Stability of in-plane delocalized vibrational modes in triangular Morse lattice

D U Abdullina1,2, M N Semenova3, A S Semenov3, D S Ryabov4, G M Chechin4, E A Korznikova1, J A Baimova1,2 and S V Dmitriev1,5

1 Institute for Metals Superplasticity Problems, 39 Khalturin st., 450001 Ufa, Russia
2 Bashkir State University, 32 Validy St. 450076 Ufa, Russia
3 North-Eastern Federal University n.a. M.K. Ammosov, Polytechnic Institute (branch) in Mirny, 5/1 Tikhonova st., 678170 Mirny, Sakha (Yakutia), Russia
4 Southern Federal University, 105 Bolshaya Sadovaya st., 344006 Rostov-on-Don, Russia
5 National Research Tomsk State University, 36 Lenin Ave., 634050 Tomsk., Russia

dina.abdullina25@gmail.com

Abstract. Delocalized nonlinear vibrational modes (DNVMs) play a very important role in the study of the dynamics of a nonlinear lattice in solid state physics. Such modes are exact solutions to the equations of motion of atoms dictated by the lattice space symmetry. If the amplitude of DNVM is above the threshold value, it is modulationally unstable. In the present study, we consider the stability of DNVMs in a two-dimensional (2D) triangular lattice with atoms interacting via the Morse potential. Critical exponents are calculated numerically as functions of the DNVM amplitude. Extrapolation to the zero value of the critical exponent gives an estimation of the DNVM amplitude, below which it is stable.

1. Introduction

Spatially localized nonlinear excitations, called discrete breathers (DBs), are actively studied in various crystals and model nonlinear lattices by means of molecular dynamics [1-21] and ab initio simulations [22,23]. Existing attempts to experimentally identify DBs in crystals were summarized in the review [2]. It has recently been demonstrated that delocalized nonlinear vibrational modes (DNVMs), synonymously called bushes of nonlinear normal modes [24], have a close relationship to DB. Particularly, it has been shown that DBs can be obtained by superimposing a bell-shaped function upon a DNVM having a frequency outside the phonon spectrum [4-6]. DBs can also emerge spontaneously from a DNVM having a frequency outside the phonon spectrum as a result of modulational instability [18-21]. From this it is clear that the stability of DNVM is a very important issue.

DNVMs are the exact solutions to the nonlinear equations governing atomic motion, and this is true for any interatomic potential used in simulations. This is so because DNVMs are found considering only the lattice space symmetry using the group theory [24]. For a two-dimensional (2D) triangular lattice, Chechin and Ryabov have recently derived eight DNVMs with in-plane atomic motion [25]. Here we study the stability of all eight DNVMs by estimating critical exponents as functions of the
initial atomic displacements that define the amplitude of DNVM. Extrapolating the results to the zero value of the critical exponent, we find the maximal initial displacement for a stable DNVM.

2. Simulation details
A two-dimensional (2D) close-packed triangular lattice is considered. The interatomic interactions are described by the classical Morse potential

\[ V(r) = A \{ \exp[-2\beta(r - r_m)] - 2 \exp[-\beta(r - r_m)] \}, \tag{1} \]

where \( r \) is the distance between the considered pair of atoms, \( A, \beta, r_m \) are the potential parameters. The function \( V(r) \) has a minimum at \( r = r_m \). \( A \) is the bond breaking energy (depth of the potential) and \( \beta \) defines the bond stiffness. With the proper choice of units of energy, distance, and time we set \( A = 1 \), \( r_m = 1 \), and the atom mass \( m = 1 \). We take \( \beta = 5 \) and the cut-off radius equal to \( 5r_m \). Then the equilibrium interatomic distance is \( \rho = 0.9881329 \). The computational cell includes \( 24 \times 24 \) atoms. Periodic boundary conditions are applied.

In figure 1 eight DNVMs with in-plane displacements of atoms are shown [22]. All arrows have equal length \( D_0 \). The initial conditions are set by setting the initial displacements according to these patterns with zero initial velocities of atoms. The choice of \( D_0 \) specifies the DNVM amplitude. To facilitate the development of the instability, random in-plane initial displacements are added to all atoms with a maximal deviation from the equilibrium position equal to \( 10^{-9} \).

![Figure 1](image_url)

**Figure 1.** Eight in-plane DNVMs supported by a triangular lattice, as found by Chechin and Ryabov [22]. The arrows have length \( D_0 \), which defines the initial amplitude of DNVM. Dotted lines show the translational cells of the displacement patterns.
3. Numerical results and discussion

In figure 2 we plot, as an example, the numerical results obtained for DNVM 2. Note that in this DNVM all moving atoms vibrate in the horizontal (x) direction. As a measure of the instability of this mode, one can analyze the appearance of displacements in the vertical (y) and out-of-plane (z) directions. It was found that the z-component of the displacements remained nearly zero but the y-component firstly remained at the level of the initial perturbation, and then started to grow exponentially with time, \( \max|\Delta y| \sim e^{\alpha t} \), with the critical exponent \( \alpha \). This is illustrated in figure 2a for three values of the initial atomic displacements, \( D_0 = 0.03, 0.04, \) and 0.05. Note that the logarithmic scale is used for the ordinate. The straight line segments show the slopes from which critical exponents were estimated. In figure 2b the critical exponent as a function of \( D_0 \) is shown for DNVM 2. The straight line represents a linear least square fit \( \alpha = a + bD_0 \) with \( a = -0.641 \) and \( b = 45.3 \). This shows that the critical exponent vanishes at \( D_0 = 0.0142 \). For smaller values of \( D_0 \), DNVM 2 is modulationally stable. The coefficient \( b \) indicates the sensitivity of the critical exponent to the amplitude of DNVM 2.

In table 1 the coefficients \( a \) and \( b \) are given for all DNVMs studied.

![Figure 2](image.png)

**Figure 2.** Results for DNVM 2. (a) Absolute value of displacement |\( \Delta y \)| as a function of time for a moving atom. Three curves give the results for three different values of the initial displacements of atoms, \( D_0 = 0.03, 0.04, \) and 0.05, as indicated in the figure. Straight lines show the slopes from which critical exponents were estimated. (b) The critical exponent as a function of the initial displacements of atoms. The straight line shows the linear least square fit.

| DNVM | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  |
|------|----|----|----|----|----|----|----|----|
| \( a \) | -0.383 | -0.641 | -1.75 | -0.811 | -3.92 | -1.49 | -0.170 | -0.05  |
| \( b \) | 13.3 | 45.3 | 70.1 | 23.8 | 125 | 73.3 | 23.4 | 11.8 |

4. Conclusions

Using molecular dynamics, the modulational instability of eight DNVMs with in-plane atomic vibrations for a triangular Morse lattice was studied. It is found that the critical value of the DNVM amplitude, above which it becomes unstable, is of the order of 1% of the interatomic distance \( \rho \). In the future studies, it would be important to analyze the effect of the computational cell size on the development of modulational instability. The stability of transverse DNVMs, as well as two-dimensional DNVMs should also be analyzed.

**Acknowledgements**

The work of A.S.S. (discussion of the numerical results) was supported by the Russian Foundation for Basic Research, grant no. 18-32-00171_mol_a. D.S.R and G.M.Ch. have worked under state
assignment no. 3.5710.2017/8.9 (derivation of DNVM and discussion of the results). E.A.K. thanks the Russian Foundation for Basic Research, grant no. 17-02-00984_a (writing the paper). Work of J.A.B. was supported by the grant of the President of the Russian Federation for state support of young Russian scientists - doctors of sciences MD-1651.2018.2 (discussion of the results). S.V.D. thanks the Russian Science Foundation, grant no. 16-12-10175, for their financial support (design of the research). This work was partly supported by the state assignment of IMSP RAS.

References
[1] Flach S and Gorbach A V 2008 Phys. Rep. 467 1
[2] Dmitriev S V, Korznikova E A, Baimova Yu A and Velarde M G 2016 Phys. Uspekhi 59 446
[3] Baimova J A, Korznikova E A, Lobzenko I P and Dmitriev S V 2015 Rev. Adv. Mater. Sci. 42 68
[4] Korznikova E A, Fomin S, Soboleva E and Dmitriev S V 2016 JETP Lett. 103 277
[5] Barani E, Lobzenko I P, Korznikova E A, Soboleva E, Dmitriev S V, Zhou K and Marjaneh A 2017 Eur. Phys. J. B 90 38
[6] Korznikova E A, Kistanov A A, Sergeev K S, Shepelev I A, Davletshin A R, Bokij D I and Dmitriev S V 2016 Letters on Materials 6 221 (in Russian)
[7] Murzaev R T, Bachurin D V, Korznikova E A and Dmitriev S V 2017 Phys. Lett. A 381 1003
[8] Evazzade I, Lobzenko I P, Korznikova E A, Ovid'ko I, Roknabadi M and Dmitriev S V 2017 Phys. Rev. B 95 035423
[9] Barani E, Korznikova E A, Chetverikov A P, Zhou K and Dmitriev S V 2017 Phys. Lett. A 381 3553
[10] Zakharov P V, Korznikova E A, Dmitriev S V, Ekomasov E G, Zhou K 2019 Surf. Sci. 679 1
[11] Haas M, Hizhnyakov V, Shelkan A, Klopop M and Sievers A J 2011 Phys. Rev. B 84 144303
[12] Murzaev R, Babicheva R I, Zhou K, Korznikova E A, Fomin S, Dubinko V I and Dmitriev S V 2016 Eur. Phys. J. B 892 168
[13] Murzaev R T, Kistanov A A, Dubinko V I, Terentyev D A and Dmitriev S V 2015 Comp. Mater. Sci. 98 88
[14] Terentyev D A, Dubinko A V, Dubinko V I, Dmitriev S V, Zhurkin E E and Sorokin M V 2015 Model. Simul. Mater. Sc. 23 085007
[15] Bachurina O V, Murzaev R T, Korznikova E A and Dmitriev S V 2017 Mater. Phys. Mech. 33 49
[16] Kiselev S A, Bickham S R and Sievers A J 1993 Phys. Rev. B 48 13508
[17] Dmitriev S V 2016 Letters on Materials 6 86
[18] Burlakov V M, Kiselev S A and Rupasov V I 1990 JETP Lett. 51 544
[19] Cretegny T, Dauxois T, Ruffo S and Torcini A 1998 Physica D 121 109
[20] Khadeeva L Z and Dmitriev S V 2010 Phys. Rev. B 81 214306
[21] Dmitriev S V, Korznikova E A, Bokij D I and Zhou K 2016 Phys. Status Solidi B 253 1310
[22] Lobzenko I P, Chechin G M, Bezuglova G S, Baimova Y A, Korznikova E A and Dmitriev S V 2016 Phys. Solid State 58 633
[23] Chechin G M, Dmitriev S V, Lobzenko I P and Ryabov D S 2014 Phys. Rev. B 90 045432
[24] Chechin G M and Sakhnenko V P 1998 Physica D 117 43
[25] Semenova M N, Semenov A S, Bebikhov Yu V, Ryabov D S, Chechin G M, Rakhamatullina Zh G, Korznikova E A and Dmitriev S V 2018 Fundamental’nye Problemy Sovremennogo Materialovedenia 15 257 (in Russian)