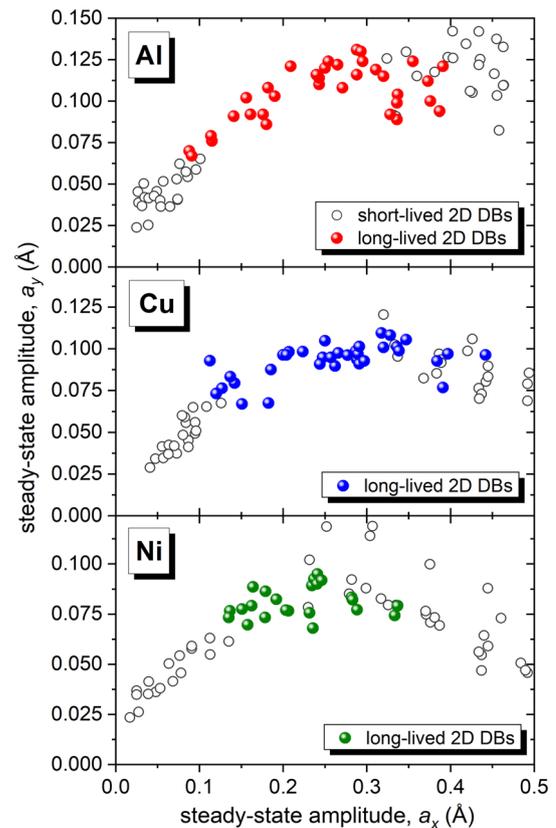


Fig. 6 The steady-state amplitudes a_x and a_y for all excited DBs in Al, Cu, and Ni. Colored volumetric circles indicate long-lived two-dimensional DBs, whose lifetime exceeds 5 ps. Empty circles depict short-lived DBs in the studied fcc metals

this spatially localized vibrational mode can be considered as a two-component two-dimensional DB. The maximum lifetimes are found to be 24.4 ps for Al, 13.9 ps for Cu, and 12.2 ps for Ni. The maximum values of vibrational energy for long-lived DBs are in the range of 0.5–1.0 eV per atom. This kinetic energy, which is localized on the oscillating atoms, can be sufficient to overcome local potential barriers, which can contribute to an increase in the diffusion rate. The studied two-dimensional DBs have a hard-type of nonlinearity in all three fcc metals, which means that the oscillation frequency increases with increasing amplitude. The ranges of steady-state amplitudes, in which long-lived two-dimensional DBs exist, were determined. These regions are quite similar for the studied fcc metals. Outside this stability range, the lifetimes of two-dimensional DBs are rather short. DB quickly radiate their vibrational energy into the crystal. The decay of two-dimensional DB occurs by a gradual decrease in its spatial dimension. First, the DB becomes a one dimensional via damping of atomic oscillations along the y -axis, and second, the kinetic energy is concentrated on 6–8 atoms in the atomic rows along the x -axis, which corresponds to a formation of zero-dimensional DB.

Table 2 Comparison of the maximal lifetime (ps) and maximal vibrational energy (eV) per atom calculated for long-lived DBs of different spatial dimensions in fcc metals (Al, Cu, and Ni)

DB type	Al		Cu		Ni	
	Lifetime	Energy	Lifetime	Energy	Lifetime	Energy
One-dimensional [20]	16.1	0.6	17.1	1.1	15.3	2.2
Two-dimensional (one-component) [23]	21.5	0.4	47.1	0.7	37.1	0.6
Two-dimensional (two-component)	24.4	0.5	13.9	0.8	12.2	1.0

A new class of long-lived spatially localized vibrational modes (two-dimensional DB), which can be excited in fcc metals on the basis of two-component DNVN, has been investigated. However, the question of the possibility of DB excitation based on the other two-component DNVNs remains open and is a natural continuation of this work. In addition, the results presented in this work will be useful in establishing the influence of two-component two-dimensional DBs on physical properties of fcc crystals.

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Author contributions

All the authors were involved in the preparation of the manuscript. All the authors have read and approved the final manuscript.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: The raw/processed data required to reproduce these findings cannot be shared at this time as the data also form part of an ongoing study.]

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