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STATISTICAL CHARACTERISTICS OF A QUASI-BREATHER WITH A HARD TYPE OF NONLINEARITY IN A CuAu CRYSTAL

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Abstract. By the method of molecular dynamics a study in the work is made of the statistical characteristics of a quasi-breather in a model CuAu crystal. 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 the quasi-breather model solution in the model considered (which uses the interatomic potential obtained by means of embedded atom method (EAM)) slightly differs from the one in the corresponding exact breather.
Keywords: quasi-breather, discrete breather, nonlinear dynamics, soliton

1. Introduction

Solitary waves are among the most interesting and important objects of nonlinear physics relevant for practical applications [1, 2]. Despite the fact that solitons were discovered more than 180 years ago, the number of studies devoted to their properties is still growing. Recently, there has been growing interest in the investigation of discrete nonlinear systems where the existence of dynamic solitons is possible. High-amplitude, spatially localized time-periodic vibrational modes in nonlinear crystals with translational symmetry called discrete breathers (DBs) belong to the class of the above mentioned dynamical solitons [3].

There are experimental evidences of formation of such localized excitations in different physical systems, including spin lattices in antiferromagnets [4], the lattices of coupled nonlinear optical waveguides [5], the assemblies of micromechanical oscillators [6]. The application of such systems as an element base of promising radio-frequency filters, magnetometers and other devices [7] determines not only a 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 [8]. In soft-type discrete breathers the frequency decreases as its amplitude grows (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 hard-type discrete breathers (they may have frequencies both in the slot and above the phonon spectrum). Discrete breathers with a soft-type of nonlinearity can be excited in diatomic crystals, for example, in NaCl [8], Pt_3Al [9-14], as well as in graphene and grafane [15]. Breathers with a hard 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 with either an infinite lifetime (in this case, the solution is always periodic in time [15] and the corresponding family of trajectories has a null measure) or with a finite lifetime, so-called

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quasi-breathers - such solutions have a non-zero probability measure and can be implemented in physical systems or in statistical numerical experiments [16]. A discrete breather, as a strictly time-periodic object, is obtained by means of numerical simulation only provided that the initial conditions of the Cauchy problem are perfectly set for a certain diversity of small dimension in the multidimensional space of all possible initial values of coordinates of individual particles and their velocities. Such fine-tuning is difficult to fulfill even within a computational experiment. Moreover, it is practically impossible to do when performing any physical experiments, particularly in cases when the breather-like objects arise spontaneously.

Therefore, the paper [16] proposed the concept of quasi-breathers as some dynamic objects localized in space, but not strictly time-periodic. For that purpose, a certain criterion of proximity of a quasi-breather to its corresponding exact breather was formulated. It is based on the calculation of mean-square deviation $\eta(t_k)$ of the oscillation frequencies of selected breather particles found at some interval in the vicinity of time t_k, and calculating the mean-square deviation of the oscillation frequencies of a selected j-th breather particle at different time intervals.

The objective of this paper is to fulfill a statistical evaluation of quasi-breathers characteristics in a model CuAu crystal. In this formulation, we will identify the concept of quasi-breather and quasi-breather model solution. The molecular dynamics method was 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 a very successful research method in condensed matter physics and materials science. This fact is due to the continuous power growth and availability of computers, development and software implementation of numerical methods. Being based on the well-tested interatomic potentials, the molecular dynamics method 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.

2. Model description and experimental procedure

We considered the biatomic system CuAu. As it has already been mentioned above, the investigation was performed by means of the well-known molecular dynamics method. This method was implemented using LAMMPS Molecular Dynamics Simulation, the package for modular dynamic modeling [17], which uses well-tested many-body interatomic potentials built according to the embedded atom method (EAM-potentials).

We considered a three-dimensional crystal containing 48000 atoms (Fig. 1). Periodic boundary conditions were imposed along all directions.

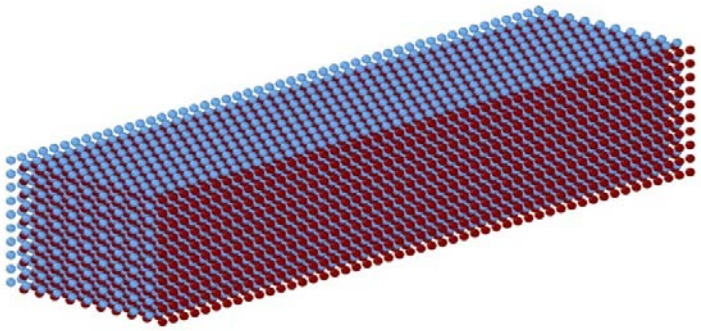

Fig. 1. The view of a 3D CuAu crystal containing 48000 atoms

The potential obtained by the method described in [18] for the Cu-Au system was used in the calculations. The process of selecting the interatomic potentials is an important task worth a detailed consideration. The home-made software [18] generates EAM-potentials of alloys using the rapid fitting procedure by combining the previously developed elemental potentials. More specifically, we applied the Finnis-Sinclair potentials for alloys determining the energy of each atom in the system, using the expression:

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

This equation consists of three types of functions: embedding functions (F), electron density functions (ρ), and pairwise interaction functions (φ). In this formula there is an embedding function for each element type, one electron density function for each permutation of two types of atoms (a, p), and a pairwise interaction function for each combination. For binary potentials, there are only three functions that need to be selected in case of using elementary conditions from existing potentials: $\rho_{\alpha\beta}$, $\rho_{\beta\alpha}$, and $\varphi_{\alpha\beta}$. Since there are no triple conditions in the Finnis-Sinclair formula, potentials with more than two elements can be created by combining all the information contained in the binary files. The method proposed by the authors of the article allows to combine elemental EAM potentials and to establish the potentials for alloys using the density functional theory (DFT) data.

Firstly, the approach of simple "rule of mixtures" is used for compensation of the difference between the lattice parameters and elasticity modulus predicted by the DFT and measured experimentally. The elastic moduli and lattice parameters calculated for intermetallic compounds are multiplied by the effective correction factor, which is the average of the elementary correction factors taken in the proportion of elements fractions. Secondly, single-element potentials are adapted to improve compatibility in binary and multicomponent potentials in such a way as to preserve all the initial states of the system. Thirdly, in the case of bonding of two elemental potentials, the maximum cut off distance is adopted for the binary potential. The electron density functions and the interaction of the original pair potentials are defined as equal to 0 at the distances greater than the cut off radius. Since most of interatomic potentials are available in a tabular format with functions defined at discrete points, this implementation uses cubic spline interpolation in order to calculate the values of functions in between the tabulated points.

The next step was the installation of cross-potentials. The Finnis-Sinclair composition for the EAM potential is used for every alloy potential considered. For a binary system, two embedding functions (F_α, F_β), four electron density functions ($f_{\alpha\alpha}$, $f_{\alpha\beta}$, $f_{\beta\alpha}$, $f_{\beta\beta}$) and three pair interaction functions ($\phi_{\alpha\alpha}$, $\phi_{\beta\beta}$) are used. Similarly to the case of single-component potentials, two-component ones are combined by converting the embedded function so that it exists on the same interval and assumes the maximum cut off radius. While the "pure" elemental potentials are used to create each double file, the electron density and interaction functions of

the pair contained in the original binaries are sufficient to create higher-order potentials without any additional equipment. In addition, the properties of each binary system and the original pure elements remain in these new potentials. The potentials created by means of the proposed technique were confirmed by comparison with the experimental results and existing potentials for the alloys. In addition, the dependence of the accuracy of binary potentials on the source of elementary potentials was estimated.

In order to analyze the possibility of the existence of DBs in CuAu crystal, the density of the phonon states of the crystal was calculated (see Fig. 2). The absence of a gap in the CuAu phonon spectrum dictates the impossibility of DB with soft nonlinearity type in this system. [19, 20]. This was confirmed in [21].

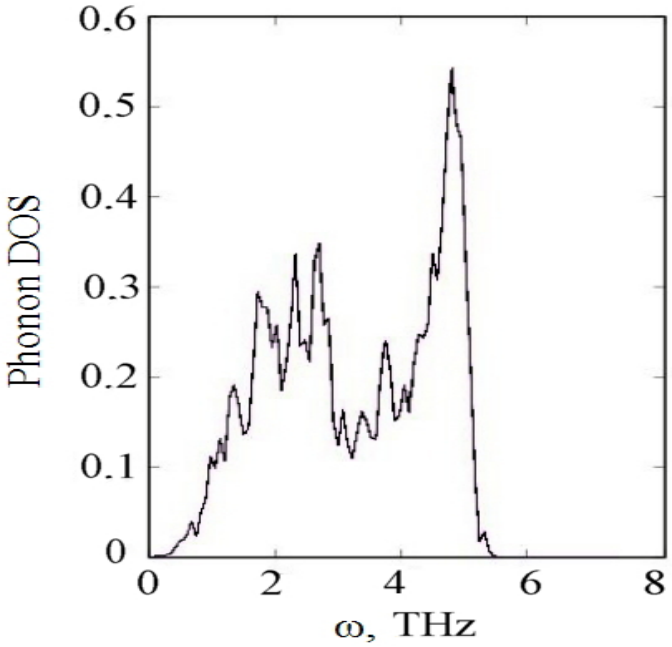

Fig. 2. The density of phonon states of CuAu crystal

The process of searching for discrete breathers in crystals involves selecting initial conditions-deviations of atoms from the equilibrium position or setting initial velocities.

For pure metals or alloys with a small difference in the atomic masses of the components, the excitation of DBs with a hard type of nonlinearity has some peculiarities. Thus, the authors of [19] proposed an ansatz for excitation of DBs in pure fcc and bcc metals, setting the DB profile in a closely packed atomic row by setting atomic displacements and velocities according to physically motivated functions. The displacements of the atoms were realized in such a way that the neighboring atoms oscillated in antiphase [22].

The Gaussian function (2), adapted for crystal conditions was used to excite a DB in the CuAu crystal

$$f(x) = A_0 e^{-\frac{x^2}{2C^2}}, \quad (2)$$

where A_0 defines the initial amplitude of the central atoms of a DB, x is the relative coordinate of a pair of atoms in a row, and parameter C is the degree of spatial localization of DB. Varying the values A_0 and C, we select the profile of the discrete breather, thereby setting the initial deviations from the equilibrium position for the atoms included in the DB oscillations.

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 including the central ones. If we estimate (with reasonable precision) the oscillation frequencies of all quasi-breather particles calculated at a certain time interval near $t = t_k$, they will not be strictly identical. In light of this, let us find the mean-square deviations $\eta(t_k)$ of the oscillation frequency of different breather particles from the average breather frequency ϖ:

$$\overline{\omega}(t_k)=\frac{1}{N}\sum_{i=1}^{N}\omega_i(t_k), \tag{3}$$

$$\eta(t_k)=\sqrt{\frac{\sum_{i=1}^{N}(\omega_i(t_k)-\overline{\omega}(t_k))^2}{N(N-1)}}. \tag{4}$$

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.

3. 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 reduced density of the phonon states of CuAu was compared with the oscillation frequencies of the quasi-breather. Below is a calculation of the statistical characteristics of a quasi-breather.

The dependence of the model quasi-breather mean-square deviation η on its lifetime t_k is shown in Fig. 3.

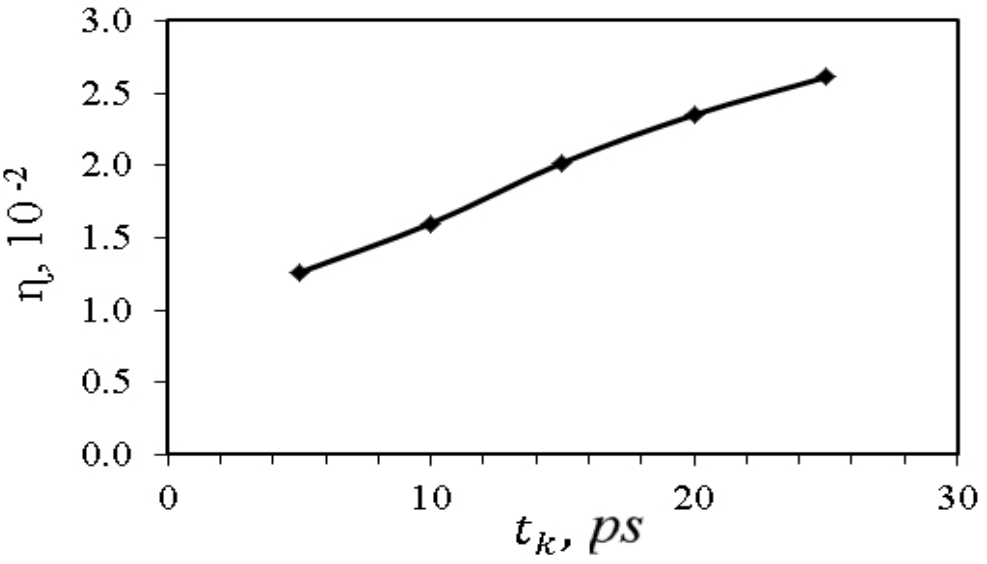

Fig. 3. Dependence of the model quasi-breather mean-square deviation η on its lifetime t_k (in picoseconds (ps))

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. 3 that the quasi-breather mean-square deviation ranges from 0.01261065 to 0.02610272, which is equivalent to slight scattering of peripheral atom frequency from the model quasi-breather nucleus frequency.

The mean-square deviation gives an absolute estimation of the measure of spread. Therefore, in order to understand how much variation is large relative to the values themselves (i.e., regardless of their scale), a relative index is required. Such an indicator is called the coefficient of variation and is calculated by the following formula:

$$V = \frac{\eta}{\omega_{cp.}}. \tag{5}$$

By this indicator, it is possible to compare the homogeneity of the most diverse phenomena, regardless of their scale and units of measurement. Table 1 shows the exponents of the coefficient of variation of V from the lifetime of the quasi-breather t_k.

Table 1. The exponent of the coefficient of variation of V from the lifetime of the quasibriser tk (in ps)

t_k	V
5	0.00220377958477173
10	0.00286022261352874
15	0.00374032727309376
20	0.00435946841613917
25	0.00491586066089457

The dependence of the model quasi-breather mean frequency ω_{mean} on its lifetime t_k is shown in Fig. 4.

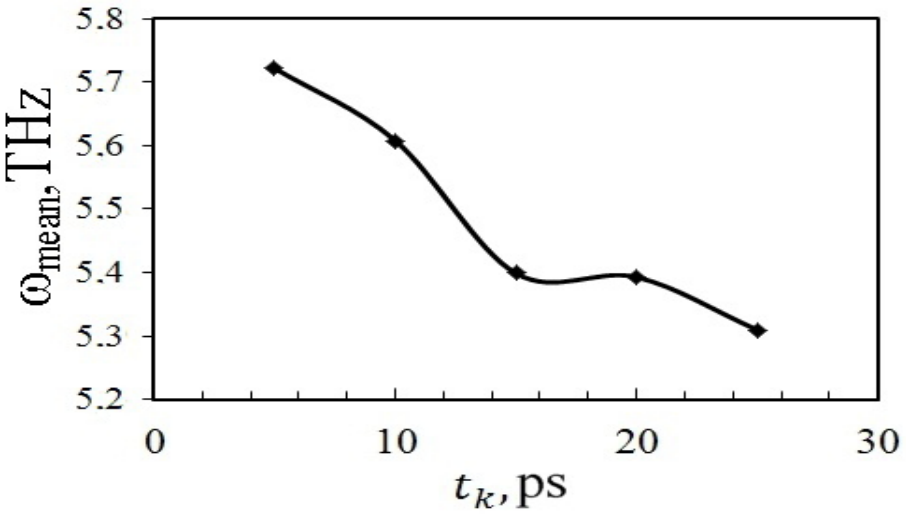

Fig. 4. Dependence of the model quasi-breather mean frequency ω_{mean} (in THz) on its lifetime t_k (in ps)

It is apparent from Fig. 3 and 4 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 5.30989773163211 THz to 5.72228656205187 THz.

For a group of atoms contained in the model quasi-breather, the mathematical expectation (the sample mean) of an ungrouped sample of the mean frequencies (5.72228656205187, 5.60811384473751, 5.39908960106847, 5.39342834099743, 5.30989773163211) is calculated by the formula:

$$M = \frac{1}{N}\sum_{i=1}^{N} X_i . \quad (5)$$

The mathematical expectation of the initial sample is 5.486563 THz, which is slightly higher than the upper limit of the phonon spectrum of the CuAu crystal (see Fig. 2).

The variance of the same ungrouped sample is calculated by the formula:

$$D = \frac{1}{N-1}\sum_{i=1}^{N}\left(X_i - M\right). \quad (6)$$

The result of the calculation by the formula above is 0.0229469. The obtained values show that within the framework of this model of the CuAu crystal, one can speak of the proximity of the model quasi-breather to the corresponding exact breather. 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.

4. Conclusion

The statistical characteristics of a quasi-breather with the hard type of nonlinearity were calculated by means of the molecular dynamics method. The main characteristics include the mean square deviation of the frequencies of some particular atoms in the breather from the mean value of the quasi-breather core frequency, as well as the coefficient of variation at different stages of life of the object under study.

It should be noted that the final quasi-breather destruction occurs at the moment when the frequencies mean square deviation exceeds the difference between the quasi-breather mean frequency and the crystal phonon spectrum upper boundary. At this moment the oscillations delocalization and the energy dissipation through the crystal in the form of low-amplitude thermal lattice vibrations occur. It is shown that the obtained quasi-breather is slightly different from the corresponding exact breather. This may indicate the stability of the obtained discrete breather in the model cells and the possibility of its excitation in real alloys of the composition examined in the work

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