Influence of elastic strain on the possibility of excitation of discrete breathers in the nanofiber crystal with A₃B stoichiometry

P.V. Zakharov  
Physics and Informatics Department  
The Shukshin Altai State Humanities Pedagogical University, Biysk, Russia;  
Physics Department  
Altai State Technical University I.I. Polzunova  
Barnaul, Russia  
E-mail: zakharovpvl@rambler.ru  

M.D. Starostenkov  
Physics Department  
Altai State Technical University I.I. Polzunova  
Barnaul, Russia  
E-mail: genphys@mail.ru  

A.M. Eremin  
Department of Mathematics and methods of teaching mathematics  
The Shukshin Altai State Humanities Pedagogical University  
Biysk, Russia  
E-mail: eam77@yandex.ru  

E.A. Korznikova  
Laboratory of nanomaterials and nanotechnologies  
Institute for Metals Superplasticity Problems of Russian Academy of Sciences  
Ufa, Russia  
E-mail: elena.a.korznikova@gmail.com  

S.V. Dmitiriev  
Laboratory of Nonlinear Physics and Mechanics of Materials  
Institute for metals superplasticity problems of Russian Academy of Sciences  
Ufa, Russia;  
Research Laboratory for Mechanics of New Nanomaterials,  
Peter the Great St. Petersburg Polytechnic University,  
St. Petersburg, Russia  
E-mail: dmitriev.sergey.v@gmail.com  

I.S. Lucenko  
Physics and Informatics Department  
The Shukshin Altai State Humanities Pedagogical University  
Biysk, Russia,  
E-mail: Lucenko.Iwan@yandex.ru  

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 A₃B 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 A3B composition for investigation
was rationalized by several factors. Alloys with A3B stoichiometry and L12 superstructure are very numerous, by
now about 190 variations of phases with A3B 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 L12 superstructure make a basis for the
development of currently existing superalloys.

It was shown previously in [12, 13] that the crystal of
Pt3Al being an example of A3B 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 A3B
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
Pt3Al 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 have 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. SIMULATION 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:

$$
\varphi_{pq}(r_{ij}) = D_{pq} \beta_{pq} \exp\left(-\alpha_{pq} r_{ij}\right) - 2 \left(\beta_{pq} \exp(-\alpha_{pq} r_{ij}) - 1\right)
$$

(1)

where $D$ is the potential depth, $\alpha$ is the bonding stiffness
parameter, $\beta$ is certain average equilibrium distance for
the coordination spheres, which takes into account the interaction
between the atoms. For the Pt3Al 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:

$$
\frac{1}{2} \sum_{i=1}^{N} \eta_i \phi_{V-V_0} = E_S, \quad \frac{1}{2} \sum_{i=1}^{N} \eta_i \left(\frac{\partial \varphi}{\partial V}\right)_{V-V_0} = 0,
$$

$$
V_0 \left(\frac{\partial P}{\partial V}\right) = K_0.
$$

(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. m., 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 \(<1\bar{1}0>\) crystallographic direction.

![Image](image.png)

**Fig. 1.** The (111) plane of the Pt₃Al 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:

\[
\varepsilon_{<11\bar{1}>} = \varepsilon_{<1\bar{1}2>} = -\mu \varepsilon_{<1\bar{1}0>},
\]

where \(\varepsilon_{<11\bar{1}>}, \varepsilon_{<1\bar{1}2>}, \varepsilon_{<1\bar{1}0>}\) are the corresponding strains along the crystallographic directions, \(\mu\) 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.

![Image](image2.png)

**Fig. 2.** Phonon DOS of Pt₃Al crystal a) initial state without strain, b) compressive strain of 3%, c) tensile strain of 3%.

Excitation of the DB in the crystal with applied compressive strain of \(\varepsilon=0.005\) along the \(<1\bar{1}0>\) direction results in formation of steady moving DB with the oscillation frequency \(\omega = 13.69\) THz. and the velocity \(V = 2.04\) Å/ps. Application of compression up to \(\varepsilon=0.01\) also results in steady moving DB formation with the velocity \(V = 1.17\) Å/ps, and frequency \(\omega = 13.33\) 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.

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 \( <110> \) 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 PtAl 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 A3B type crystal.

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