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Analysis of the statistical characteristics of the discrete breather in CuPt₇ crystal by the method of molecular dynamics by GPU-calculations

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Abstract. The article uses the molecular-dynamic method to calculate the statistical characteristics of a quasi-breather in a CuPt₇ model crystal. In the calculations, a high-performance computing complex based on a GPU accelerator was used, which provided the necessary speed and accuracy of calculations. The phonon spectrum of this model crystal was calculated, and the dependences of the standard deviation, coefficient of variation, and average frequency of the model quasi-breather on its lifetime were revealed. The analysis of statistical data allows concluding that in the model under consideration, using the interatomic interaction potential obtained by the immersed atom (EAM) method, the quasi-breather model solution does not differ significantly from the corresponding exact breather. Moreover, the final destruction of the quasi-breather occurs at a time when the standard deviation of the frequencies exceeds the difference between the average frequency of the quasi-breather and the upper boundary of the phonon spectrum of the crystal. At this moment, the delocalization of vibrations and the dissipation of energy through the crystal in the form of low-amplitude thermal vibrations of the lattice occur. This may indicate the stability of the obtained discrete breather and the possibility of excitation in real alloys of the considered composition.

1. Introduction

The existence of such types of solutions as discrete breathers (DBs) in discrete structures was predicted a little over thirty years ago [1–2]. This concept means high-amplitude localized excitation in discrete systems with translational symmetry [3]. These systems primarily include crystals of various compositions and stoichiometries. During this time, the study of these objects was carried out both from the standpoint of theoretical methods, based primarily on solving differential equations, and using experimental methods, for example, by studying the density of phonon states at various crystal temperatures.

The detection of discrete breathers in experiments indicates their contribution to the properties of systems and prospects of application. Thus, in a number of works [4–7], discrete breathers were found in spin gratings in antiferromagnets, in coupled nonlinear optical waveguides, and in ensembles of micromechanical oscillators. It seems promising to use such objects as high-frequency filters, for controlling heat fluxes and as information carriers. From the position of discrete breathers, a number of authors explain the effect of nonlinear supratransmission [8].

To excite the DB, a number of conditions must be met. Depending on the conditions, a discrete system may support one or another type of breather. Two types of breathers are distinguished: with a



soft type of nonlinearity and with a hard type of nonlinearity. The type of nonlinearity is determined by the dependence of the frequency on the amplitude, in case the frequency decreases with increasing amplitude, they speak of a soft type, if it increases, they say that it is hard. Discrete breathers with a soft type of nonlinearity exist in biatomic crystals, for example, in NaCl, Pt₃Al, as well as in graphene and graphane [9–17]. Breathers with a rigid type of nonlinearity exist both in monoatomic metals and in biatomic ones.

In this paper, we will talk about excitations with a soft type of nonlinearity. For such discrete breathers, the presence of a forbidden band in the phonon spectrum of the crystal is necessary. For example, for graphene, it is known that uniform elastic deformation can lead to the appearance of a gap in its phonon spectrum. Using the molecular dynamics method, the possibility of excitation of a slit discrete breather in elastically deformed graphene has recently been shown, and clusters consisting of several closely spaced DBs have been studied [18]. Clusters of discrete breathers regularly located in the form of a two-dimensional array also attract particular attention. For the first time, methods of the density functional theory were used for modeling discrete breathers in graphene [19]. The absence of a clear gap in the phonon spectrum allows the presence of discrete breathers in crystals [20–22].

Turning to the strict definition of a discrete breather, in experimental works, the observed objects should be called quasi-breathers, since they have a finite lifetime and not a strict periodicity in time. For this reason, the concept of quasi-breathers as localized in space but not strictly periodic in time objects appeared in [23]. At the same time, a certain criterion was formulated for the proximity of the quasi-breather to the corresponding exact breather, based on the calculation of the standard deviation $\eta(t_k)$ vibration frequencies of individual breather particles found over a certain interval in the vicinity of a moment in time t_k , and calculating the standard deviation of the vibration frequencies of the selected j -th particle of the breather at different time intervals.

The purpose of the present work is to analyze the statistical estimation of the characteristics of quasi-breathers in the CuPt₇ crystal under consideration. The method of research in our work is the method of molecular dynamics (MD method). There are several reasons for this. In the first place, DBs are rather difficult to observe in a real experiment, since they are dynamic objects and do not affect the structure of the material, have a lifetime of about 0.1 ns, in addition, they can move with considerable speeds in metals. At the same time, the MD method is a very effective research method in condensed matter physics and material science, which is due to the constant increase in the power and availability of computers, the development and implementation of numerical methods. Speaking about the selected CuPt₇ material, we note that this is a rather rare phase of the combination of copper and platinum, but it is promising. Platinum compounds are used in many fields, including where heat-resistant alloys are required. It is at high temperatures that spontaneous excitations of quasi-breathers in crystals are possible, which led to the choice of this particular alloy for investigation.

To solve this problem by the molecular dynamics method, a high-performance computing cluster based on Tesla k40 graphics accelerators was used, which allows performing double-precision calculations for a large number of particles in the model. Let us pay attention to the fact that a computational experiment in physics at the moment is as recognized a method as theory and field experiment. The uses of high-performance calculators allows building models close to real objects, and reduce the calculation time to an acceptable one.

2. Research methods

In this work, we considered the CuPt₇ biatomic system containing $5 \cdot 10^5$ atoms and having a cubic crystal lattice. As already emphasized, the method of molecular dynamics was chosen as the method, which proved itself well in studies of such processes. This method was implemented using the molecular dynamics modeling package LAMMPS Molecular Dynamics Simulator [24], which uses proven multiparticle interatomic potentials created by the immersed atom method (EAM potentials). In computational chemistry, the immersed atom model is used to approximately describe the interaction energy between two atoms, taking into account the presence of neighboring atoms. The choice of potential and the correct use of it for a specific task is an important stage in the modeling.

The total energy E of the crystal is expressed as $E = \frac{1}{2} \sum_{i,j \neq i} \varphi_{ij}(r_{ij}) + \sum_i F_i(\rho_i)$, where φ_{ij} represents the pair energy of interaction of atoms i and j located at a distance r_{ij} from each other, and F_i – attachment energy associated with placing atom i in a location with electron density ρ_i . The electron density considers the position of the surrounding atoms and can be calculated by the formula $\rho_i = \sum_{j, j \neq i} f_j(r_{ij})$, where $f_j(r_{ij})$ – electron density at a site of atom i located at a distance r_{ij} from the atom j .

The EAM potential of a pure element is determined by three functions: pair energy φ , electron density ρ , and embedding energy F . For an alloy, the EAM potential contains not only three functions φ , ρ , and F and for each of the constituent elements, but also paired energies φ_{ab} between different elements a and b ($a \neq b$). In this regard, the functions φ , ρ , and F , calculated for pure metals, can not be directly applied to alloy or multilayer systems. At the same time, the procedure for generalizing EAM potentials and their “trimming” distances by normalizing EAM potentials and introducing an alloy model was proposed by the author of [23]. This procedure makes it possible to build EAM potentials of alloys from EAM potentials for individual elements. Such potentials of alloys were used in molecular modeling and led to good experimental results [25]; we used this kind of potential for a CuPt₇ crystal.

The described model was a bulk crystal containing $5 \cdot 10^5$ atoms (see figure 1). Along all directions, periodic boundary conditions were imposed.

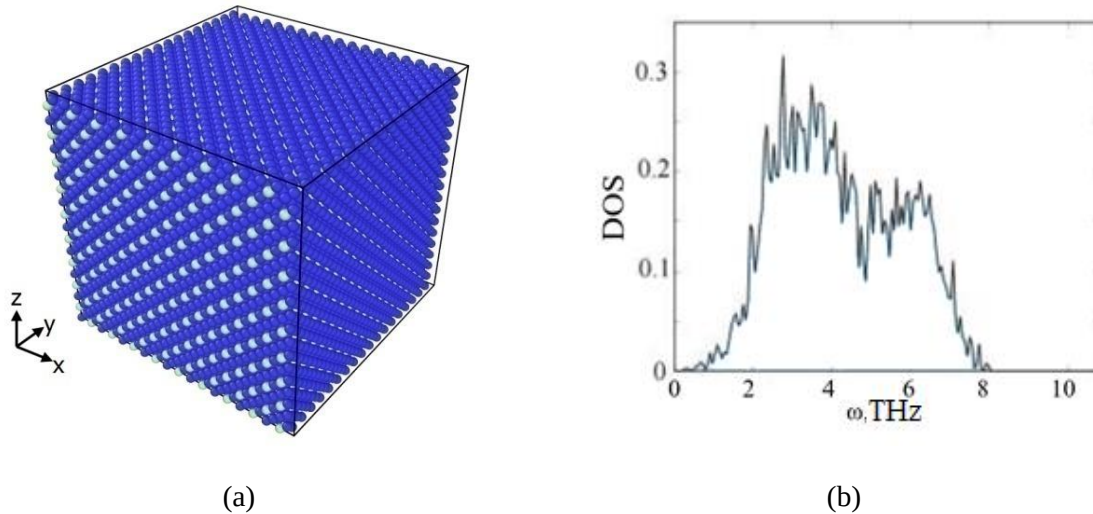


Figure 1. Crystal Model CuPt₇: (a) volumetric view of a crystal fragment; (b) density of phonon states.

In contrast to exact discrete breathers, quasi-breathers are not strictly periodic in time dynamic objects, although they are localized in space. They arise for any sufficiently small deviations from exact breather solutions in the multidimensional space of all possible initial conditions when solving the Cauchy problem. That is why, “weakening of the dictatorship” from the side of the nucleus (central atoms) of the breather leads to the presence in the breather solution of small contributions having different frequencies. These small contributions can be found in the vibrations of all particles of the chain, in particular, and central ones. If we find accurately enough the vibration frequencies of all particles of the quasi-breather, calculated on a certain time interval near $t = t_k$, then they will not be exactly the same. In connection with these considerations, we find the standard deviations $\eta(t_k)$ of

the oscillation frequency of various particles of the breather from the average breather frequency $\bar{\omega}(t_k)$:

$$\bar{\omega}(t_k) = \frac{1}{N} \sum_{i=1}^N \omega_i(t_k), \quad (1)$$

$$\eta(t_k) = \sqrt{\frac{1}{N \cdot (N-1)} \sum_{i=1}^N (\omega_i(t_k) - \bar{\omega}(t_k))^2}. \quad (2)$$

The larger 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 time t_k .

3. Results and discussion

The following is a calculation of the statistical characteristics of the quasi-breather. Figure 2 shows the dependence of the standard deviation $\eta(t_k)$ of the frequencies of the model quasi-breather on its lifetime t_k .

The standard deviation $\eta(t_k)$ describes a measure of the dispersion of the data. In the case under consideration, this is the deviation of the frequencies of the peripheral atoms of the model quasi-breather from the core frequency of the quasi-breather. Figure 2 shows that the standard deviation of the quasi-breather varies from 0.0064977295 to 0.0264001837, which corresponds to insignificant scattering of the frequency of peripheral atoms from the core frequency of the model quasi-breather.

Figure 3 shows the average frequency $\omega_{mean}(t_k)$ of the model quasi-breather from the time of its existence t_k .

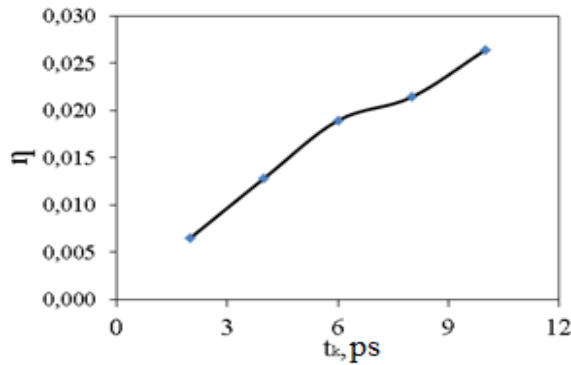


Figure 2. The dependence of the standard deviation η of the frequencies of the model quasi-breather on the time of its existence t_k (in picoseconds, ps).

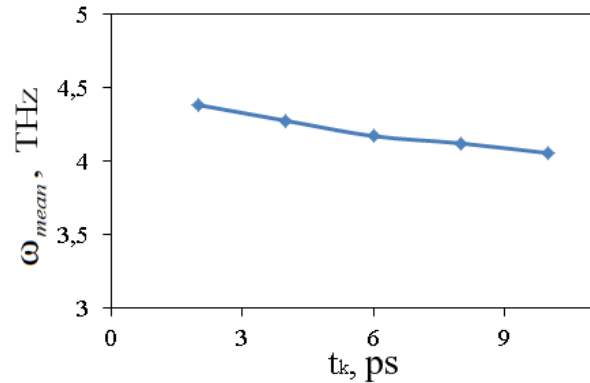


Figure 3. The average frequency $\omega_{mean}(t_k)$ (in THz) of the model quasi-breather from the time of its existence t_k (in picoseconds, ps).

Figures 2-3 show that the deviation of the frequency of the peripheral atoms of the model quasi-breather from the frequency of the core of the quasi-breather is extremely small. Moreover, the average frequency varies from 4.052869801 THz to 4.379309626 THz.

For a more detailed analysis, a grouped statistical series of absolute frequencies was constructed. The lengths, boundaries, and centers of the grouping intervals are found. For each grouping interval, the number of sample elements that fell in this interval was found. The results are shown in table 1. The ratio of the number of sample elements for a given interval to the frequency value of the center of the interval is additionally visualized in figure 4 as a polygon.

The standard deviation $\eta(t_k)$ indicates the absolute estimate of the scatter measure. In this regard, in order to understand how wide the spread is relative to the values themselves (i.e., regardless of their scale), a relative indicator is needed. This indicator is called the coefficient of variation and is calculated by the following formula:

$$V(t_k) = \frac{\eta(t_k)}{\omega_{mean}(t_k)} = \frac{\eta(t_k)}{\bar{\omega}(t_k)}. \quad (3)$$

According to this indicator, it is possible to compare the homogeneity of a variety of phenomena, regardless of their scale and units. The graph shows the coefficients of the coefficient of variation $V(t_k)$ on the lifetime of the quasi-breather t_k (figure 5).

Table 1. The data of the grouped statistical series.

Interval Number k	Interval Center ω_k	Interval Boundaries	Amount in the interval n_k	n_k / ω_k
1	4.08551	4.05287... 4.11816	1	0.244767
2	4.15080	4.11816... 4.18345	2	0.481835
3	4.21609	4.18345... 4.24873	0	0
4	4.28138	4.24873... 4.31402	1	0.23357
5	4.34667	4.31402... 4.37931	1	0.230061

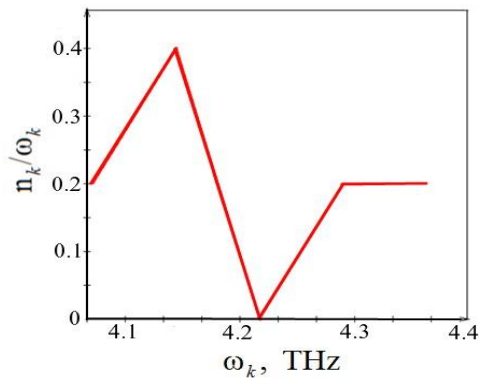


Figure 4. The ratio of the number of sample elements to the frequency value of the center of the interval.

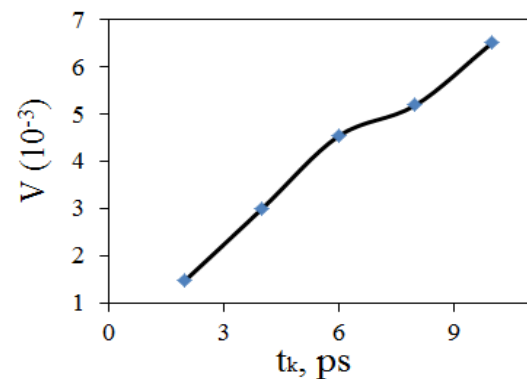


Figure 5. Dependence of the coefficient of variation V on the lifetime of a quasi-breather t_k (ps).

Estimation of the mathematical expectation (sample average) of an ungrouped sample of the average frequencies of a group of atoms included in the model quasi-breather ($\{\omega_{cp}(t_k); k = 1, 2, 3, 4, 5\} = \{4.3793096261; 4.2731326617; 4.1684584381; 4.1194172774; 4.0528698013\}$) calculated by the formula:

$$M(\omega_{mean}) = \frac{1}{N} \sum_{k=1}^N \omega_{mean}(t_k). \quad (4)$$

The estimate of the mathematical expectation $M(\omega_{mean})$ of this sample is 4.198638 THz.

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

$$D(\omega_{mean}) = \frac{1}{N-1} \sum_{k=1}^N (\omega_{mean}(t_k) - M(\omega_{mean}))^2. \quad (5)$$

Calculating the sample variance $D(\omega_{mean})$ by the formula (5), we obtain the value 0.016657. Calculated estimates of mathematical expectation and variance show, that within the framework of this CuPt₇ crystal model, it can be argued that the model quasi-breather is close to the corresponding exact breather. Similarly, within the framework of this model, the following statistical characteristics and dependencies were calculated: a grouped statistical series of absolute and relative frequencies, histogram of relative frequencies and polygon of absolute and relative frequencies, empirical distribution function of the original sample.

Comparing with the results in [20, 21], where the statistical data for breathers in Pt₃Al and CuAu crystals were calculated, we note that in this crystal the lifetime of such objects is much shorter. Moreover, the statistical values are quite comparable. The main role is played by the geometry of the crystal, which determines the density of phonon states and also the features of interatomic bonds.

4. Conclusion

Based on the use of the molecular-dynamic method, the statistical characteristics of the quasi-breather are calculated. A high-performance computing complex based on a GPU accelerator made it possible to provide the necessary speed and accuracy of calculations. The root mean square deviations of the frequencies of individual atoms were calculated entering the breather from the average frequency of the quasi-breather core and also the coefficient of variation at various stages of the existence of the object in question.

It is shown in the paper that the obtained quasi-breather differs from the corresponding exact breather. This may be the reason for the relatively short lifetime of the obtained vibrations in the CuPt₇ crystal. This is also affected by the absence of the band gap in the spectrum of phonon vibrations of the lattice.

Acknowledgments

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