



# Influence of two-dimensional discrete breathers on the macroscopic properties of fcc metals

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**Abstract.** Delocalized nonlinear vibrational modes (DNVMs) in crystals are precise solutions to the equations governing atomic motion that are determined solely by the symmetry of the lattice. This study investigates the influence of two-dimensional discrete breathers (DBs) excited using four one-component DNVMs on the macroscopic properties of three-dimensional fcc single crystals of Al, Cu, and Ni. All results were obtained using molecular dynamics simulations. Key findings include the observation that the lifetime of two-dimensional DBs is significantly influenced by both the symmetry of the DNVM and the initial oscillation amplitude. The two-dimensional DBs exhibit hard-type nonlinearity, characterized by an increase in oscillation frequency with increasing initial amplitude. The excitation of the DBs leads to a reduction in the crystal's heat capacity, which becomes more pronounced with increasing amplitude. The presence of two-dimensional DBs induces thermal expansion within the crystal, suggesting an impact on the mechanical properties of the material. This research provides new insights into the role of DBs, in influencing the macroscopic properties of fcc metals.

## 1 Introduction

Chechin and Sakhnenko have developed a general theory of delocalized nonlinear vibrational modes (DNVM), which they originally called bushes of nonlinear normal modes, in dynamical systems with discrete symmetry using a group-theoretical approach [1–3]. DNVM is an exact solution of the nonlinear dynamical equations governing atomic motion. These vibrational modes are delocalized in space and periodic for systems with translational symmetry. Since only the symmetry of the lattice is taken into account, the solution of the dynamical equations for a given lattice is independent of the nature of the interaction between particles and the amplitude of their oscillations. This approach has recently been employed in the analysis of all possible DNVMs in both triangular and square lattices [4, 5].

The vibrational modes in crystalline lattices can be classified according to their spatial dimensionality and the number of components. A DNVM that is governed by  $n$  coupled equations of motion is characterized by  $n$  degrees of freedom and is referred to as an  $n$ -dimensional mode. One-dimensional DNVMs are constrained to a single spatial dimension within the lattice. In defect-free crystals, such modes often

take the form of linear chains where the vibrational energy propagates primarily along the chain. Two-dimensional DNVMs are delocalized along two spatial dimensions while exhibiting localization along the third. Three-dimensional DNVMs extend across all spatial dimensions within the crystal. The number of components corresponds to the number of independent parameters that characterize a given vibrational mode, namely the amplitude of atomic displacements from the equilibrium lattice sites. Presently, the majority of research in this field is focused on the investigation of one-component DNVMs in materials with different crystalline structures [6–15]. Due to the considerable diversity and complexity of two- and three-component DNVMs, their investigation has been relatively limited [16–18].

One of the interesting and promising practical applications of DNVM, as recently elucidated in Ref. [19], is the possibility of assessing the precision of the interatomic potential via analysis of the trajectories of atomic motion, as an alternative to the conventional approach of analyzing the configuration of atoms.

Discrete breathers (DBs), also known as time-periodic and spatially localized vibrational modes, represent a unique type of nonlinear oscillation in defect-free, nonlinear lattices. DBs can be excited through

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(1) spontaneous generation through thermal fluctuations [20–23], (2) the effect of an external periodic force at frequencies beyond the phonon spectrum of a crystal [24–26], and (3) modulation instability resulting in energy localization [27, 28]. Furthermore, DBs can be excited by imposing a localizing function on DNVMs [29–34].

Over the past decade, DBs have attracted considerable attention from researchers and have been analyzed in various crystals [8, 35–47]. The consequence of the modulation instability of the DNVM is the formation of chaotic DBs that oscillate with a frequency lying outside the phonon spectrum of the crystal. Such DBs are formed as a result of the decay of the DNVM and the concentration of vibrational energy on specific particles. The formation of chaotic DBs and the effect of the relative stiffness of the first- and second-neighbor interactions have recently been the subject of intensive investigation in a number of different crystal lattices using the Fermi-Pasta-Ulam-Tsingou interatomic potential [48–51].

The main properties of DNVMs and DBs excited on their basis in various crystals have been well investigated, but their influence on the macroscopic properties of crystals remains very limited [10, 48, 52]. The aim of the present work is molecular dynamics study of the influence of two-dimensional DBs on the macroscopic properties of fcc metals, namely Al, Cu and Ni, with particular emphasis on the effects on heat capacity and thermal expansion. The two-dimensional DBs were excited in a three-dimensional crystal lattice based on the previously studied four stable one-component DNVMs [13], which are characterized by a single parameter (vibrational amplitude). By exploring these vibrational modes and their impact on material properties, this work contributes to a broader understanding of nonlinear dynamics in crystal lattices and their potential applications.

## 2 Stable delocalized nonlinear vibrational modes in an fcc lattice

Using a group-theoretical approach, Chechin and Ryabov [53, 54] have derived eight one-component DNVMs for a two-dimensional triangular lattice. Notably, the (111) plane of an fcc crystal corresponds to a two-dimensional triangular lattice, meaning that these DNVMs can be used as initial configurations to excite two-dimensional DBs within an fcc lattice. DNVMs are exact solutions to the nonlinear equations of motion for a two-dimensional triangular lattice. However, when a (111) plane of the fcc lattice is excited, they are no longer the exact solutions due to the presence of the neighboring atomic planes in the crystal structure. The excited plane shares part of its energy with the other planes, and in some cases, a significant part of the energy transferred to the plane remains localized in the plane for a long time. This phenomenon

is referred to as long-lived two-dimensional DBs, characterized by their localization in the direction normal to the excited plane while remaining delocalized in the other two spatial dimensions.

As stated in Ref. [54], these DNVMs exhibit different symmetries. DNVMs 1, 2, 4, and 5 are symmetrical, meaning the maximal positive and negative atomic displacements from equilibrium lattice sites are equal in magnitude. In contrast, DNVMs 3, 6, 7, and 8 are asymmetrical, as the positive and negative displacements differ in magnitude. This distinction in symmetry affects how these DNVMs behave under certain conditions.

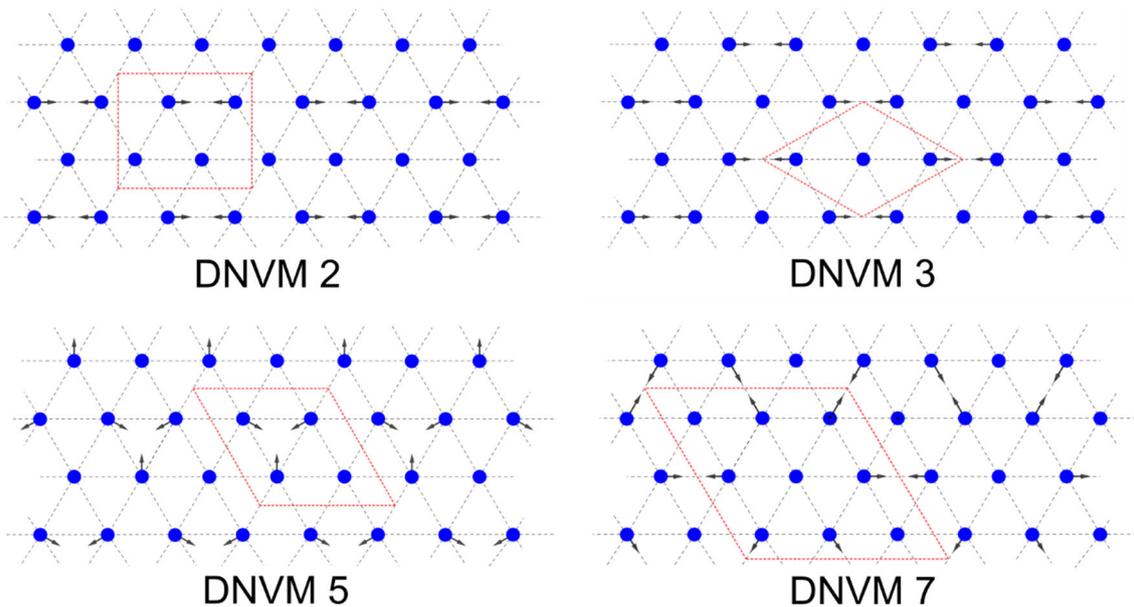
The results of recent molecular dynamics studies [13] indicate that only four of the eight one-component DNVMs are stable. The stability of the mode means that it can maintain periodic oscillations for a time longer than 5 ps. These are DNVMs 2, 5, and 7 for Al and DNVMs 2, 3, 5, and 7 for Cu and Ni. This implies that they are capable of maintaining periodic oscillations for a time of the order of several picoseconds, as well as accumulating and storing their vibrational energy. Figure 1 illustrates these four stable one-component DNVMs, namely 2, 3, 5, and 7, which were selected for study in this work. For the sake of clarity, the previously used DNVMs numbering [13] has been retained in the present paper. The black arrows in Fig. 1 indicate the displacement of atoms from their equilibrium lattice sites. The length of all displacement vectors at the initial moment of time is identical for all DNVM atoms and is equal to  $A$ .

## 3 Computational details

Molecular dynamics simulations were carried out using the LAMMPS software package [55], a widely recognized tool for simulating the behavior of atomic systems. The interatomic forces in the selected fcc metals Al, Cu, and Ni were modeled using the embedded atom method (EAM) potentials. These potentials, sourced from the LAMMPS library [56, 57], are well-established for accurately describing the interactions in metallic systems. In our simulations, the equilibrium lattice constants at absolute zero temperature ( $T = 0$  K), as reproduced by the selected EAM potentials, were found to be 4.05 Å for Al, 3.62 Å for Cu, and 3.54 Å for Ni.

The computational supercells, comprising  $22 \times 12 \times 11$  translational cells (46,464 atoms) were used for the simulation of symmetrical DNVMs 2 and 5, while  $21 \times 9 \times 11$  translational cells (33,264 atoms) were employed for the simulation of asymmetrical DNVMs 3 and 7. The axes of the Cartesian coordinate system  $x$ ,  $y$ , and  $z$  is aligned with the crystallographic directions  $[10\bar{1}]$ ,  $[\bar{1}2\bar{1}]$ , and  $[111]$  within the computational cell.

One of the primary challenges in conducting molecular dynamics simulations is identifying the initial conditions under which the desired excitation of DB can be observed. In light of these circumstances, a systematic



**Fig. 1** Four stable one-component DNVMs derived for triangular lattice in Refs. [53, 54]. DNVMs 2 and 5 are symmetrical, while DNVMs 3 and 7 are asymmetrical. The black arrows indicate initial atomic displacements from the equilibrium lattice sites. The red dashed line outlines the unit cell of the vibrational state within the atomic plane. The length of all displacement vectors at the initial moment of time is the same for across all atoms in the DNVMs and is denoted as  $A$

variation in the initial amplitudes of atomic displacements from their equilibrium lattice sites was conducted across a broad range from 0.05 to 0.70 Å. Only a subset of atoms belonging to DNVM and lying in the same atomic plane within the computational cell was displaced, while the remaining atoms were left undisturbed at their equilibrium positions. Furthermore, all atoms were assigned zero initial velocities in order to eliminate any pre-existing kinetic energy that could interfere with the excitation of the vibrational mode.

The simulations were conducted with a timestep of 1 fs, which is sufficiently small to ensure the accurate integration of the equations of motion for the atoms. This is crucial for capturing the rapid atomic oscillations occurring during the excitation of DNVMs. In order to ensure that the simulated behavior of the system accurately reflects the bulk material properties, periodic boundary conditions were applied along all three orthogonal directions. This approach mimics an infinite crystal lattice and prevents the potential issues associated with edge effects.

All molecular dynamics simulations were performed at an initial temperature of  $T = 0$  K using the NVE ensemble (constant number of atoms, volume, and energy). The selection of zero temperature is of significant importance for this type of simulation, as it eliminates the influence of thermal noise. At finite temperatures, thermal fluctuations from neighboring atoms would interfere with the coherent oscillations of the DNVM atoms, making it difficult to isolate and analyze the vibrational modes under investigation. The duration of each simulation was limited to 40,000 timesteps, which is equivalent to 40 ps. This timescale was selected to achieve an optimal balance between computational

efficiency and the necessity of capturing sufficient vibrational dynamics for comprehensive analysis.

## 4 Computational results and discussion

DNVMs 2, 5, and 7 excited in Al and DNVMs 2, 3, 5, and 7 excited in Cu and Ni support stable periodic oscillations. The excitation of a time-stable vibrational mode based on DNVM 3 in Al was not possible over the full range of amplitudes, which is related to the softness of the interatomic bonds. Atomic oscillations of the selected four two-dimensional DNVMs remain localized to a single atomic plane within the three-dimensional crystal structure, from which they were initially initiated. The amplitude of atomic oscillations exhibits an exponential decay with increasing distance from this plane. The four stable DNVMs can thus be classified as spatially localized modes. According to the established definition, DBs are localized vibrational modes characterized by atomic oscillations confined to a small region of the lattice, with the surrounding atoms remaining relatively stationary. Consequently, the vibrational energy of DBs is highly localized to a few atoms or a small cluster of atoms. DNVMs are extended modes where atomic oscillations occur across the entire lattice, involving many atoms oscillating according to a given pattern. In contrast to DBs, the vibrational energy of DNVMs is evenly distributed throughout the lattice, rather than being concentrated in a specific region. Since stable DNVMs meet the broader definition of a DB, the concept of a DB can be expanded to include

DNVM. In this context, a DB can be considered two-dimensional, with its dimensionality corresponding to that of the DNVM used to excite it. Throughout the paper, the terms stable DNVM and two-dimensional DB will be used as synonyms. When a two-dimensional DB is excited in a densely packed atomic plane of an fcc crystal, the atoms vibrate strictly in-plane, without any displacement components perpendicular to it. Such perpendicular components only appear when the DB becomes unstable and is subsequently destroyed.

For the sake of completeness, it should be noted that the remaining DNVMs 1, 3, 4, 6, and 8 for Al and DNVMs 1, 4, 6, and 8 for Cu and Ni were found to be unstable upon excitation (for further details see [13]). The latter means that after several periods of oscillation, they dissipated their vibrational energy on neighboring atoms in the form of low-amplitude waves, which led to the rapid destruction of the structure of these modes.

The oscillation frequency as function of the initial amplitude  $A$  for the four stable DNVMs 2, 3, 5, and 7 is depicted in Fig. 2. A hard-type of nonlinearity is observed for all two-dimensional DBs, whereby the oscillation frequency increases as the amplitude rises. In all metals, the slope of the curves differs at low amplitudes compared to higher ones. This is due to the fact that at larger atomic displacements from equilibrium lattice sites, the core of the interatomic potential contributes more significantly to the system's dynamics, whereas at smaller displacements, the softer part of the potential is more influential. The oscillation frequencies of the DNVMs are consistently higher than the upper edge of the phonon spectrum for each fcc metal. This ensures that the DBs remain dynamically isolated from the lattice phonons, preventing energy transfer to the surrounding atoms and allowing the DBs to maintain their localized vibrational state for extended periods. This separation from phonon modes plays a critical role in sustaining the stability of the DBs. Consequently, these characteristics of hard nonlinearity and frequency isolation make the DBs resilient to decay, enhancing their potential influence on the material's properties at the nanoscale.

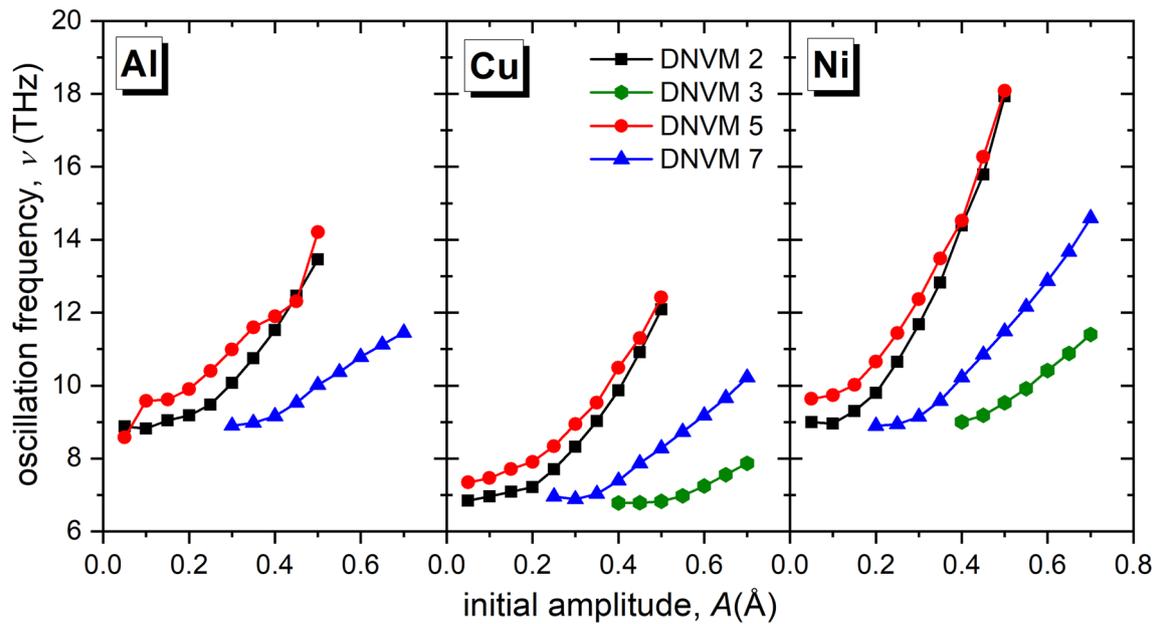
Figure 3 illustrates the relationship between lifetime and initial amplitude  $A$  for the four stable DNVMs 2, 3, 5, and 7. At small initial amplitudes, specifically  $A = 0.05\text{--}0.15$  Å for Al,  $A = 0.05\text{--}0.10$  Å for Cu, and  $A < 0.05$  Å for Ni, the DNVMs exhibit short lifetimes that do not exceed 5 ps. The latter suggests that the vibrational energy dissipates rapidly at low amplitudes. Therefore, such DBs excited based on the four selected DNVMs are unstable according to our specific criterion introduced in the previous section. The maximum lifetimes are achieved for DBs excited based on DNVM 2, with lifetimes of 23 ps for Al, 47 ps for Cu, and 37 ps for Ni at initial amplitudes of 0.25, 0.20, and 0.20 Å, respectively. DBs excited using DNVM 5 exhibit the second longest lifetimes, namely 18 ps for Al, 25 ps for Cu, and 17 ps for Ni, with the similar initial amplitudes as those for DNVM 2. DNVM 3 can maintain periodic oscillations in time for the order of several picoseconds only

at large initial amplitudes exceeding 0.35 Å. Therefore, DNVM 3 can be classified as a quasi-stable vibrational mode, and, consequently, two-dimensional DB excited on its basis in Cu and Ni can be considered as a quasi-stable DB. It should be noted that the classification of DBs is somewhat arbitrary and is based solely on the lifetime of the vibrational mode. This may vary depending on the interatomic potential used and, to a lesser extent, on the size of the computational cell. The aforementioned observations can be also applied to DNVM 7, which exhibits slightly enhanced lifetime in comparison to DNVM 3, as illustrated in Fig. 2. It is noteworthy that the longest lived DBs are observed at relatively low initial amplitudes, while at high amplitudes, the lifetime is significantly reduced. This indicates that the atoms, due to significant deviations from the equilibrium lattice sites, begin to rapidly dissipate their vibrational energy on neighboring atoms that were not initially excited. Thus, the investigated two-dimensional DBs are only stable within a specific amplitude range. Outside this range, the lifetimes are markedly reduced.

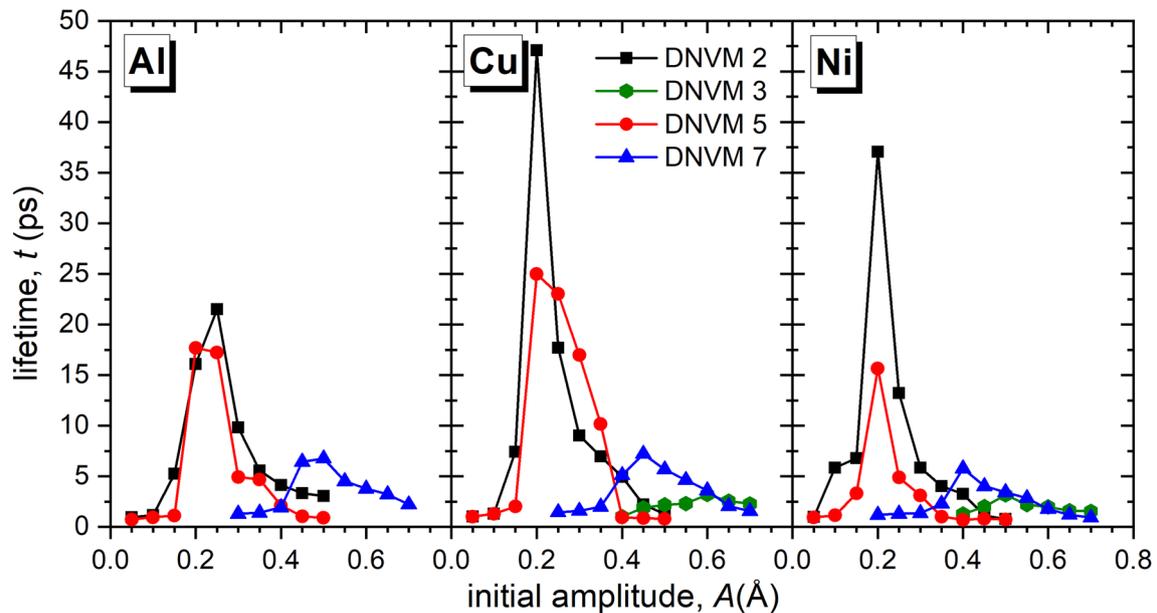
Another point to note is that the initiation of DB excitation in Ni occurs at smaller initial amplitudes than in Al and Cu. This behavior can be attributed to the stronger interatomic bonds in the Ni crystal lattice, which require less displacement to generate the necessary conditions for DB excitation. The difference in bond strength affects the dynamic properties of DBs in various metals, thereby underscoring the importance of atomic interactions in determining DB stability and lifetime across different materials.

One of the most straightforward methods to evaluate the nonlinearity of a crystal due to the excitation of a vibrational mode is to calculate the ratio of the system's total energy to its period-averaged kinetic energy, represented as  $C = E_{\text{total}}/\bar{E}_k$ . This ratio serves as an indicator of changes in the crystal's heat capacity. In harmonic systems, the averaged kinetic energy over a period is equal to the averaged potential energy, or  $\bar{E}_k = \bar{E}_p$ , which yields  $C = 2$ . In contrast, in nonlinear systems,  $\bar{E}_k \neq \bar{E}_p$ , resulting in  $C \neq 2$ . Therefore, the degree of deviation from  $C = 2$  reflect the degree of the nonlinearity of the system.

The dependence of the ratio  $C$  on the initial amplitude for the four two-dimensional DBs, excited the basis of DNVMs 2, 3, 5, and 7, is shown in Fig. 4. As can be seen, the degree of the nonlinearity of DNVMs 2 and 5 remains relatively small within the initial amplitudes not exceeding 0.20 Å, with the ratio  $C$  varying by less than 1%. A similar phenomenon is observed for DNVMs 3 and 7, albeit at higher initial amplitudes. The primary distinction between DNVMs 2 and 5 and the aforementioned vibrational modes is that their excitation begins at markedly higher initial amplitudes, specifically 0.20 Å for DNVM 7 and 0.40 Å for DNVM 3. This is due to the fact that the frequency of the atomic vibrations in this amplitude range is below the upper edge of the phonon spectrum. For all four DNVMs, an increase in the initial amplitude results in a roughly analogous decrease in the ratio  $C$ , which corresponds to



**Fig. 2** The oscillation frequency of the four stable DNVMs as functions of initial oscillation amplitude  $A$  calculated for Al, Cu, and Ni. The solid lines connecting the data points are provided as visual guides

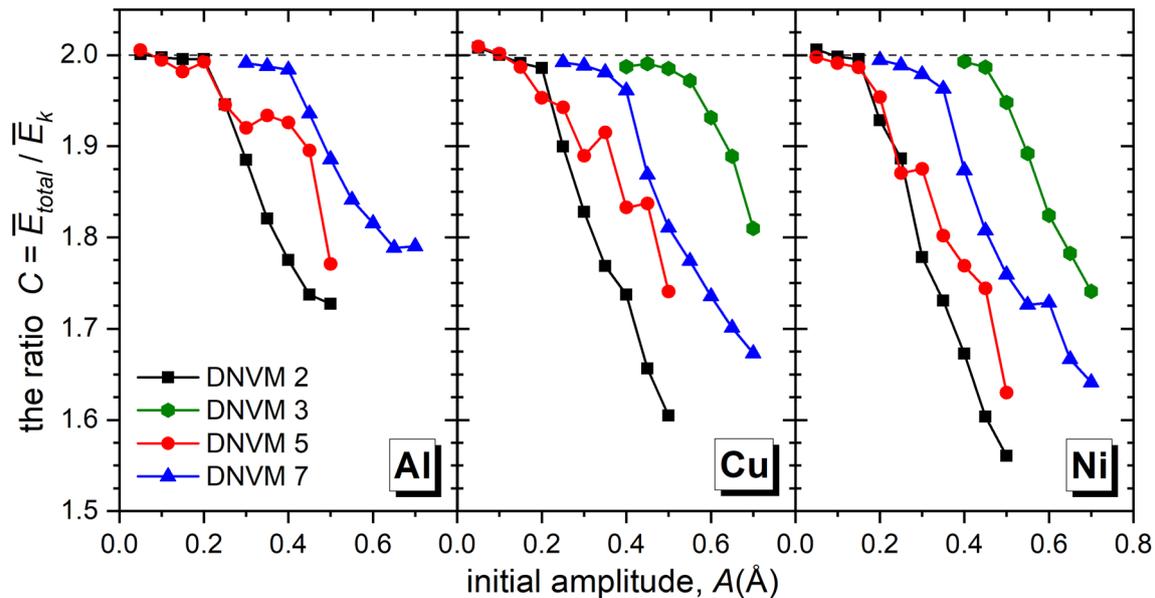


**Fig. 3** The lifetime of the four stable DNVMs as functions of initial oscillation amplitude  $A$  calculated for Al, Cu, and Ni. The solid lines connecting the data points are provided as visual guides

an increase in the deviation of the system from its equilibrium state. It can thus be concluded that the presence of a vibrational mode in a system exhibiting a hard type of nonlinearity invariably results in a reduction in the ratio  $C$  with an increase in the initial amplitude of atomic oscillations. In contrast, in materials with a soft type of nonlinearity, the ratio  $C$  tends to increase with increasing of initial amplitude [58]. It should also be noted that at this stage of the research, it is not possible to conclude which mode, based on its symmetry,

has the most pronounced effect on the ratio  $C$ , i.e., on the specific heat of the system.

Another interesting question is how the presence of an excited vibrational mode in the lattice affects the thermal expansion of the crystal. To investigate this, the dependence of the stress components  $\sigma_{xx}$ ,  $\sigma_{yy}$ , and  $\sigma_{zz}$  within the computational cell resulting from the excitation of two-dimensional DBs with respect to variations in the initial amplitude was analyzed. As a consequence of the inherent symmetry of the system (see



**Fig. 4** The ratio  $C$  (degree of the nonlinearity of the system) for the four stable DNVMs as functions of initial oscillation amplitude  $A$  calculated for Al, Cu, and Ni. The horizontal dashed line illustrates the value of  $C = 2$ , which is characteristic of harmonic systems, where the kinetic energy is equal to the potential energy. The solid lines connecting the data points are provided as visual guides

Fig. 1), two stress components exhibit approximate equality depending on the specific DNVM excited as demonstrated in Fig. 5. Namely, the relationship  $\sigma_{xx} \approx \sigma_{yy}$  is applicable to DNVMs 5 and 7, whereas the relevant relationship for DNVMs 2 and 3 is  $\sigma_{yy} \approx \sigma_{zz}$ . Additionally, the magnitude of the stress component  $\sigma_{xx}$  for the symmetrical DNVM 2 and 5 are comparable, while it differs significantly from those for the asymmetrical DNVM 3 and 7.

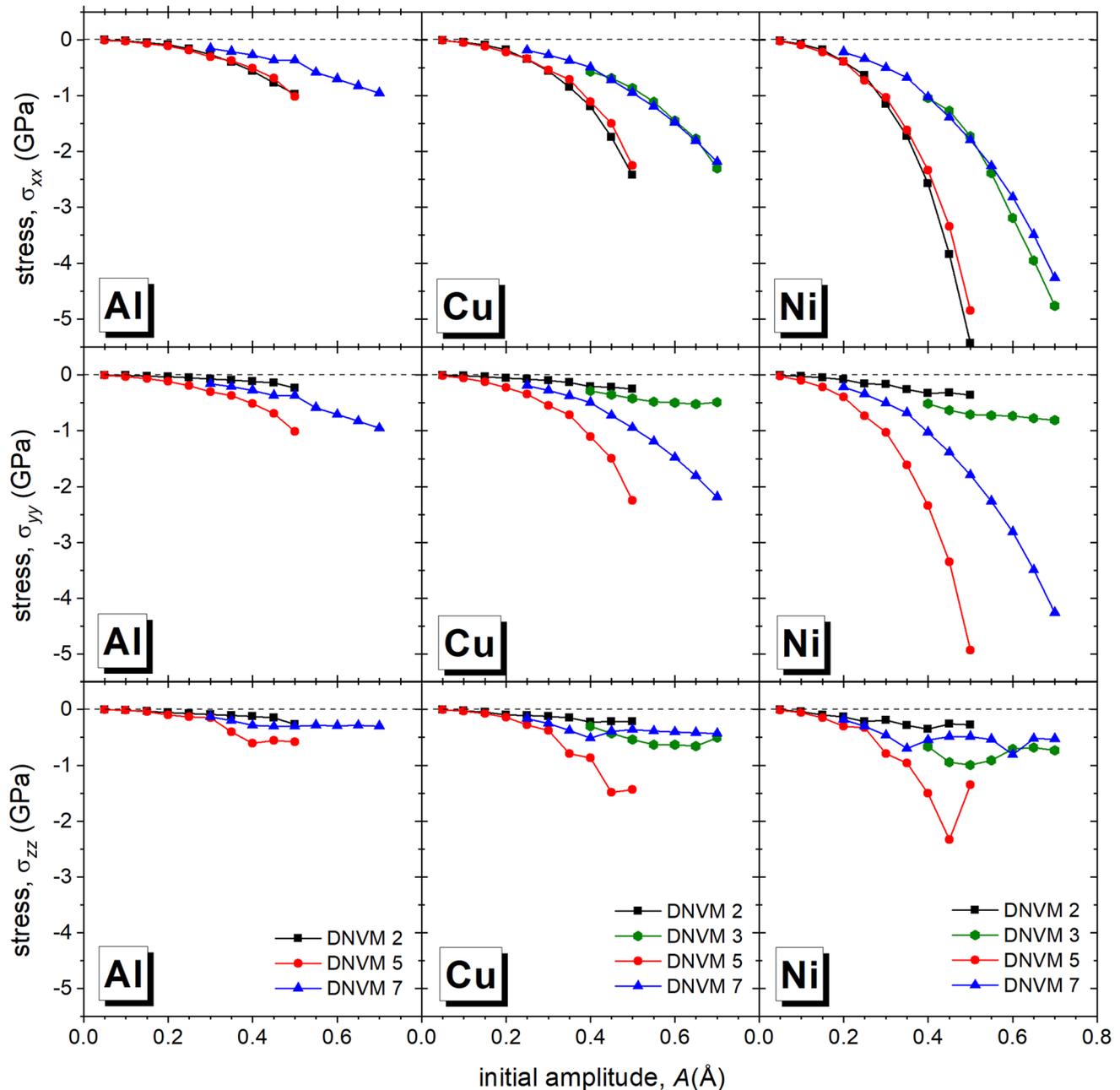
The results presented in Fig. 5 reveal that increasing the initial amplitude of atomic oscillations enhances compressive stresses within the crystal lattice. This behavior indicates that the excitation of two-dimensional DBs indeed induces thermal expansion within the crystal structure. This phenomenon occurs as a result of the increased atomic displacements from equilibrium sites, which amplify lattice strains and, consequently, generate internal stresses. Moreover, the stresses induced by symmetric and asymmetric DNVMs are of an approximately equal magnitude across all the studied fcc metals.

The observed decay of one-component DBs differs significantly from the previously reported behavior of two-component DBs [59]. In contrast to the gradual reduction in spatial dimension observed for two-component DBs, where oscillating chains (one-dimensional DBs) form first in the initial plane, followed by the dissipation of vibrational energy onto neighboring atoms, no such process is observed here. The decay of the one-component DBs occurs abruptly at a specific point in time when one or more of the oscillating atoms deviates from its initial displacement vector. This deviation is caused by the loss of vibrational energy as the atoms interact with their nearest neighbors, which then

initiates a rapid displacement cascade that propagates through the plane.

Following a few oscillation periods, the majority of the atoms return to their equilibrium lattice positions. Nevertheless, a minor proportion of the atoms undergo transitions to neighboring interstitial sites, where they remain until the end of the simulation. These jumps, which are critical to the evolution of the defect structure, only occur at larger initial amplitudes. For example, for the asymmetric DNVM 7, the initial amplitudes necessary for such jumps are  $A \geq 0.65$  Å for Al,  $A \geq 0.6$  Å for Cu, and  $A \geq 0.65$  Å for Ni. The discrepancy in these threshold amplitudes can be attributed to differences in the bond stiffness of the fcc metals, which are directly correlated with the differences in their lattice parameters. Among the metals studied, Al exhibits the largest lattice parameter  $a_0$ , while Ni has the smallest. As a result, the ratios  $A/a_0$  are 0.160 for Al, 0.166 for Cu, and 0.184 for Ni, with the ratio increasing in accordance with the bond stiffness of the material.

The energy released during the decay of two-dimensional DBs has the potential to displace atoms from their equilibrium lattice sites, thereby creating interstitial atoms that are critical in the evolution of the defect structure. These atomic displacements, driven by the excitation and subsequent decay of vibrational modes, can have a substantial influence on the material's macroscopic properties, particularly affecting its mechanical strength, thermal stability, and response to extreme environments like high temperatures or irradiation. This study highlights the significance of understanding these dynamic processes, as they shed light on the atomic-scale mechanisms that contribute to material performance and reliability.



**Fig. 5** The stress components  $\sigma_{xx}$ ,  $\sigma_{yy}$ , and  $\sigma_{zz}$  arising in the computational cell as a result of excitation of the four stable DNVMs as functions of initial oscillation amplitude  $A$  calculated for Al, Cu, and Ni. The horizontal dashed line shows the zero stress level characteristic of the system at the initial time instant. The solid lines connecting the data points are provided as visual guides

The effect on macroscopic properties depends on the statistical mechanics of DBs, specifically on their concentration. The probability of DB generation from thermal fluctuations can be estimated using the Arrhenius formula, with DB energy values obtained from molecular dynamics simulations. DBs localized in three spatial dimensions can accumulate energy up to several electronvolts [37, 38]. These estimations suggest that the equilibrium concentration of DBs is generally low, especially for high-energy DBs [60, 61]. However, as

highlighted in the literature, the significance of DBs in crystals increases substantially in non-equilibrium processes [38, 62], such as their excitation by lasers operating at frequencies above the phonon spectrum. In such cases, phonons are not directly excited. Instead, DBs with frequencies above the phonon spectrum are generated, and their energy is subsequently dissipated as thermal energy. Specifically, the two-dimensional DBs studied in this work can be excited by lasers due to the

relatively large laser spot size. High-power lasers operating at terahertz frequencies are now available [63].

## 5 Conclusions

The influence of two-dimensional DBs excited on the basis of stable one-component DNVMs, which are localized along one spatial direction and delocalized along two others, on the macroscopic properties of three-dimensional single crystals of Al, Cu, and Ni was investigated using molecular dynamics simulations. The main findings are summarized as follows.

The lifetime of a two-dimensional DB is highly dependent on both the symmetry of DNVM used for its excitation and the initial oscillation amplitude. It is noteworthy that the maximum lifetimes were observed to reach up to 24–47 ps for the symmetrical DNVM 2, which demonstrates greater stability under specific conditions. Two-dimensional DBs demonstrate hard-type nonlinearity, characterized by an increase in oscillation frequency with rising initial amplitude. The excitation of two-dimensional DBs results in a reduction in the heat capacity of the crystal. This decrease becomes more pronounced as the initial amplitude of the atomic oscillations increases, which reflects the impact of the DB on the crystal's energy storage and transfer mechanisms. The excitation of a two-dimensional DB induces thermal expansion within the crystal, thereby indicating that DBs have the potential to affect the mechanical properties of the crystal.

In summary, the present study provides novel insights into how localized vibrational modes, such as two-dimensional DBs, can influence both the thermal and mechanical properties of fcc metals. This work paves the way for further research into the impact of DBs of different dimensions on the macroscopic properties of other crystalline structures.

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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** 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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