Analysis of Statistical Characteristics of Quasi-Breather with Soft-Type of Nonlinearity in the Crystals of A_3B Stoichiometry

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Abstract. The research of quasi-breather statistical characteristics in the model crystal of A_3B stoichiometry is conducted by means of molecular dynamics method in the paper by the example of Pt_3Al. The phonon spectrum of this model crystal, the dependences of mean-square deviation, the coefficient of variation and the average frequency of the model quasi-breather on the time of its existence are obtained. The statistical data analysis allows for the conclusion that a quasi-breather model solution slightly differs from the exact breather corresponding to it in the model under consideration using the interatomic potential obtained by means of embedded atom method (EAM).

Introduction

The research of discrete breathers in the condensed media arises much interest in recent years. Discrete breather is a spatially localized, strictly periodic vibrational modes of large amplitude in nonlinear lattice systems [1–2]. There are experimental evidences of origin of such localized excitations in different physical systems, including spin lattices in antiferromagnets [3], the lattices of coupled nonlinear optical waveguides [4], the assemblies of micromechanical oscillators [5]. The application of such systems as an element base of promising radio-frequency filters, magnetometers and other devices [6] determines not only fundamental but also a practical interest for the breathers.

Discrete breathers can be divided into two types based on the nature of their frequency dependence on the amplitude [7]. In soft-type discrete breathers the frequency decreases with increasing its amplitude (such discrete breathers can only exist in the crystals having a slot in the phonon spectrum: their frequency lies in the phonon spectrum slot, and therefore they are called slotted), while a reverse situation occurs with the rigid-type discrete breathers (they may have frequencies both in the slot and higher the phonon spectrum). Discrete breathers with a soft-type of nonlinearity can be excited in diatomic crystals, for example, in NaCl [7], Pt_3Al [8-10], as well as in graphene and grafane [11]. Breathers with a rigid type of non-linearity exist in pure metals with FCC –, BCC –, and HCP – structures.

Depending on the problem formulation we speak of the discrete breathers either with an infinite lifetime, in this case, the solution is always periodic in time [12] and the corresponding family of trajectories has a null measure or with a finite lifetime, so-called quasi-breathers, such decisions have a non-zero probability measure and can be implemented in the physical systems or in the statistical numerical experiment. Discrete breather, as an object strictly periodic in time, is obtained by means of numerical simulation only in case of ideal setting the initial conditions of the Cauchy problem for a certain diversity of small dimension in the multidimensional space of any and all possible initial values of coordinates of individual particles and their velocities. Such fine-tuning is difficult to fulfill even during performance of computational experiment. Moreover, it is practically impossible to do when setting any physics experiments, particularly in cases where the breather-like objects arise spontaneously.

Therefore, the quasi-breather concept was proposed in paper [13] as some localized in space, but as dynamic objects not strictly periodic in time. In this case, it was formulated a certain criterion of quasi-breather proximity to its corresponding exact breather based on the calculation of mean-square deviation $\eta(t_k)$ of oscillation frequencies of breather individual particles found at some interval in the vicinity of time t_k, and calculating the mean-square deviation of the oscillation frequencies of allocated breather j-th particle at different time intervals.

The objective of this paper is to fulfill a statistical evaluation of quasi-breathers characteristics in the model lattices of A_3B composition. In this formulation, we will identify the concept of quasi-breather and quasi-breather model solution. A molecular dynamics method is selected as a research method in our paper. The choice of the method is due to a number of factors. Discrete breathers are very difficult to observe in a full-scale experiment given the fact that they are not topological defects; they have a lifetime of several thousand periods of atomic oscillations, which is about 0.1ns. Besides, they can move at high velocities in metals. At the same time, computer simulation has become very successful research method in condensed matter physics and materials science. This fact is due to continuous power growth and availability of computers, development and software implementation of numerical methods. The molecular dynamics method being based on the well proven interatomic potentials is one of the most effective methods of studying discrete breathers. When we speak of the molecular dynamics method in more detail, it should be noted that it provides an opportunity to solve the issues related to the problems of structural energy transformations both in crystalline and non-crystalline materials. Besides, this method makes it possible to design many properties of the system both thermodynamical (e.g., energy, pressure, entropy) and kinetic (diffusion coefficients, frequencies of atom oscillations). Moreover, the process dynamics is studied on a real time basis in this method.

Model description and experimental procedure

The simulation was being performed using the LAMMPS Molecular Dynamics Simulator molecular dynamics package [15]. The model being studied represented a bulk FCC crystal of A_3B stoichiometry. Pt_3Al crystal, containing 50,000 atoms, was being considered as a special case.

Alloys of A_3B stoichiometry with $L1_2$ superlattice structure are the most numerous ones. Searching the currently known systems having $L1_2$ structure made it possible to identify about 190 of such phases in the field of A_3B composition. Besides, the alloys with the given structure are the model ones most frequently and are chosen for fundamental research with a view to develop structural and physical basics of creating new structural and functional materials with different unique properties. Alloys with $L1_2$ structure form the development basis of currently existing superalloys.

The potential obtained by the embedded atom method (EAM) [16] was used for simulating the interatomic interaction. In computational chemistry, the embedded atom model is applied for approximate description of two atoms interaction energy. The energy is a function F of the sum of functions $\rho(r_{ij})$ depending on the distance between the i-th atom under consideration and its j-th neighbors. The function ρ represents an electron density.

$$E_i = F_a\left(\sum_{i\neq j}\rho_\alpha\left(r_{ij}\right)\right)+\frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}\left(r_{ij}\right), \quad (1)$$

where r_{ij} – distance between the i-th and j-th atoms $\phi_{\alpha\beta}$ - pair potential function, ρ_α - contribution to the charge density of the electrons from the j-th atom at the location of the i-th atom, F – function of "embedding", which represents the energy necessary to contain the i-th atom of α-type into electronic cloud. EAM method is a many-body potential and, for the reason that the electronic cloud density is a sum of the contribution of a large number of atoms, the number of neighbors is often limited via so-called "truncation radius" in practice in order to reduce the complexity and, therefore, the computation time. It was 8 Å in our situation.

The model quasi-breather excitation was being observed while deflecting Al atom along the <100> direction.

Unlike the exact discrete breathers, quasi-breathers are not dynamic objects strictly periodic in time, although they are localized in space. They arise in any sufficiently small deviations from the exact breather solutions in multidimensional space of any and all initial conditions while solving the Cauchy problem for the original differential equations, since there is no complete suppression of contributions from the oscillations of peripheral particles with their natural frequencies in this case. Thus, "dictatorship weakening" on the part of the breather nucleus (a single central particle forms a nucleus as well in case of a symmetric breather considered by us, and it is being formed by its two central particles in case of an antisymmetrical breather) leads to the presence of small contributions with different frequencies in the breather solution. These small contributions may be detected in the oscillations of all chain particles, in particular, and in the central ones. If finding pretty exactly the oscillation frequencies of all quasi-breather particles calculated at a certain time interval near $t = t_k$ then they will not be strictly identical. In light of this, we will find the mean-square deviations $\eta(t_k)$ of the oscillation frequency of the breather different particles from the average breather frequency ϖ:

$$\overline{\omega}(t_k)=\frac{1}{N}\sum_{i=1}^{N}\omega_i(t_k), \tag{2}$$

$$\eta(t_k)=\sqrt{\frac{\sum_{i=1}^{N}(\omega_i(t_k)-\overline{\omega}(t_k))^2}{N(N-1)}}. \tag{3}$$

The more the value $\eta(t_k)$, the more the quasi-breather solution differs from the exact breather solution, for which $\eta(t_k)=0$ at any particular time t_k.

Results and discussion

The distribution of the phonon modes, i.e. the crystal phonon spectrum is important for the existence of quasi-breather on a first-priority basis. The density of Pt_3Al crystal cell phonon states is shown in Fig. 1.

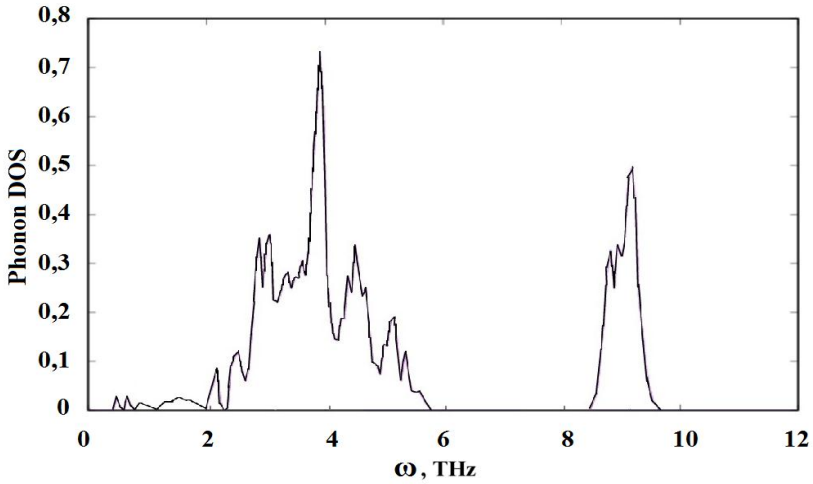

Fig. 1. Density of Pt_3Al crystal phonon states

The dependence of the model quasi-breather mean-square deviation η on its lifetime t_k is shown in Fig. 2.

The mean-square deviation characterizes the measure of data scattering. In our case, this is a deviation of peripherical atom frequencies of model quasi-breather from the quasi-breather nucleus frequency. It is apparent from Fig. 2 that the quasi-breather mean-square deviation ranges from

0.05351804 to 0.07872487, which is equivalent to slight scattering of peripheral atom frequency from the model quasi-breather nucleus frequency.

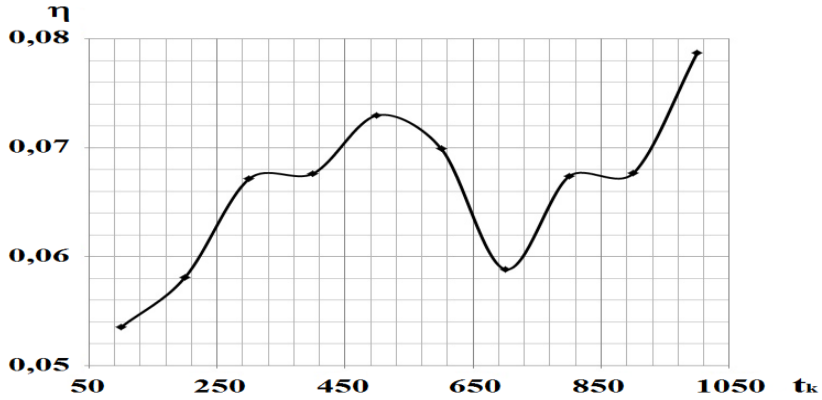

Fig. 2. Dependence of the model quasi-breather mean-square deviation η on its lifetime t_k (in picoseconds (ps))

The dependence of the model quasi-breather mean frequency ω_{mean} on its lifetime t_k is shown in Fig. 3.

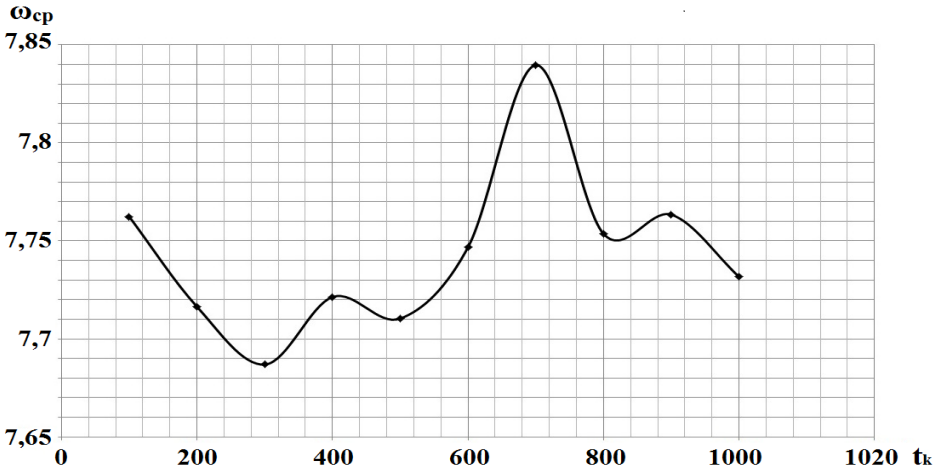

Fig. 3. Dependence of the model quasi-breather mean frequency ω_{mean} (in THz) on its lifetime t_k (in ps)

It is apparent from Fig. 2 and 3 that the deviation of the model quasi-breather frequency of peripherical atoms from the quasi-breather nucleus frequency is extremely negligible. Moreover, the medium frequency ranges from 7.68688603 THz to 7.83960979 THz, which is equivalent to the slot of Pt_3Al crystal phonon spectrum (See Fig. 1). Consequently, we may talk of the proximity of model quasi-breather to its corresponding exact breather within the limits of this Pt_3Al crystal model.

Besides, the following statistical characteristics and functions were calculated within the limits of this model: grouped statistical array of absolute and relative frequencies, range of absolute and relative frequencies, histogram of relative frequencies, empirical distribution function, estimation of expectation and variance of the original sample. The analysis of these statistical functions will be discussed in our further papers.

Conclusion

It has been established via molecular dynamics method that a quasi-breather model solution slightly differs from its corresponding exact breather in the model of A_3B stoichiometry crystal being considered by the example of Pt_3Al using the interatomic potential obtained by the embedded

atom method (EAM). This is the evidence of the obtained discrete breather stability in the model cells and the possibility of considered composition excitation in real alloys.

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