Influence of elastic strain on the possibility of excitation of discrete breathers in the nanofiber crystal with A_3B stoichiometry

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***Abstract* – A molecular dynamics investigation of the influence of strain on the existence of moving discrete breathers with hard type nonlinearity in the nanofiber crystal with A_3B stoichiometry is performed. It is found that a small strain can affects the characteristics of the mobile discrete breather together with its excitement possibility. In some strains possible rebirth of a breather in the mobile discrete stationary.**

***Keywords* – discrete breather; quasi-breather; phonon spectrum; nonlinear localized mode; deformation.**

I. INTRODUCTION

Nanomaterials are usually considered as a special class of functional and structural materials. Among them one can name metallic nanowires [1–8] presenting an elongated almost defect-free [1] crystals with lateral size not exceeding 100 nm.

Application of nanowires can be found in different areas, namely medicine, bioengineering, electronics, gases, liquids filtration facilities and composite materials [6].

Wide possibilities of application of nanofibers are due to their unique set of properties. Strength of the nanofibers grows with decreasing its diameter approaching the theoretical strength limit [2–8].

Creation of nanofibers is accompanied by various impacts that can result in crystal structure transformation. Those changes can result in formation of soliton-type objects able to perform the energy transport along the nanofiber. Discrete breathers are among those soliton type objects.

Discrete breathers (DB) are spatially localized strictly periodic large amplitude vibrational modes in nonlinear periodic lattices [9, 10]. DB have been found in the form of exact solutions of equations of motion for a number of nonlinear discrete systems. DB do not radiate energy in the form of small amplitude vibrations because their frequency is located out of the phonon spectrum of the crystal.

DB can demonstrate soft or hard nonlinearity. In the former (later) case DB frequency decreases (increases) with increasing amplitude. Decrease of the frequency of the soft

nonlinearity DB with growing amplitude can result in entering the phonon spectrum gap, if it exists. For the DB of hard type nonlinearity the frequency growing with increasing amplitude can cross the upper edge of the phonon spectrum. Hereinafter DB with soft (hard) nonlinearity type will be denoted as DB1 (DB2).

It should be mentioned that in real crystals one should use the concept of quasi-breathers having limited lifetime and not satisfying the exact time-periodicity condition [11].

Quasi-breathers considered in this paper here and after will be denoted as DB.

The choice of alloy with A_3B composition for investigation was rationalized by several factors. Alloys with A_3B stoichiometry and L_{12} superstructure are very numerous, by now about 190 variations of phases with A_3B composition are known. Another reason for our choice is that alloys with mentioned composition are commonly used as model materials in research oriented on development of new materials with unique properties. One can also recall that alloys with L_{12} superstructure make a basis for the development of currently existing superalloys.

It was shown previously in [12, 13] that the crystal of Pt_3Al being an example of A_3B composition can support the existence of two DB types – with soft (DB1) and hard (DB2) nonlinearity. DB2 have a possibility to move in the crystal along closely packed atomic rows. This feature can be useful in frames of searching for new directions of DB applications to enhance materials properties. Potential roles of DB2 in improvement of state of the art materials have been addressed in [12]. Among them one can recall the assistance of DB2 in analysis of purity and defect structure of the alloy of A_3B composition, energy or information transport along the nanofibers, exc.

In order to estimate the role of DB2 in potential application perspectives in the variety of systems, including nanofibers a detailed study of the influence of different factors should be performed. One of the most relevant directions of those studies is the analysis of the influence of external conditions on the ability of mobile DB2 excitations and their characteristics.

The aim of this work is to establish the elastic strain effect on the possibility of excitation the mobile discrete breathers in Pt_3Al crystal.

The work was performed by means of computer simulation method, namely molecular dynamics. Choice of this method was determined by the features of the objects being studied. DBs has a very short lifetime and too small scale for experimental investigation. In the same time molecular dynamics is a perfect method for analysis of small topological defects having a lifetime of several thousand periods of atomic vibrations, which is about 0.1 ns, with an optional ability of high speed movement along the crystal. Molecular dynamics and ab initio simulations are to date the most effective methods in studying the properties of DBs in crystals and the existence of DBs by means of those methods has been demonstrated for a number of pure metals [14], graphene[15-18], and other lattices [19-21].

Growth of the impact of simulation methods in the area of material structure and properties is caused by constant increase of the power and accessibility of computers, software development and numerical methods implementation. Molecular dynamics based on well approved interatomic potentials as a part of simulation methodology gains considerable attention as a perfect tool for investigation different features of materials including DB. One should also mention that by means of molecular dynamics one can consider the tasks related to the structural and energetical transformations, both in crystalline and non-crystalline materials. Moreover, this method allows the calculation of various properties of the system like thermodynamic (e.g., energy, pressure, entropy) and kinetic (diffusion coefficients, frequency of atomic vibrations) ones. Moreover this method allows tailoring the dynamics of the processes with real time.

II. SUMULATION DETAILS

The considered model is the bulk crystal of A3B stoichiometry, and the size of 225.71 x 29.32 x 20.73 Å, containing 8640 particles, periodic boundary conditions were set along the <110> direction and free surfaces in other directions. Interaction of atoms was described by pairwise Morse potential:

$$\varphi_{PQ}(r_{ij}) = D_{PQ}\beta_{PQ}\exp(-\alpha_{PQ}r_{ij})\cdot \cdot(\beta_{PQ}\exp(-\alpha_{PQ}r_{ij})-2) \quad (1)$$

where D is the potential depth, α is the bonding stiffness parameter, β is certain average equilibrium distance for the coordination spheres, which takes into account the interaction between the atoms. For the Pt_3Al those parameters were taken from [21]: $D_{AlAl} = 0.318$, $\beta_{AlAl} = 27.4979$, $\alpha_{AlAl} = 1.02658$, $D_{PtPt} = 0.710$ $\beta_{PtPt} = 102.89$, $\alpha_{PtPt} = 1.582$, $D_{PtAl} = 0.5048$, $\beta_{PtAl} = 63.124$, $\alpha_{PtAl} = 1.3501$, where they were fitted using standard method considering the following three conditions:

$$\frac{1}{2}\sum_{i=1}^{z}\eta_i\varphi_{V=V_0} = E_S,\ \frac{1}{2}\sum_{i=1}^{z}\eta_i\left(\frac{\partial\varphi}{\partial V}\right)_{V=V_0} = 0,$$
$$V_0\cdot\left(\frac{\partial P_S}{\partial V}\right) = K_0. \quad (2)$$

Here E_S is the sublimation energy of the alloy at 0 K, K_0 is the bulk elastic modulus. The value of the interatomic distance is $a_0 = 2.83$. Weights of platinum and aluminum atoms are: $m_{Pt} = 195.23$, $m_{Al} = 26.97$ a. e. м., and the lattice constant is $a_0 = 3.99$ Å.

The method of excitation of DB2 was described in [12] where two atoms of light sublattice were given an initial shifts from the equilibrium position in opposite directions. The value of the initial shift was set accordingly to the maximum speed

of DB2 obtained after the relaxation of the undeformed crystal (Figure 1).

Deformation of the nanofibers was set in accordance with the Poisson's rule. The main attention was paid to the direction of DB2 movement, which corresponds to $<\bar{1}10>$ crystallographic direction.

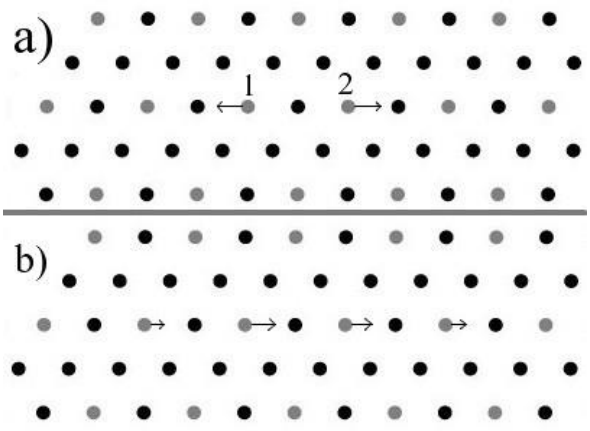

Fig. 1. The (111) plane of the Pt_3Al crystal. a) The initial conditions for the excitation of the mobile DB2 with a hard nonlinearity type. b) Moving DB2 arising after the 2 ps transition process.

The two others perpendicular directions were subjected to strain according to a formula:

$$\varepsilon_{<111>} = \varepsilon_{<1\bar{1}2>} = -\mu\,\varepsilon_{<1\bar{1}0>}, \qquad (3)$$

where $\varepsilon_{<111>}$, $\varepsilon_{<1\bar{1}2>}$, $\varepsilon_{<1\bar{1}0>}$ are the corresponding strains along the crystallographic directions, μ is the Poisson ratio.

III. Results and Discussion

Application of the strain leads to significant changes of the crystal properties. One of the most important effects of the applied strain is the shift of phonon density of states (DOS) which has a direct impact on the possibility of DB existence and its properties. In order to analyze the effect of deformation on the phonon DOS we have performed the heating of the cell up to 5 K with following estimation of the cell oscillation frequency and calculating the corresponding distributions [23]. This approach is convenient to describe the phonon DOS at finite temperatures for the crystal under train.

Fig.2 presents phonon DOS for different strain values. Presented results demonstrate a slight difference from the theoretical calculations for other crystals [23, 24], however, the revealed trend is similar. The compressive strain leads to the shift of the optical branch of phonon DOS towards higher frequencies, while tensile deformation results in branch shift to the lower frequencies.

Analysis of the effect of strain on the possibility of excitation of DB2 have shown that even a moderate values of strain can significantly affect the characteristics of DB2.

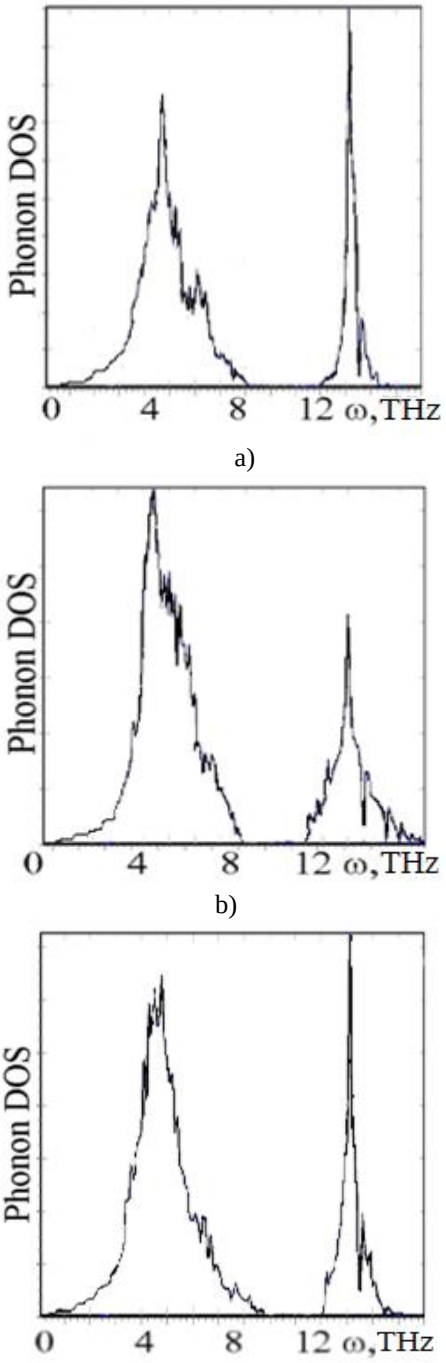

Fig. 2. Phonon DOS of Pt_3Al crystal a) initial state without strain, b) compressive strain of 3%, c) tensile strain of 3%.

Excitaiton of the DB in the crystal with applied compressive strain of ε=-0.005 along the $<\bar{1}10>$ direction results in formation of steady moving DB with the oscillation frequency ω = 13,69 THz. and the velocity V = 2.04 Å/ps. Application of compression up to ε=0.01 also results in steady moving DB formation with the velocity V = 1.17 A / ps, and frequency ω = 13,33 THz.

Increase of strain values results in the formation of structure that does not support the existence of moving DB. However, one should mention that the crystal subjected to compressive strain in the interval ε=0.015 -0.03 can support the existence of unstable nonlinear vibrational mode, with lifetime about 6 ps and following excitation of DB1 with soft nonlinearity type those frequency lies in the phonon spectrum gap. Lifetime of DB1 makes about 30 ps.

Similar effect has been considered in [25] where it was caused by corresponding interatomic potential parameters. In present case the formation of gap DB1 is caused by compression induced phonon DOS changes.

An example of transition from DB2 to DB1 is shown on Fig. 3.

Application of preliminary compression with ε>0.03 have resulted in structure that does not support mobile or stationary DBs.

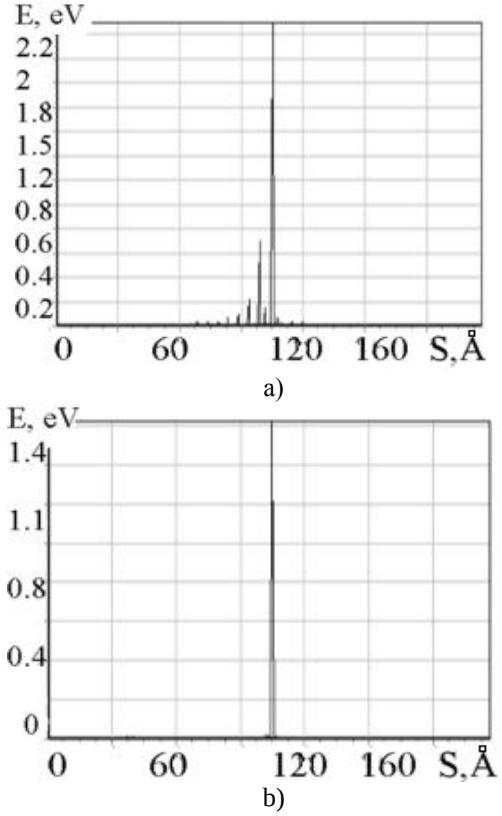

Fig. 3. Energy distribution over atoms along the nanofiber, a) initial stage, 5 ps, b) steady DB formed after 15 ps.

Formation of DB2 in stretched nanofibers could not be observed even in case of very small strains (ε<0.005). In the structure subjected to 2.5% tensile strain a formation of unstable nonlinear vibrational mode is observed. Lifetime of the latter mode makes about 5 ps and it is followed by excitation of DB1 with frequency ω = 10.9890 THz corresponding to the phonon DOS gap frequency interval. The lifetime of this DB1 was more than 40 ps. One should note that the DB2 polarization direction corresponds to the $<\bar{1}10>$ crystallographic direction and DB1 is polarized along the $<100>$ direction. Thus one can conclude that the process of DB1 excitation is accompanied by the change of polarization of nonlinear localized mode oscillations.

IV. Conclusions

The influence of the strain of the Pt_3Al crystal on the possibility of excitation of discrete breathers with hard nonlinearity type was investigated. It was revealed that even very small values of strain make a considerable impact on the properties of DB2. It was shown that one can excite the gap type DB1 with the initial conditions designed for excitation of mobile DB2. The latter feature is the result of strain induced phonon DOS transformations. The obtained results can contribute to the estimation of role of both DB1 and DB2 in the structure and properties of A_3B type crystal.

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References

[1] R.A. Andrievski, A.M. Glezer. Strength of nanostructures. Physics-Uspekhi. Vol. 52, 4 (2009), pp. 315.

[2] A.I. Potekaev, M.D. Starostenkov, N.V. Sinitsa, A.V. Yashin. Mechanisms of structure rearrangements in a nanofiber model of intermetallic compound Ni_3Al, containing long-period antiphase boundaries, in the course of high-speed uniaxial tensile loading. Russian Physics Journal. Vol. 53, Issues 8 (2011), pp. 818-826.

[3] S.J.A. Koh, H.P. Lee. Molecular dynamics simulation of size and strain rate dependent mechanical response of FCC metallic nanowires. Nanotechnology. Vol. 17 (2006), pp. 3451.

[4] H. Gleiter. Deformation of polycrystals. Proc. 2-nd RISO Inter. Sympos. Metallurgy and Materials Science. Ed. Hansen N. et al. Denmark, Roskilde: RISO Nat. Lab. (1981), pp. 15.

[5] M.D. Starostenkov, A.V. Yashin, E.A. Dudnik, N.V. Sinitsa. Investigation of structural transitions in the Ni_3Al alloy under uniaxial tension. Deformation and fracture of materials. № 6 (2009), pp. 28-31.

[6] A.T. Matveev, I.M. Afanasov. Getting nanofibers by electrospinning. Moskva.: MSU publ. (2010), 83 p.

[7] R.I. Babicheva, K.A. Bukreeva, S.V. Dmitriev et al. Strengthening of NiAl nanofilms by introducing internal stresses. Intermetallics. Vol. 43 (2013), pp. 171–176.

[8] K.A. Bukreeva, R.I. Babicheva, S.V. Dmitriev, K. Zhou, R.R. Mulyukov. Inhomogeneous elastic deformation of nanofilms and nanowires of NiAl and FeAl. Alloys. Vol. 98, № 2 (2013), pp. 91-95.

[9] A.J. Sievers, S. Takeno. Intrinsic Localized Modes in Anharmonic Crystals. Phys. Rev. Lett. 61, 8 (1988), pp. 970.

[10] S. Flach, A.V. Gorbach. Discrete breathers advancer in theory and application. Phys. Rep. 467 (2008), pp. 1-116.

[11] G.M. Chechin, G.S. Dzhelauhova, E.A. Mehonoshina. Quasibreathers as a generalization of the concept of discrete breathers. Phys. Rev. E. V.74 (2006), pp. 036608.

[12] P.V. Zakharov, A.M. Eremin, M.D. Starostenkov, N.N. Medvedev, S.V. Dmitriev. Simulation of the interaction between discrete breathers of various types in a Pt_3Al crystal nanofiber. Journal of Experimental and Theoretical Physics. Vol. 121, № 2 (2015), pp. 217-221.

[13] M.D. Starostenkov, A.I. Potekaev, S.V. Dmitriev, A.M. Eremin. Dynamics of discrete breathers in the Pt_3Al crystal. Russian physics journal. Vol. 58, 9 (2015), pp. 136-140.

[14] S.V. Dmitriev, E.A. Korznikova, J.A. Baimova, M.G. Velarde. Discrete breathers in crystals. Phys. Usp. 59, 5 (2016), DOI: 10.3367/UFNe.2016.02.037729
[15] J.A. Baimova, E.A. Korznikova, S.V. Dmitriev, I.P. Lobzenko. Discrete breathers in carbon and hydrocarbon nanostructures. Reviews on Advanced Materials Science. Vol. 42, № 1 (2015), pp. 68-82.
[16] I.P. Lobzenko, G.M. Chechin, G.S. Bezuglova, Yu.A. Baimova, E.A. Korznikova, S.V. Dmitriev. Ab Initio Simulation of Gap Discrete Breathers in Strained Graphene. Fizika Tverdogo Tela. Vol. 58, №. 3 (2016), pp. 616–622.
[17] E.A. Korznikova, Y.A. Baimova, S.V. Dmitriev, R.R. Mulyukov, A.V. Savin. Discrete breather on the edge of the graphene sheet with the armchair orientation. Journal of Experimental and Theoretical Physics Letters (JETP Letters). Vol. 96, № 4 (2012), pp. 222-226.
[18] E.A. Korznikova, J.A. Baimova, S.V. Dmitriev. Effect of strain on gap discrete breathers at the edge of armchair graphene nanoribbons. EPL. Vol. 102, № 6 (2013), pp. 60004.
[19] E.A. Korznikova, S.Yu. Fomin, E.G. Soboleva, S.V. Dmitriev. Highly Symmetric Discrete Breather in a Two-Dimensional Morse Crystal. JETP Letters. Vol. 103, №. 4 (2014), pp. 277–281.
[20] A.A. Kistanov, E.A. Korznikova, S.Yu. Fomin, K. Zhou, S.V. Dmitriev. Properties of discrete breathers in 2D and 3D Morse crystals. Letters on materials. Vol. 4, № 4 (2014), pp 315.
[21] N.N. Medvedev, M.D. Starostenkov, M.E. Manley Energy localization on the Al sublattice of Pt_3Al with L12 order. J. Appl. Phys. Vol. 114 (2013), pp. 213506.
[22] P.V. Zakharov. The module for calculating the phonon density of states of the model crystal by means of molecular dynamics. Rospatent. Certificate of state registration of the computer program № 2015614597 from April 21 (2015).
[23] S.V. Dmitriev, Yu.A. Baimova. Effect of elastic deformation on phonon spectrum and characteristics of gap discrete breathers in crystal with NaCl type structure. Technical Physics Letters. Vol. 37, №. 5 (2011), pp. 451–454.
[24] S.V. Dmitriev, Yu. A. Baimova. Influence of elastic strain on the density of phonon states and characteristics of discrete breathers in the gap of the phonon spectrum of a crystal with a NaCl structure. Technical Physics. Vol. 56, №. 11 (2011), pp. 1612–1618.
[25] N.N. Medvedev, M.D. Starostenkov, P.V. Zakharov, S.V. Dmitriev. Exciting discrete breathers of two types in a computer 3D model of Pt_3Al crystal. Technical Physics Letters. Vol. 41, № 10 (2015), pp. 994-997.