



Two-dimensional discrete breathers in fcc metals

O.V. Bachurina^{a,*}, A.A. Kudreyko^b

^a Ufa State Petroleum Technological University, Kosmonavtov str. 1, 450062 Ufa, Russia

^b Bashkir State Medical University, Lenina str. 3, 450008 Ufa, Russia

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ABSTRACT

The interest in discrete breathers (DB), i.e. a time-periodic and spatially localized vibrational mode in a defect free nonlinear lattice, is related to their ability to localize vibrational energy of the order of several eV. In the present work, for the first time, a systematic study of eight nonlinear vibrational modes localized in one spatial dimension and delocalized in the two other dimensions is performed by means of molecular dynamics simulations in defect-free single crystals of fcc metals (Al, Cu and Ni). For this goal, the standard embedded atom method potentials are employed. Calculations are performed at a zero temperature in three-dimensional computational cells. Excitation of DBs takes place via displacement of the specified atoms from their equilibrium lattice sites according to the patterns corresponding to the delocalized nonlinear vibrational modes (DNVMs) found earlier for a two-dimensional triangular lattice. It is revealed that only four out of the eight studied DNVMs can support stable two-dimensional DBs with the lifetimes in the range of 24–47 ps and accumulate vibrational energy of the order of 2 eV per atom. All excited DBs are characterized by a hard type of nonlinearity, i.e. the frequency increases with the increasing oscillation amplitude. Obtained results indicate the presence of a wide variety of nonlinear, spatially localized vibrational modes in three-dimensional lattices of fcc metals.

1. Introduction

In recent decades, there has been considerable interest in physical and technological processes in which materials are exposed to influence of high-energy particles [1]. This, in turn, causes a significant displacement of atoms from their equilibrium positions in a crystal lattice, where the nonlinear nature of interatomic interactions is fully manifested. In this case, describing the scattering channels of external energy and mechanisms of matter transport are very important. Nonlinear lattice oscillations, which are responsible for the spatial localization of vibrational energy, play a significant role in these processes. In particular, vibrational energy localized on a few atoms can help them to overcome potential barriers and contribute to evolution of a defect structure.

Nonlinear lattice oscillations can be classified as delocalized and spatially localized. In the first case, a group of atoms oscillates with amplitudes significantly higher than the other atoms in a crystal lattice and possesses a translational symmetry in all coordinate directions; in the second case, only a small group of atoms oscillates with high amplitudes. This stimulates for searching the ways to classify lattice oscillations according to various criteria, including their spatial dimension, different types of crystal lattice and chemical bonds. In this regard,

the study of various vibrational modes of large amplitude in metals is an actual task of modern nonlinear physics.

A time-periodic and spatially localized vibrational mode in a defect free nonlinear lattice is called discrete breather (DB). Three different mechanisms of DB excitation in nonlinear crystals are known: (1) spontaneous thermofluctuational generation at thermodynamic equilibrium [2–6]; (2) an external periodic force with a frequency outside the phonon spectrum of the system [7–9]; (3) modulation instability of a short wave length vibrational mode, which results in spatial energy localization in the form of large-amplitude DBs [10,11].

Intensive development of molecular dynamics methods and interatomic potentials has allowed to study the properties of zero-dimensional (conventional) and one-dimensional DBs in materials with different crystal lattices [12–27], while the properties of two-dimensional DBs, i.e. localized in one spatial dimension and delocalized in the two other dimensions, have not yet been sufficiently investigated in three-dimensional lattices. Recently, such an attempt has been made in Ref. [28], where only one (out of the eight possible) delocalized nonlinear vibrational modes (DNVMs) has been used for excitation of two-dimensional DBs in fcc crystals (Al, Cu, and Ni). It turned out that DBs excited in the (1 1 1) plane demonstrate a hard type of nonlinearity and can exist in all three fcc metals during the time range of 17–22 ps.

* Corresponding author.

E-mail address: obachurina@yahoo.com (O.V. Bachurina).

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The present work is aimed to study two-dimensional DBs excited using eight DNVMs in three-dimensional fcc single crystals (Al, Cu, and Ni) by means of molecular dynamics simulations. It should be emphasized that only one-component DNVMs characterized by a single parameter (oscillation amplitude) are considered here in contrast to the two-component DNVMs (with two different oscillation amplitudes within the same mode) studied recently in Ref. [29].

2. Model description and simulation setup

DNVMs are exact solutions of nonlinear equations of atomic motion, which are completely determined by the symmetry of a crystal lattice [30] and therefore do not depend on the type of the used interatomic potential. Chechin and Ryabov with the help of group-theoretical approach [31,32] have derived eight one-component DNVMs in a two-dimensional triangular lattice, which are schematically illustrated in Fig. 1. Since a close-packed (1 1 1) plane in fcc crystal exactly represents a two-dimensional triangular lattice, these DNVMs can be used as the start configurations for excitation of two-dimensional DBs in fcc lattice. It should be noted that according to Ref. [32], DNVMs 1, 2, 4, and 5 are symmetrical, in which the maximal positive and negative deviations from the equilibrium lattice positions are equal in absolute value, while DNVMs 3, 6, 7, and 8 are asymmetrical, since for them the positive and negative deviations are not equal.

Further, these eight DNVMs are excited and their lifetimes are investigated. If the frequency of atomic oscillations of DNVM (1) increases with increasing amplitude, (2) is above the upper edge of the phonon spectrum of the crystal, and (3) its lifetime exceeds 15 oscillations, then such DNVM can be called as stable two-dimensional DB, since atomic oscillations are localized in one direction and delocalized in the two other directions.

Molecular dynamics simulations are performed with the use of the LAMMPS software package [33]. Interatomic interactions in the chosen fcc metals are described via the embedded atom method potentials taken from the LAMMPS library [34,35]. These interatomic potentials have been previously used to study, in particular, one-dimensional DBs in fcc metals [26] and two-component DNVM in Ni [29]. The equilibrium lattice constants at $T = 0$ K reproduced by the used interatomic potentials are 4.05 Å for Al, 3.62 Å for Cu, and 3.54 Å for Ni.

One of the main difficulties emerging during molecular dynamics simulations is the search of initial conditions at which DBs can be successfully excited. Therefore, the amplitudes of initial atomic displacements from the equilibrium lattice sites are varied in the wide range of 0.05 to 0.75 Å, while the other atoms have zero initial displacements. All atoms at the beginning of the simulation have zero initial velocities. The time step is chosen equal to 1 fs, which is sufficient for this type of simulations. Periodic boundary conditions are applied along the three orthogonal directions of the computational cell.

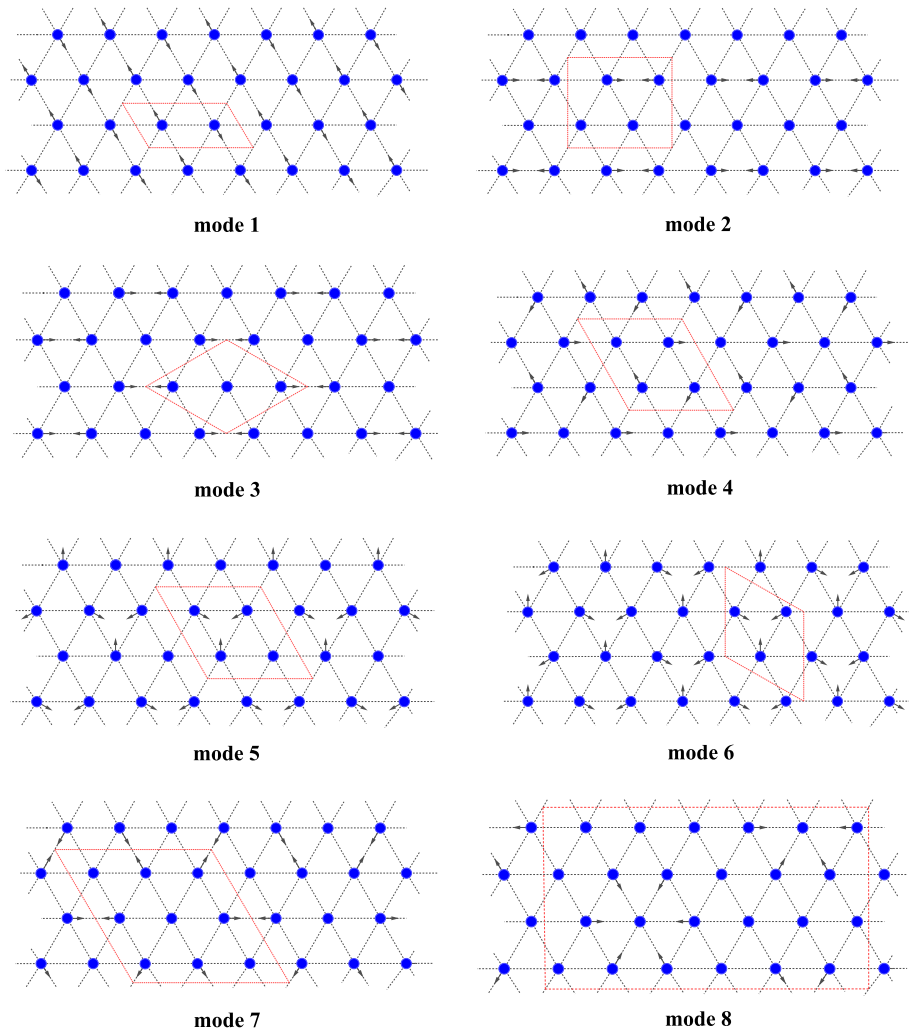


Fig. 1. Eight one-component DNVMs found in Refs. [31,32]. DNVMs 1, 2, 4, and 5 are symmetrical, DNVMs 3, 6, 7, and 8 are asymmetrical. The red dashed line shows the unit cell of the vibrational state in the plane. The black arrows indicate atomic displacements from the equilibrium lattice sites. The length of all displacement vectors at the initial moment of time is the same for all atoms in DNVM and equal to A .

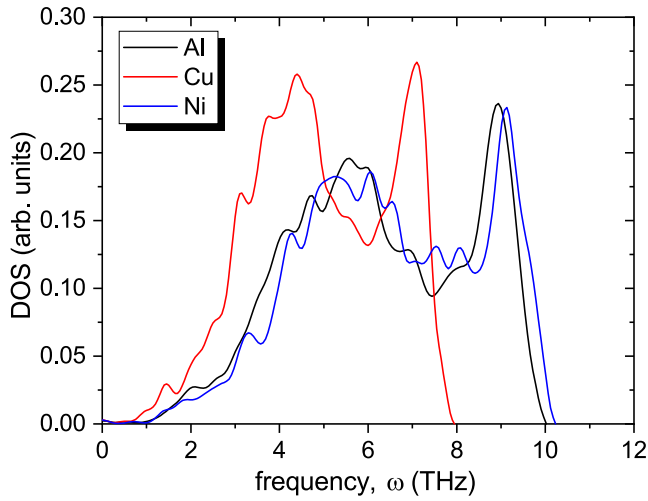


Fig. 2. The phonon density of states (DOS) calculated for fcc metals (Al, Cu, and Ni).

All molecular dynamics simulations are performed at zero initial temperature $T = 0$ K using the NVE thermodynamic ensemble (constant number of atoms, volume, and energy). It should be noted that the usage of zero temperature is preferable for the observation of the studied phenomena, since the thermal fluctuations of neighboring atoms considerably disturb oscillation of the atoms belonging to DNVM and thus reduce the lifetime of two-dimensional DB. The duration of simulations is limited to 4×10^4 timesteps, which corresponds to 40 ps.

The phonon density of states (DOS) is calculated according to the standard method implemented in LAMMPS. The Green's function molecular dynamics method involves calculation of the dynamical matrix based on fluctuation–dissipation theory for a group of atoms and described in detail in Refs. [33,36]. The measure of the Green's function is occurred every 10 timesteps, and totally 10 million timesteps at a constant temperature of 20 K using NVT thermodynamic ensemble (constant number of atoms, volume, and temperature) are performed. The DOS calculated for Al, Cu, and Ni are presented in Fig. 2. The upper edges of phonon spectrum, which are the most important for this study, are 10.0 THz for Al, 7.9 THz for Cu, and 10.3 THz for Ni.

The relevant data regarding the sizes of the computational cell, the number of atoms in them, equilibrium lattice constants at $T = 0$ K and the upper edge of phonon spectrum for the studied fcc metals are summarized in Table 1.

3. Simulation results and discussion

Molecular dynamics simulations reveal that only DNVMs 2, 3, 5, and 7 out of the eight illustrated in Fig. 1 can support stable two-dimensional DBs, while DNVMs 1, 4, 6, and 8 are found to be unstable in all three fcc metals and dissipate their vibrational energy during a few oscillation periods on the neighboring atoms in the form of small-amplitude waves. It should be reminded that DNVMs 2 and 5 are symmetrical and DNVMs 3 and 7 are asymmetrical. The simulation results

are summarized in Table 2. All atomic oscillations of the stable two-dimensional DBs are localized in one atomic plane of the three-dimensional crystal, where they were initially excited. The amplitude of atomic oscillations decreases exponentially with the distance from this plane.

The dependences of the lifetime, oscillation frequency, and total vibration energy per atom for four stable DBs excited based on DNVMs 2, 3, 5, and 7 on the initial amplitude A are shown in Fig. 3. In the range of small initial amplitudes $A = 0.05$ – 0.15 Å for Al, $A = 0.05$ – 0.10 Å for Cu, and $A < 0.05$ Å for Ni, the lifetimes are short and do not exceed 5 ps. It is interesting to note that the lifetime maxima are reached for DBs excited based on DNVM 2 and are equal to 23, 47, and 37 ps at initial amplitudes of 0.25, 0.20, and 0.20 Å for Al, Cu, and Ni, respectively. The second long-lived DBs (18 ps for Al, 25 ps for Cu, and 17 ps for Ni) are excited by means of DNVM 5 at almost the same initial amplitudes as for DNVM 2. The corresponding lifetimes of DBs excited using DNVM 7 are noticeably lower than those for DNVM 2 and 5. DB based on DNVM 3 can be excited only at higher amplitudes and its lifetime is considerably lower in comparison with the other stable DBs. As seen in Fig. 3, the lifetimes of two-dimensional DBs are rather short outside the range of initial amplitudes specified in Table 2. The fact that excitation of DBs in Ni begins at lower initial amplitudes as compared with Al and Cu is due to the harder bonds between atoms in the crystal lattice.

All two-dimensional DBs excited on the basis of one-component DNVM 2, 3, 5, and 7 obtain a hard type of nonlinearity, i.e. demonstrate an increase of the oscillation frequency with the increasing amplitude. For all metals, the slope of the dependences frequency vs. initial amplitude at low amplitudes differs from that at higher amplitudes. It is related to the fact that at larger atomic displacements from the equilibrium lattice sites the core of the interatomic potential contributes more significantly to the dynamics of the system as compared to its soft tail. The oscillation frequencies of all stable DBs are above the upper edge of the phonon spectrum of the corresponding fcc metals, thus providing noninteraction with the lattice phonons.

The full (kinetic plus potential) vibrational energy per oscillating atom of DBs excited using DNVMs 2, 3, 5, and 7 as function of initial amplitude is demonstrated in Fig. 3. As expected, the energy increases with the increasing amplitude. At low initial amplitudes ($A \leq 0.2$ Å), the differences between the dependences $E(A)$ for all four stable DBs are very small, and the data points are almost overlay each other. At higher amplitudes ($A \geq 0.2$ Å) the behaviors of the curves for Al are noticeably different for different DBs. In particular, a clear saturation of the vibrational energy vs. initial amplitude is seen for DBs excited by means of DNVMs 2 and 5, but it does not occur for DB excited based on DNVM 7, and the energy continues to increase with the increasing amplitude. At the same time, these differences are not so distinctly pronounced for Cu and Ni even at high initial amplitudes (see Fig. 3) and corresponding curves for these two metals behave similarly. Two-dimensional DBs with the lifetimes longer than 5 ps can accumulate up to 0.6 eV for Al, 1.0 eV for Cu, and 1.5 eV for Ni of the vibrational energy per atom. At higher initial amplitudes and lower lifetimes, accumulated vibrational energy of two-dimensional DBs can reach the values of 3 eV. It is worth noting the following tendency, which directly follows from the obtained

Table 1

The sizes of the three-dimensional computational cells along the x-, y- and z-directions, number of atoms (N) used for calculation of eight DNVMs, lattice constant a_0 at $T = 0$ K and the upper edge of phonon spectrum (ω) for the studied fcc metals.

Metal	a_0 (Å)	ω (THz)	computational cell (Å)		N	
			DNVMs 1, 2, 4, 5	DNVMs 3, 6, 7, 8	DNVMs 1, 2, 4, 5	DNVMs 3, 6, 7, 8
Al	4.05	10.0	$125.1 \times 78.8 \times 76.6$	$119.4 \times 59.1 \times 76.6$	46,464	33,264
Cu	3.62	7.9	$112.5 \times 70.8 \times 68.9$	$107.4 \times 53.1 \times 68.9$	46,464	33,264
Ni	3.54	10.3	$109.5 \times 68.9 \times 67.1$	$104.5 \times 51.7 \times 67.1$	46,464	33,264

Table 2

Summary of the simulation results of eight DNVMs in fcc metals (Al, Cu and Ni). The sign “+” means that stable two-dimensional DB exists, and the “-” sign means that excitation of DB based on this DNVM does not occur. The range of initial amplitudes (in Å) at which long-lived two-dimensional DBs can be excited is presented below.

Metal	DNVMs							
	1	2	3	4	5	6	7	8
Al	-	+	-	-	+	-	+	-
		$0.15 \leq A \leq 0.55$			$0.15 \leq A \leq 0.40$		$0.40 \leq A \leq 0.70$	
Cu	-	+	+	-	+	-	+	-
		$0.15 \leq A \leq 0.50$	$0.50 \leq A \leq 0.70$		$0.15 \leq A \leq 0.35$		$0.40 \leq A \leq 0.70$	
Ni	-	+	+	-	+	-	+	-
		$0.10 \leq A \leq 0.45$	$0.45 \leq A \leq 0.70$		$0.15 \leq A \leq 0.30$		$0.35 \leq A \leq 0.65$	

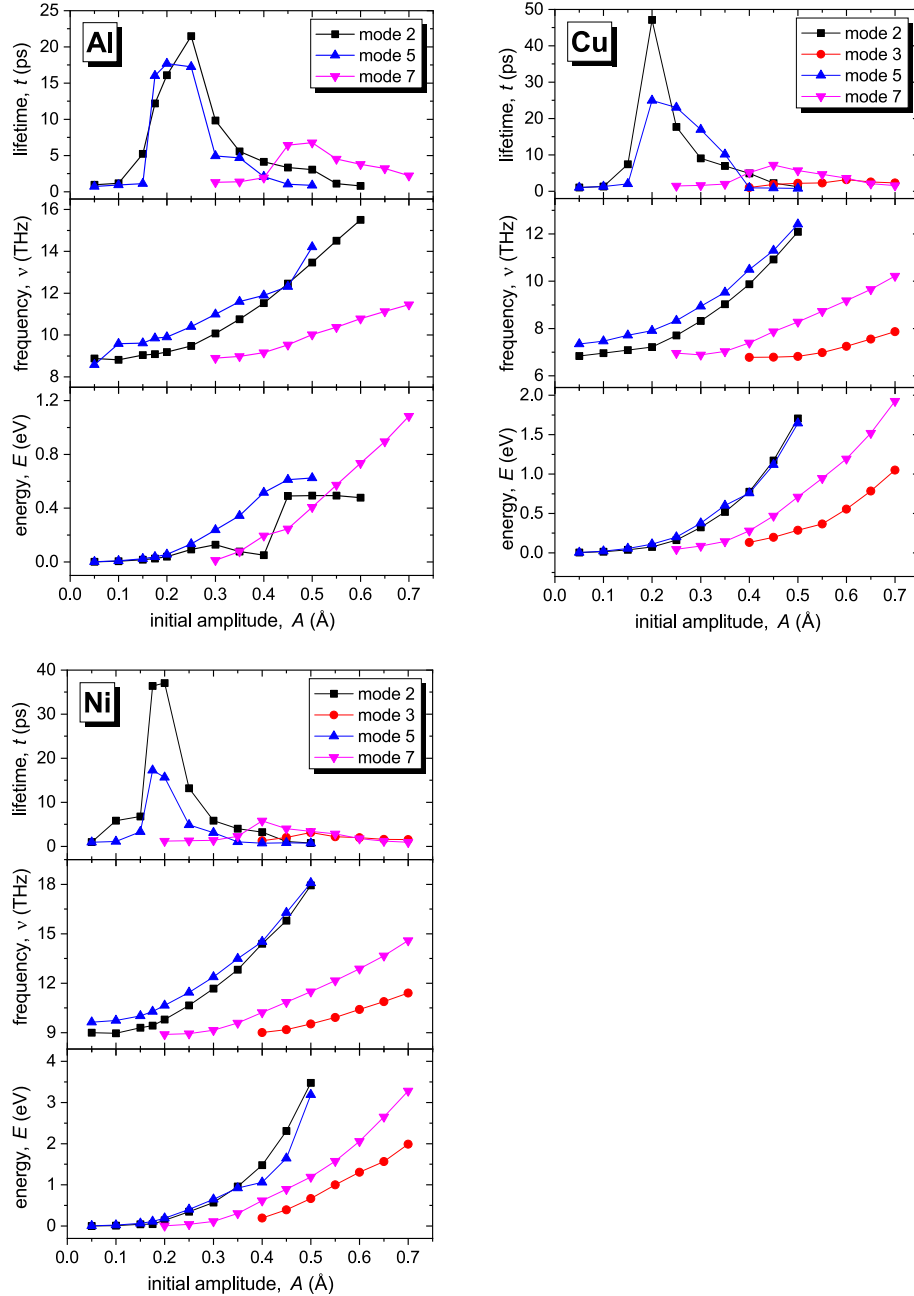


Fig. 3. The lifetime, oscillation frequency, and full vibration energy per atom of two-dimensional DBs as functions of initial oscillation amplitude A calculated for fcc metals (Al, Cu, and Ni). The numbers in the legend indicate the corresponding DNVMs illustrated in Fig. 1, based on which two-dimensional DBs are excited. The results are presented only for stable two-dimensional DBs. The solid lines interpolating the data points are guides to the eye.

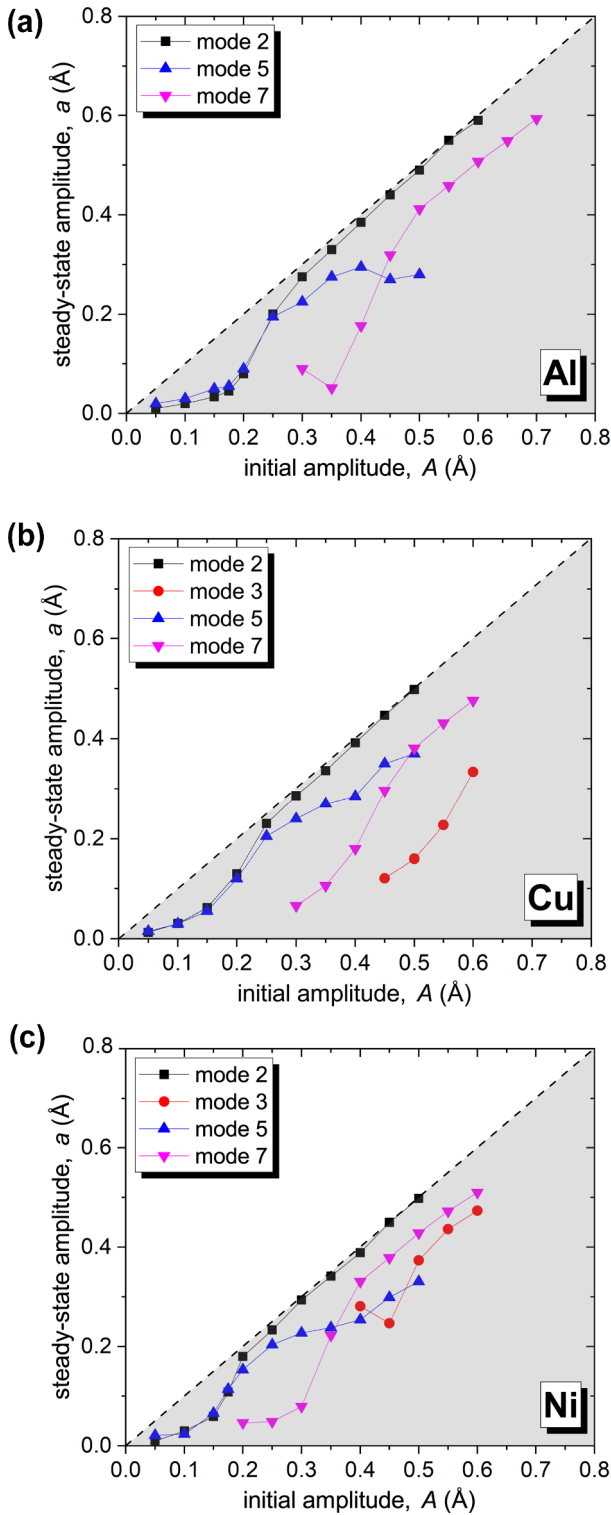


Fig. 4. Steady-state amplitude of two-dimensional DBs as functions of initial displacement amplitude calculated for Al, Cu, and Ni. The numbers in the legend indicate the corresponding DNVMs illustrated in Fig. 1, based on which two-dimensional DBs are excited. The results are presented only for stable two-dimensional DBs. The dashed line, as a guide, demonstrates the dependence of $a = A$. The gray area shows the region where $a < A$. The solid lines interpolating the data points are guides to the eye.

results. Namely, the harder the bonds between atoms in crystal lattice, the less the vibrational energy differentiation between the stable DBs.

The dependences of the steady-state amplitude (a) vs. the initial

amplitude (A) for Al, Cu, and Ni are demonstrated in Fig. 4. For DBs, excited on the basis of DNVM 2, after a certain transient period occurring at low amplitudes, the linear dependence $a(A)$ is observed at $A \geq 0.25$ Å. Note that the data points for DNVM 2 are rather close to the line $a = A$, but still below it, i.e. an inequality $A > a$ is always fulfilled. The steady-state amplitudes for DB excited using DNVM 5 are also always less than the corresponding initial ones. This is a clear demonstration of the fact that the energy initially given to the atoms of DNVMs dissipates during several oscillation periods in the form of low-amplitude oscillations onto neighboring atoms.

Similar ratio $A > a$ is observed for asymmetrical DNVMs 3 and 7, while DNVM 3 in Al is found to be unstable (see Fig. 4). As shown by the preliminary calculations, which are not included in the present paper, this ratio can be violated for asymmetrical DNVMs, i.e. $A \leq a$, and depends on the direction along which the atomic displacements are initiated. This fact can be easily explained in the following way. Inasmuch as the maximal positive and negative displacements of atoms from their equilibrium lattice sites are not equal in absolute value for asymmetrical DNVMs (for details see Ref. [32]), then there are always “the long” and “the short” arms in atomic oscillations. Initial displacement A along “the long” arm will lead to a displacement A/α along “the short” arm, where the coefficient $\alpha > 1$. In the case when initial displacement A is assigned along “the short” arm, atomic displacement along “the long” arm from the equilibrium site results in α -times larger displacement, i.e. $\alpha \times A$. Thus, initiation of atomic displacements along “the short” arm in the chosen amplitude range provoked fast energy dissipation on neighboring lattice atoms and, as consequence, instability of asymmetrical DNVMs. Therefore initial atomic displacements for all asymmetrical DNVMs in this work were performed along “the long” arm.

Molecular dynamics simulations of two-dimensional DBs excited on the basis of the one-component DNVM 5 have been performed for three fcc metals (Al, Cu, and Ni) in a larger computational cell [28], which gives an opportunity to elucidate a dependence of the simulation results on the cells size. Comparative analysis shows that an increase of computational cell does not lead to noticeable altering of the all three dependencies (steady-state amplitude, lifetime, and frequency as the functions of initial displacement amplitude).

Due to the lack of the simulation data, the following comparison with DBs of different dimensions is of preliminary character. Nevertheless, let us compare the maximal lifetimes of one-dimensional DBs [26] and two-dimensional DBs excited on the basis of the two-component DNVM [29] with the present results. Comparison is made only for Ni, due to the lack of the results for the other fcc metals in Ref. [29]. The maximal lifetimes are 15 ps for one-dimensional DB [26], 9.5 ps for two-dimensional DBs excited using two-component DNVM [29], and 38 ps for two-dimensional DBs excited on the basis of the one-component DNVM 5 (see Fig. 3). Therefore, it can be concluded that the two-dimensional DBs are the most long-lived ones among the studied earlier, which opens up new perspectives of their experimental observation.

The decay of one-component DBs investigated here differs from that previously found for two-component DBs [29]. Namely, no gradual decrease of its spatial dimension via first formation of oscillating chains (one-dimensional DBs) in the origin plane, and further dissipation of their vibrational energy onto neighboring atoms are observed. On the contrary, the decay of one-component DBs occurs at some moment of time by the deviation of one (or several) oscillating atoms from the given displacement vector, which is caused by the loss of vibrational energy due to interaction with nearest neighbors, and results in a displacement cascade that propagates very quickly in a given plane. After several oscillation periods, most atoms return to their equilibrium lattice sites, and only a few of them jump into the neighboring interstitial lattice sites and remain there up to the end of the simulation. It is obvious, that such jumps can occur only at large initial amplitudes, which, for example, for DB excited on the basis of asymmetrical DNVM 7 are

$A \geq 0.65 \text{ \AA}$ (Al), $A \geq 0.6 \text{ \AA}$ (Cu), and $A \geq 0.65 \text{ \AA}$ (Ni). It is worth noting that this discrepancy between the initial amplitude and the bond stiffness of the fcc metals can be easily explained by the difference in the lattice parameters. Namely, among the studied fcc metals Al has the largest lattice parameter a_0 (see Table 1), while Ni has the smallest one. Therefore, the ratios A/a_0 are 0.160 (Al), 0.166 (Cu), and 0.184 (Ni), i.e. they increase as expected with increasing bond stiffness. Thus, the energy released during the destruction of two-dimensional DBs can lead to the knocking out of atoms from the crystal lattice sites and to an appearance of interstitial atoms contributing to evolution of a defect structure.

4. Conclusions

For the first time, the possibility of existence of two-dimensional DBs localized along one direction and delocalized along the two other spatial directions in three-dimensional single crystal of fcc metals (Al, Cu, and Ni) was demonstrated via molecular dynamics simulations. The eight one-component DNVs determined earlier by Chechin and Ryabov for two-dimensional triangular lattice by means of group-theoretical approach were used for excitation of two-dimensional DBs. It was found that stable DBs can be excited on the basis of four out of the eight DNVs (2, 3, 5, 7). The lifetimes of these DBs are in the range of 24–47 ps. DBs can accumulate vibrational energy of the order of 0.6–1.5 eV per atom, which is more than sufficient to overcome potential barriers and locally facilitate diffusion processes. The stable two-dimensional DBs in fcc metals are characterized by a hard type of nonlinearity, i.e. the frequency increases with the oscillation amplitude. The other four DNVs (1, 4, 6, 8) are found to be unstable in three-dimensional lattice and quickly radiate their vibrational energy into the crystal.

Obtained results broaden our understanding of variety of nonlinear spatially localized vibrational modes in fcc metals and opens up new class of two-dimensional DBs which are yet to be explored in the near future in materials with different crystal lattice. A logical continuation of the present work will be an investigation of possibility of excitation of plane-radial DBs by imposing a localized radial function on the stable DNVs, similar to that studied recently in Ref. [28]. It is also tempting to investigate two-dimensional DNVs on the close-packed surfaces of fcc and hcp metals [37]. The final goal of studying DBs in crystals is to understand their possible contribution to macroscopic [38] and tribological [39,40] properties of materials.

CRedit authorship contribution statement

O.V. Bachurina: Data curation, Formal analysis, Investigation, Validation, Visualization, Writing - original draft, Writing - review & editing. **A.A. Kudreyko:** Formal analysis, Visualization, Writing - review & editing.

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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