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ANALYSIS OF STATISTICAL CHARACTERISTICS OF QUASI-BREATHER IN MONOATOMIC FCC METALS Au, Cu, Ni, Pd AND Pt

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Abstract. The molecular dynamics method is used to calculate and analyze the statistical characteristics of a quasi-breather with a hard type of nonlinearity in monoatomic FCC metals, for example, Cu, Au, Pt, Ni and Pd. Within the framework of this model, the following statistical characteristics and dependencies were calculated for quasi-breathers: a grouped statistical series of absolute and relative frequencies, a polygon of absolute and relative frequencies, a histogram of relative frequencies, an empirical distribution function, an estimate of the mathematical expectation and variance of the original sample. The densities of phonon states are calculated for all crystals. Statistics allow you to understand the causes of the destruction of breathers and more fully describe the process of their dissipation of energy.

Keywords: crystal, quasi-breather, discrete breather, nonlinear dynamics, soliton, molecular dynamics.

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INTRODUCTION

One of the most interesting and important objects of nonlinear physics for practical application are soliton-type waves (solitary waves) [1–2]. Despite the fact that solitons are known to science for more than 180 years, they have been little studied in many fields of knowledge. So, recently interest to discrete nonlinear systems in which the existence of dynamic solitons is possible increases. An example of a dynamic soliton can serve as discrete breathers (DB) – localized in space and periodic in time high-amplitude excitations in nonlinear discrete structures with translational symmetry [3].

It is assumed that the DBs participate in various solid-state processes. In particular, DB can increase the catalytic properties of nanoparticles with a disordered structure, lead to radiation-stimulated growth of pores in metals, contribute to diffusion, transport electric charge, lead to annealing of defects, reduce the energy barrier of chemical reactions in crystalline solids, etc. [4–5].

Discrete breathers can be divided into two types according to the nature of their frequency dependence on the amplitude [6]. In discrete breathers of a soft type, the frequency decreases with increasing amplitude (such discrete breathers can exist only in crystals having a gap in the phonon spectrum: their frequency lies in the slit of the phonon spectrum and therefore they are called slotted), and in discrete hard type breather the opposite occurs (they can have frequencies, both in the gap and above the phonon spectrum). Discrete breathers with a soft type of nonlinearity can be excited in biatomic crystals, for example, in NaCl [6], Pt_3Al [7–14], as well as in graphene and graphane [15]. Breather with a hard type of nonlinearity exist in pure metals with FCC-, BCC-, and HCP-structures. For pure metals or ordered alloys with a small difference in mass, the conditions for excitation of a DB with a hard type of nonlinearity are more specific than when exciting slit DBs with a soft type of nonlinearity.

It is necessary to make a terminological reservation. In mathematical physics, DB means strictly periodic, non-local oscillations localized in space, continuous in time, at one frequency, but in real systems where the presence of all possible perturbations is inevitable, one should consider quasi-breathers having a non-strict periodicity of oscillations with frequencies in a certain range and finite life time [16]. Unlike idealized DB, quasi-breathers have an infinite, but rather long, lifetime. Quasi-breathers arise in the presence of small deviations from accurate breather solutions in the multidimensional space of all possible initial conditions in the solution of

the Cauchy problem for nonlinear differential equations, since in this case there is no complete suppression of the contributions from oscillations of peripheral particles with their own frequencies. Thus, weakening of the leading vibration of the breather core (in our calculations, the core of a symmetric breather forms one particle, and in the case of an antisymmetric breather, two of its central particles) leads to the presence of additional vibration frequencies in the breather solution. These small contributions can be found in the vibrations of all quasi-breather particles, in particular, central ones. If the frequencies of oscillations of all quasi-breather particles computed at a certain time interval near $t = t_k$ are determined sufficiently accurately, then they will not be strictly identical. Further, the terms breather, discrete breather and quasi-breather will be used as synonyms.

The monoatomic FCC metals Cu, Au, Pt, Ni and Pd are considered in this paper. The main goal of the paper is to calculate and analyze the statistical characteristics of quasi-breathers with a hard type of nonlinearity in the specified materials. The data obtained will make it possible to characterize the evolution of a quasi-breather over time.

COMPUTER MODEL AND DESCRIPTION OF THE EXPERIMENT

The models we are considering are bulk crystals containing 10^5 to $3\cdot10^5$ particles interacting via a potential obtained by the immersed atom method (EAM potential). The simulation was carried out using the LAMMPS package [17].

In computational chemistry, the immersed atom model is used to approximate the interaction energy between two atoms, taking into account the presence of neighboring atoms. The choice of the potential and the validity of its use for a specific task is an important stage in the modeling.

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

The EAM potential of a pure element is determined by three functions: the pair energy φ, the electron density ρ, and the embedding energy F. For the alloy, the EAM potential contains not only the three functions φ, ρ, and F for each of the constituent elements, but also the pair energies φ_{ab} between the different elements a and b ($a\neq b$). As a result, the functions φ, ρ, and F calculated for pure metals can not be directly applied to the alloy or multilayer systems. Nevertheless, the procedure for generalizing EAM potentials and their trimming distance by normalizing EAM potentials and introducing an alloy model was proposed by the author of [18]. This procedure enables the construction of EAM potentials of alloys from EAM-potentials for individual elements. Such potentials of alloys were used in molecular modeling and gave good results in experiments [18]; we used this potential for the CuAu crystal [19].

The main factor determining the lifetime of the DB in real crystals is the remoteness of its frequency from the frequencies of the phonon spectrum, and therefore dispersion curves and phonon-state densities for the crystals under study were calculated (see Fig. 1). The calculations used the software package LAMMPS, which includes the procedures necessary for these purposes, based on the Fourier transform of the autocorrelation functions of atomic displacements versus time.

Next, the statistical characteristics of DB in monoatomic crystals Cu, Au, Pt, Ni and Pd will be calculated and analyzed.

RESULTS AND DISCUSSIONS

The main statistical characteristics of the quasi-breather are the standard deviation $\eta(t_k)$ (Fig. 2) and the mean value of the frequency $\bar{\omega}$ of atomic vibrations, where t_k is the quasi-breather lifetime [20–21]:

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

$$\bar{\omega}\left(t_k\right) = \frac{1}{N}\sum_{i=1}^{N}\omega_i\left(t_k\right), \qquad (2)$$

The lifetime of these quasi-breathers was divided into five equal parts. Thus, five points were obtained for analyzing the statistical characteristics of breathers (see Fig. 2). That is, there was a sample of five elements – frequencies of quasi-breathers, see Table 1.

Next, we constructed the statistical series of absolute frequencies for this sample, i.e. the sequence of pairs of numbers (ω_1^*, n_1^*), (ω_2^*, n_2^*), … ,(ω_m^*, n_m^*), where ω_k^* is the center of the k-interval of the grouping and n_1^* is the number of sampling elements in k-interval. The numbers. n_k^* (k = 1, …, m) are called absolute frequencies. We find the minimum and maximum sample elements, they correspond to

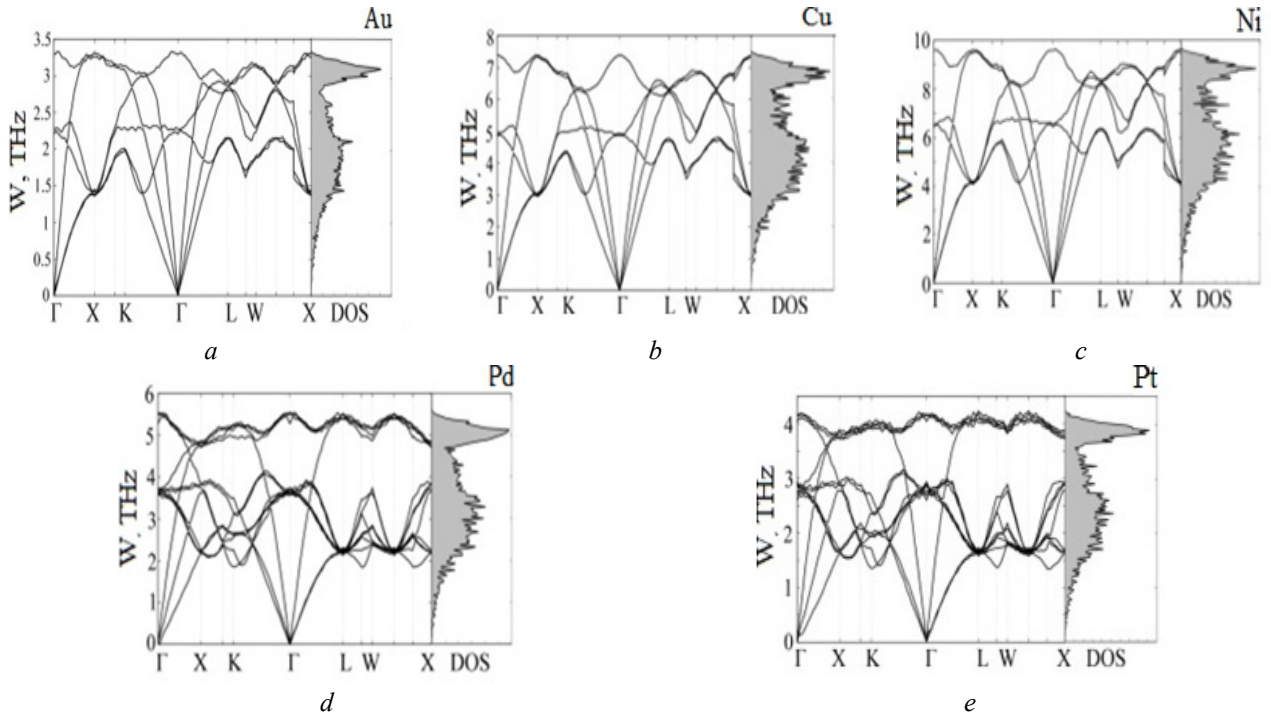

Fig. 1. Dispersion curves and densities of phonon states for metals: *a* - Au, *b* - Cu, *c* - Ni, *d* - Pd, *e* – Pt

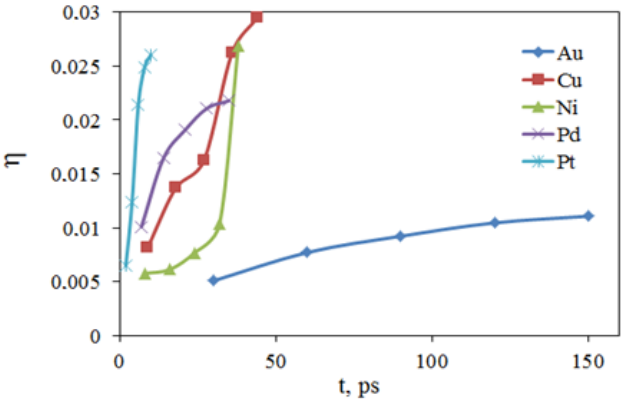

Fig. 2. Dependence of the root-mean-square deviation of vibration frequencies of quasi-breather atoms on their lifetime for Cu, Au, Pt, Ni, and Pd

Table 1. Frequency sampling of a quasi-breather

Model	ϖ_1, THz	ϖ_2, THz	ϖ_3, THz	ϖ_4, THz	ϖ_5, THz
Cu	8.18301	7.87534	7.72063	7.42053	7.33631
Au	3.56532	3.51414	3.48136	3.42447	3.37433
Pt	4.47930	4.37063	4.22345	4.12226	4.04060
Ni	10.52174	10.33132	10.16977	9.99958	9.85306
Pd	5.85093	5.69786	5.61925	5.49998	5.40357

the extreme values for each model in Table 1. Find the length of the grouping interval by the formula:

$$h = (\omega_{max} - \omega_{min}) / m. \quad (3)$$

We find the right boundaries of the grouping intervals:

$$\omega_k = \omega_{min} + k\,h\ (\kappa = 1, ..., 5). \quad (4)$$

We find the centers ω^*_k intervals of the grouping by the formula:

$$\omega^*_k = \omega_k - h / 2\ (\kappa = 1, ..., 5). \quad (5)$$

For each grouping interval (ω_{k-1}, ω_k) we find the number n_k^* of sample elements that fall in this interval. It is important that each sample element is assigned to one and only to one interval, and if the value of the element falls on the interval boundary, then we will refer it to the interval with the lowest number. The minimum element is always referred to the first interval, the maximum to the last. The results are shown in Table 2.

We build a grouped statistical series of relative frequencies, which is a sequence of pairs of numbers $(\omega_1^*, n_1^*/n)$, $(\omega_2^*, n_2^*/n)$, … , $(\omega_m^*, n_m^*/n)$, where n_k^*/n are the relative frequencies and n is the sample size (see Table 3).

Based on Table 3, we construct the relative frequency polygons for each of the crystal models (see Fig. 3).

To complete the statistical picture of the cha-racteristics of quasi-breathers, we estimate the mathematical expectation and variance, and also construct empirical distribution functions.

Estimate of the mathematical expectation (sample mean) of a grouped sample is calculated using the formula:

Table 2. Supporting table of statistical data

Model	Number of interval k	Center of interval ω_k^*, THz	Limits of interval, THz
Cu	1	7.42098	7.33631...7.50565
	2	7.59032	7.50565...7.67499
	3	7.75966	7.67499...7.84433
	4	7.92900	7.84433...8.01367
	5	8.09834	8.01367...8.18301
Au	1	3.39343	3.37433...3.41253
	2	3.43162	3.41253...3.45072
	3	3.46982	3.45072...3.48892
	4	3.50802	3.48892...3.52712
	5	3.54622	3.52712...3.56532
Pt	1	4.08447	4.04060...4.12834
	2	4.17221	4.12834...4.21608
	3	4.25996	4.21608...4.30383
	4	4.34770	4.30383...4.39157
	5	4.43544	4.39157...4.47931
Ni	1	9.91993	9.85306...9.98680
	2	10.05366	9.98680... 10.12053
	3	10.18740	10.12053...10.25427
	4	10.32114	10.25427...10.38800
	5	10.45487	10.38800...10.52174
Pd	1	5.44831	5.40357...5.49305
	2	5.53778	5.49305...5.58252
	3	5.62725	5.58252...5.67199
	4	5.71673	5.67199...5.76146
	5	5.80620	5.76146...5.85093

Table 3. Grouped statistical series of relative frequencies

Cu	ω_k^*, THz	7.42098	7.59032	7.75966	7.92900	8.09834
	n_k^*/n	0.40000	0.00000	0.20000	0.20000	0.20000
Au	ω_k^*, THz	3.39343	3.43162	3.46982	3.50802	3.54622
	n_k^*/n	0.20000	0.20000	0.20000	0.20000	0.20000
Pt	ω_k^*, THz	**4.08447**	**4.17221**	**4.25996**	**4.34770**	**4.43544**
	n_k^*/n	**0.40000**	**0.00000**	**0.00000**	**0.40000**	**0.20000**
Ni	ω_k^*, THz	9.91993	10.05366	10.18740	10.32114	10.45487
	n_k^*/n	**0.40000**	**0.00000**	**0.20000**	**0.20000**	**0.20000**
Pd	ω_k^*, THz	**5.44831**	**5.53778**	**5.62725**	**5.71673**	**5.80620**
	n_k^*/n	**0.20000**	**0.00000**	**0.40000**	**0.20000**	**0.20000**

$$M^* = \frac{1}{n}\sum_{k=1}^{n}\omega_k. \quad (6)$$

The estimation of variance, not grouped sample, is carried out according to the formula:

$$D^* = \frac{1}{n-1}\sum_{k=1}^{n}(\omega_n - M^*)^2. \quad (7)$$

For the models we are considering, we have obtained the values given in Table 4.

Table 4. Mathematical expectation and variance for model crystals

Model	M^*	D^*
Cu	7.707168	0.118647
Au	3.471924	0.005593
Pt	4.269478	0.033139
Ni	10.155099	0.080553
Pd	5.634324	0.026402

For clarity, we construct empirical distribution functions *F(ɯ) (see Fig. 4).*

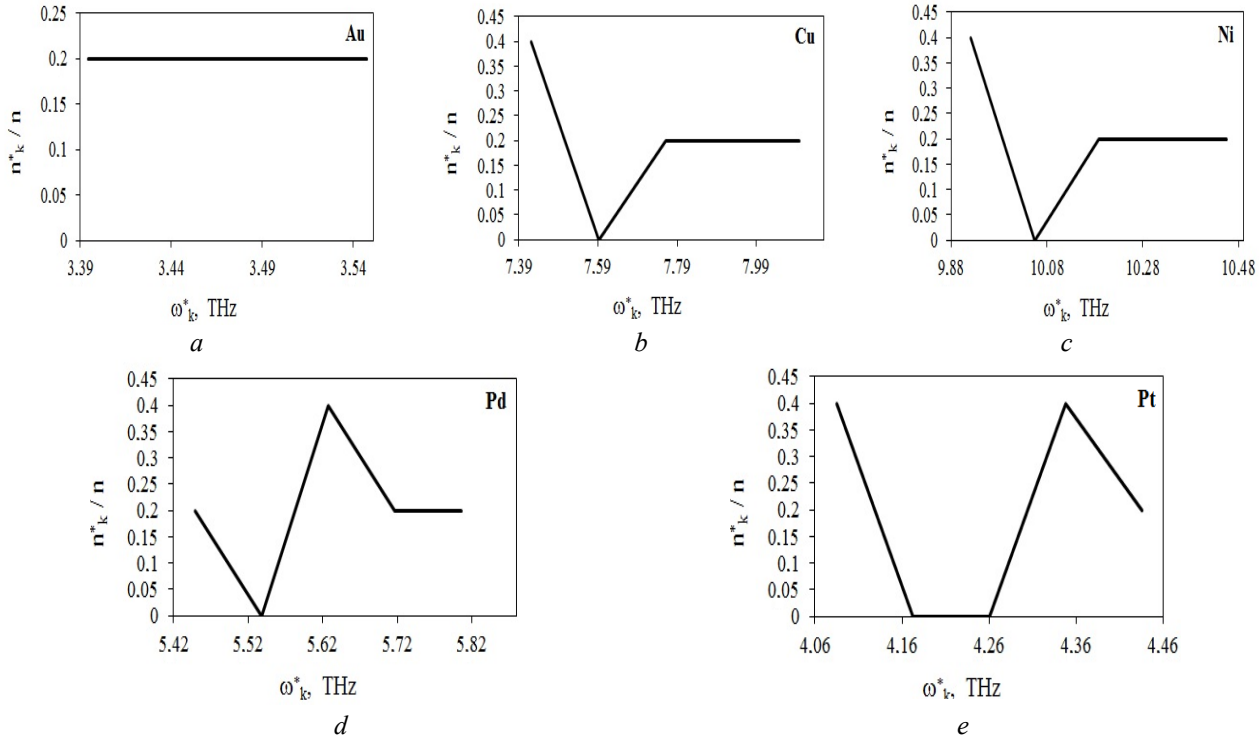

Fig. 3. Polygons of relative frequencies of discrete breathers: *a* - Au, *b* - Cu, *c* - Ni, *d* - Pd, *e* – Pt

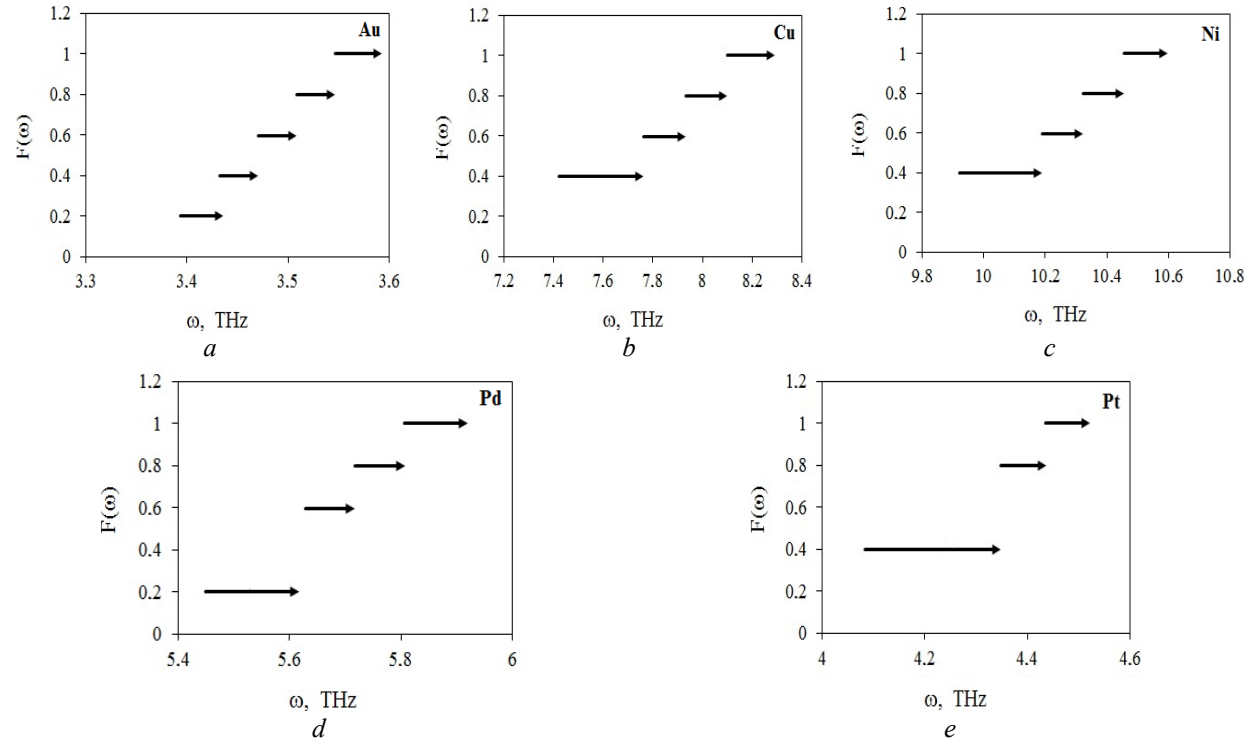

Fig. 4. Empirical distribution functions: *a* - Au, *b* - Cu, *c* - Ni, *d* - Pd, *e* - Pt

The obtained statistical data show the process of energy dissipation by breathers on the whole interval of their lifetime. The destruction of quasi-breathers occurs at a time when the root-mean-square deviation exceeds the difference between the average frequency of the breather and the nearest boundary of the phonon spectrum of the crystal. In this case, this process may not be uniform, which is primarily due to the properties of the crystals, as well as the method of exciting the breathers.

CONCLUSION

In the work of molecular dynamics using the statistical approach, quasi-breathers in monoatomic FCC crystals Cu, Au, Pt, Ni, and Pd are considered. Dispersion curves and densities of phonon states are calculated for all crystals. All the basic statistical characteristics of quasi-breather frequencies are calculated: the standard deviation of the frequencies of the atoms, the mean frequencies of the quasi-breather, the polygons of the relative frequencies, the mathematical expectation, the variance, and the empirical distribution functions. It is established that the root-mean-square deviation of vibration frequencies of quasi-breather atoms, that is, the degree of their quasi-breathing, increases with time (see Fig. 2), and the average frequency of their oscillations decreases, approaching the upper boundary of the phonon spectrum (see Table 1). Quasi-breathers are destroyed when the root-mean-square deviation of the vibration frequencies exceeds the difference between the average frequency of the breather and the nearest boundary of the phonon spectrum of the crystal. The obtained statistical data allow describing the process of degradation of DB with the passage of time. It is important that the described approaches make it possible to establish that quasi-breathers having a shorter lifetime dissipate energy at the initial stages of existence, which is caused both by the method of exciting the breathers and by the properties of model crystals.

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УДК 538.913

АНАЛИЗ СТАТИСТИЧЕСКИХ ХАРАКТЕРИСТИК КВАЗИ-БРИЗЕРОВ В МОНОАТОМНЫХ ГЦК МЕТАЛЛАХ Au, Cu, Ni, Pd И Pt

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Аннотация. Методом молекулярной динамики проводится расчёт и анализ статистических характеристик квази-бризера с жёстким типом нелинейности в моноатомных ГЦК металлах, на примере Cu, Au, Pt. Ni и Pd. В рамках данной модели для квази-бризеров были рассчитаны следующие статистические характеристики и зависимости: группированный статистический ряд абсолютных и относительных частот, полигон абсолютных и относительных частот, гистограмма относительных частот, эмпирическая функция распределения, оценка математического ожидания и дисперсии исходной выборки. Для всех кристаллов рассчитаны плотности фононных состояний. Статистические данные позволяют вникнуть в причины разрушения бризеров и более полно описать процесс рассеяния ими энергии.

Ключевые слова: кристалл, квази-бризер, дискретный бризер, нелинейная динамика, солитон, молекулярная динамика.

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