ISSN 1063-7761, Journal of Experimental and Theoretical Physics, 2017, Vol. 125, No. 5, pp. 913–919. © Pleiades Publishing, Inc., 2017.
Original Russian Text © P.V. Zakharov, S.V. Dmitriev, M.D. Starostenkov, A.M. Eremin, E.A. Korznikova, 2017, published in Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki, 2017, Vol. 152, No. 5, pp. 1073–1080.

STATISTICAL, NONLINEAR, AND SOFT MATTER PHYSICS

Stationary Quasi-Breathers in Monatomic FCC Metals

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Received May 10, 2017

Abstract—The characteristics of quasi-breathers in monatomic fcc metals are investigated by the molecular dynamics method. The standard deviations of the frequencies of atoms constituting a breather from the fundamental frequency of oscillations are calculated. It is shown that the quasi-breather lifetime in the models under investigation depends on the initial excitation conditions as well as on the metal type.

DOI: 10.1134/S1063776117100181

1. INTRODUCTION

The concept of energy localization and transport in crystals by soliton-type waves has been intensely developed in recent years. In particular, discrete breathers (DBs), which are defined as spatially localized large-amplitude strictly periodic in time vibrational modes of in nonlinear lattices, aroused special interest [1, 2]. However, the search for the initial conditions leading to DB excitation corresponding to the given rigorous definition for 3D crystals that can be described by realistic interatomic potentials appears as a complicated problem (the possibility of solution of this problem has not been proved theoretically). Such an exact tuning of the initial conditions cannot be easily performed in the course of molecular dynamic simulation; the more so, such a tuning cannot be attained in any physical experiment, in which various perturbations are inevitably present [3, 4]. This circumstance led Chechin et al. [5] to develop the concept of a quasi-breather, which is a long-lived spatially localized nonlinear oscillation that does not exhibit temporal periodicity [5]. They formulated a certain criterion of closeness of a quasi-breather to the corresponding exact DB, which is based on the calculation of the standard deviation $\eta(t_k)$ of the oscillation frequencies of individual breather particles in a certain time interval in the vicinity of instant t_k, as well as the standard deviation of oscillation frequencies of a selected DB particle on various time intervals. Such an approach makes it possible to characterize the DB evolution with time. In the present study, quasi-breathers will be referred to as DBs for brevity.

Considering the topicality of studying DBs in crystals, we note that in a number of recent publications, such objects were considered as main carriers of energy from the source of external action to the bulk of the crystal. For example, annealing of defects in the plasma treatment of germanium at a considerable distance from the crystal surface was considered in [6]. The authors of this work believe that the energy is transported precisely by discrete breathers. In a large number of publications, the possibility of a contribution of such objects to the lattice dynamics of crystals and their contribution to the properties of various crystalline structures was indicated [7]. In this connection, it is necessary to study localized objects in crystals such as breathers. It is important to analyze not only static characteristics of particle vibrations, but also their lifetime, depending on the properties of crystals.

It should be noted DBs can be divided into two classes as regards the form of the dependence of the frequency of atomic vibrations on the amplitude. For a soft-type DB, the frequency decreases with increasing its amplitude (such discrete breathers can exist only in crystals with a gap in the phonon spectrum because their frequency lies in the phonon spectrum gap; breathers of this type are known as gap breathers). For hard-type DBs, the frequency increases with the amplitude (the frequencies of such breathers can lie in the gap or above the phonon spectrum). Discrete breathers with the soft type of nonlinearity can be excited in diatomic crystals as well as in graphene and

Table 1. Properties of fcc metals under investigation [24, 25]

Parameter/Metal	Pt	Ni	Cu	Pd	Au
a_0, Å	3.92	3.52	3.615	3.89	4.078
E_0, eV/at	−5.77	−4.45	−3.54	−3.91	−3.93
c_{11}, 10^{11} Pa	3.47	2.63	1.75	2.35	1.97
c_{12}, 10^{11} Pa	2.53	1.54	1.24	1.8	1.65
c_{44}, 10^{11} Pa	0.78	1.27	0.79	0.82	0.45
Elastic modulus, GPa	282	186	141	188	178
Young modulus, GPa	180	217	46	127	78
Shear modulus, GPa	65	84	48	46	27.5
Poisson ratio	0.36	0.35	0.38	0.39	0.4
Density, g/cm^3	21.45	8.91	8.92	12.02	19.32

graphane [7–17]. Breathers with the hard type of nonlinearity exist in graphene [18] and in pure fcc, bcc, and hcp structures [19–21], as well as in alpha-uranium [22] and diamond [23].

In this work, we consider hard-type quasi-breathers. As the objects of investigation, we chose the following metals with the fcc structure: Pt, Ni, Cu, Pd, and Au. Such a choice of the crystals makes it possible to establish correlations between the DB lifetime and the properties of the materials under investigation. The main properties of the crystals in question are given in Table 1.

2. MODEL AND EXPERIMENTAL TECHNIQUE

According to information available in the literature, the DB lifetime in different crystals and under different conditions amounts to from dozens to thousands of periods of vibrations (i.e., attains values on the order of 1 ns). Breathers are spatially localized on a small group of atoms from units to dozens (i.e., on a scale of about 1 nm). Investigation of quasi-breathers in crystals in actual experiments is difficult in view of their short lifetime and small size. For this reason, the computer simulation method was chosen for their investigation, which is quite efficient in analysis of the physics of condensed state and in material science. One of the most popular methods of DB analysis in crystals is the molecular dynamics method based on well-tested interatomic potentials. It is important to note that the nonlinear dynamics of the crystal lattice is investigated in this method in real time.

Simulation was carried out using the LAMMPS molecular dynamics package that was successfully used earlier [26]. For the interatomic potentials, we used the potentials obtained by the embedded atom method (EAM). The embedded atom method is used in computational chemistry for obtaining an approximate description of the energy of interaction between two atoms. The potential energy of a crystal in the given case can be represented as the sum of the pair interaction energy of atoms and the energy of interaction of atoms with the electron gas:

$$E = \frac{1}{2}\sum_{i,j,i\neq j}\varphi_{ij}(r_{ij}) + \sum_i F_i(\rho_i), \qquad (1)$$

where φ_{ij} is the pair interaction energy between the ith and jth atoms separated by distance r_{ij}, and F_i is the energy of embedding of the ith atom in the electron subsystem characterized by electron density ρ_i. The electron density can be calculated by the formula

$$\rho_i = \sum_{i,j\neq i} f_j(r_{ij}),$$

where $f_j(r_{ij})$ is the electron density at the point of location of the ith atom separated by distance r_{ij} from the jth atom. Therefore, the EAM potential of a pure element is described by three functions of pair energy φ, electron density ρ, and embedding energy F. More detailed information on the functions and methods for obtaining their parameters can be found on LAMMPS site [26] and, for example, in [27].

The rated blocks of crystals in the form of cubic cells contained from 5×10^4 to 5×10^5 atoms. Computation cells of such a size are sufficient for avoiding the effect of the boundary conditions on the lifetime of

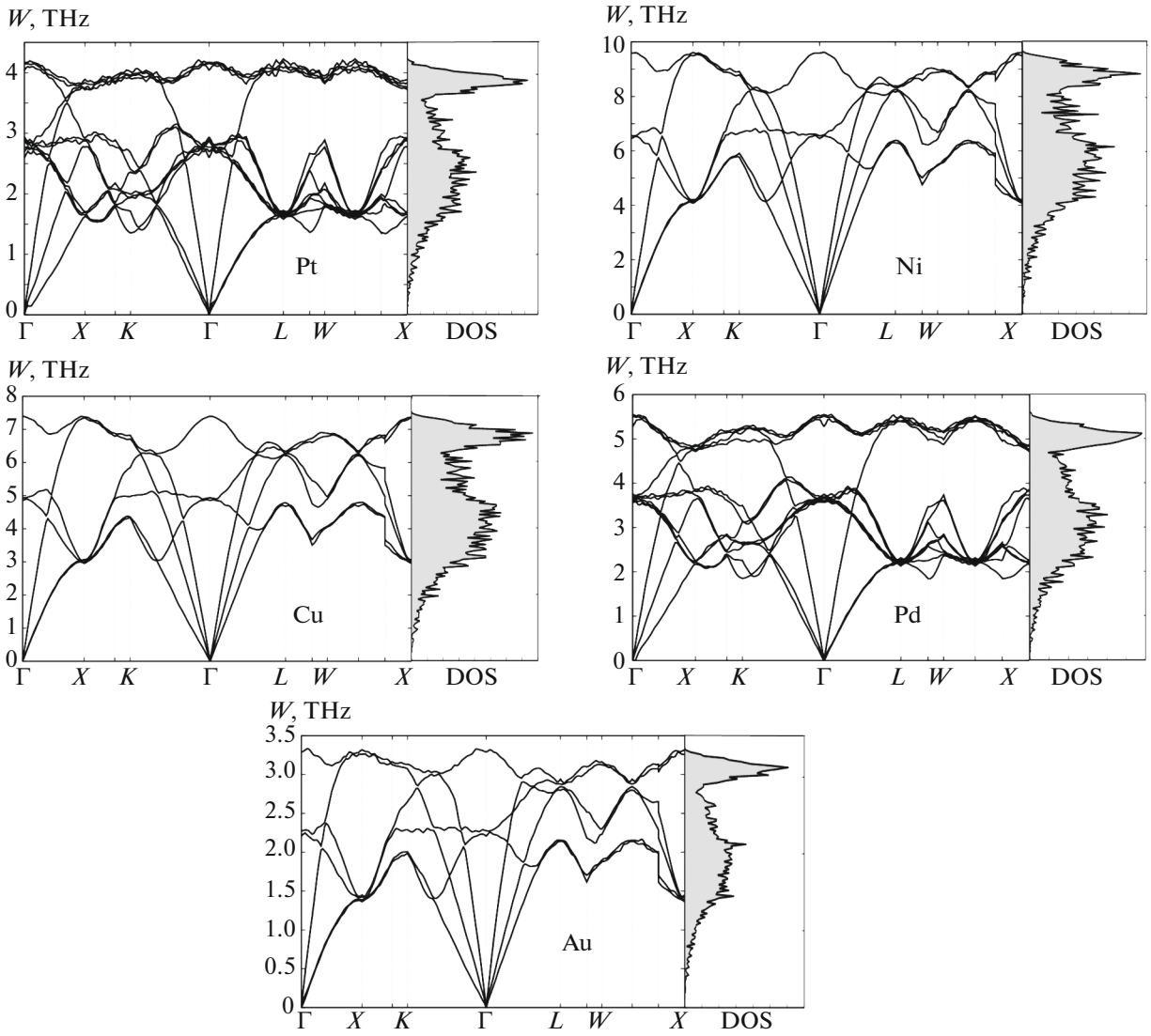

Fig. 1. Dispersion curves and phonon densities of state (DOS) for different metals.

quasi-breathers on account of their high degree of spatial localization. Periodic boundary conditions that make it possible to eliminate the effect of the surface of the DB dynamics were imposed along three coordinate axes.

The equations of motion of atoms were integrated using the numerical algorithm of the fourth order of accuracy with an integration step of 0.5 fs.

The main factor determining the DB lifetime in real crystals is the closeness of its frequency to the frequencies of the phonon spectrum; for this reason, we calculated the dispersion curves and the phonon densities of state for the crystals under investigation (Fig. 1). In our calculations, we used the LAMMPS program package that includes the required procedures based on the Fourier transform of the autocorrelation functions of atomic displacements depending on time [26].

Hard-type breathers are localized predominantly in one closely packed atomic row in which atoms are labeled by index n. The coordinate x axis was chosen along this row. Atoms in the DB core vibrate along the

Table 2. Maximal lifetime of quasi-breathers and parameters of Eq. (3), used for their excitation in different fcc metals

Parameter/Metal	Pt	Ni	Cu	Pd	Au
DB lifetime, ps	14	39	49	74	154
Parameter of Eq. (3) A	0.58	0.45	0.46	0.5	0.65
Parameter of Eq. (3) β	0.18	0.07	0.12	0.05	0.25
Parameter of Eq. (3) B	0.3	0.51	0.41	0.3	0.45
Parameter of Eq. (3) γ	0.5	0.46	0.55	0.46	0.5

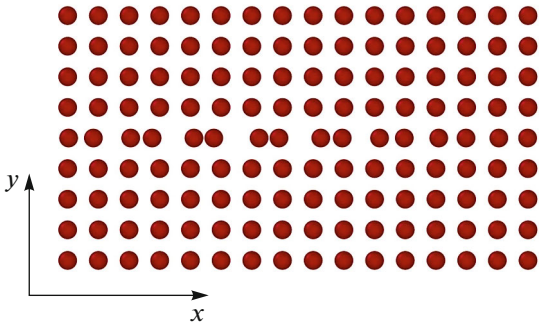

Fig. 2. (Color online) Initial deviations of atoms in an fcc crystal for excitation of a stationary discrete breather with the hard-type nonlinearity; the x-axis is directed along the densely packed crystallographic direction ⟨110⟩.

densely packed row in antiphase with the nearest neighbors. The initial conditions for exciting a stationary DB with the hard type of nonlinearity were specified, according to [28], as

$$x_n^0 = T_n + S_n, \quad \dot{x}_n^0 = 0, \tag{2}$$

where x_n^0 and $\dot{x}_n^0$ are the components of initial displacement vectors and initial velocities of the nth atom of the densely packed row in the crystal. All remaining atoms of the crystal had zero initial displacements and initial velocities. Functions T_n and S_n describe the amplitudes of vibration and displacements of the centers of vibration of atoms, respectively. Therefore,

$$T_n = \frac{1}{2}(x_{n,\max} - x_{n,\min}), \quad S_n = \frac{1}{2}(x_{n,\max} + x_{n,\min}),$$

where $x_{n,\max}$ and $x_{n,\min}$ are the maximal and minimal values of function $x_n(t)$ describing the motion of the nth atom. These functions have the form

$$T_n = \frac{(-1)^n A}{\cosh[\beta(n - x_0)]}, \quad S_n = \frac{-B(n - x_0)}{\cosh[\gamma(n - x_0)]}, \tag{3}$$

where parameter A determines the DB amplitude, parameter B determines the amplitude of displacements of the centers of vibrations of atoms, parameters β and γ specify the degree of spatial localization of the DB, and x_0 is its initial position [28].

Figure 2 shows the form of the initial displacements of atoms from their equilibrium positions.

3. RESULTS AND DISCUSSION

By selecting parameters of Eq. (3), we obtained DBs in all investigated fcc crystals. Depending on the values of parameters in Eq. (3), the DB lifetime can vary significantly. By way of example, we consider the dependence of the DB lifetime in Pd on the variation of the amplitude (Fig. 3a) and parameter γ (Fig. 3b).

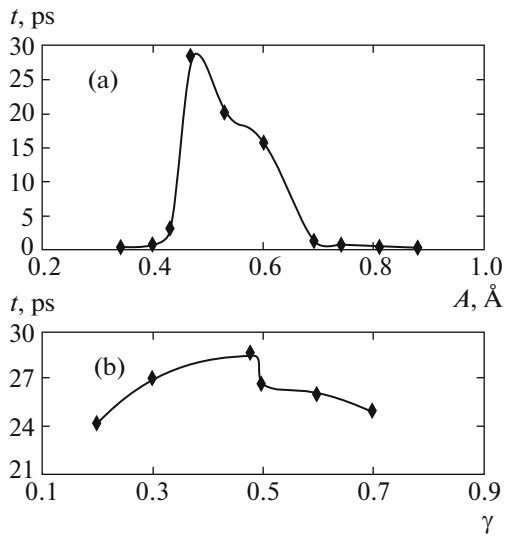

Fig. 3. Dependence of the lifetime of a quasi-breather in a Pd crystal on (a) initial amplitude and (b) parameter γ in Eq. (3).

Analogous dependences were also observed for other crystals under investigation. The choice of parameters was carried out by the trial-and-error method so as to obtain the maximal breather lifetime. The maximal lifetime attained in our numerical experiments and the corresponding values of parameters of Eq. (3) are given in Table 2.

We failed to increase the DB lifetime significantly by a further selection of parameters of Eq. (3). Therefore, the DB lifetime obviously not only depends on the initial conditions, but a certain correlation with the properties of the crystals is also observed (Fig. 4). In particular, the dependence of the lifetime on the shear modulus is manifested most clearly. In the whole, a tendency is observed for the crystals under investigation, in which the breather lifetime increases upon a decrease in the shear modulus.

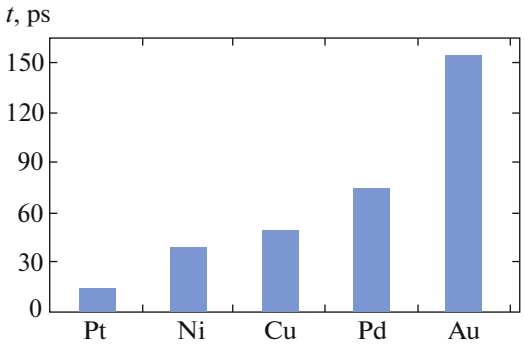

Fig. 4. (Color online) Maximal lifetime of a quasi-breather for different metals.

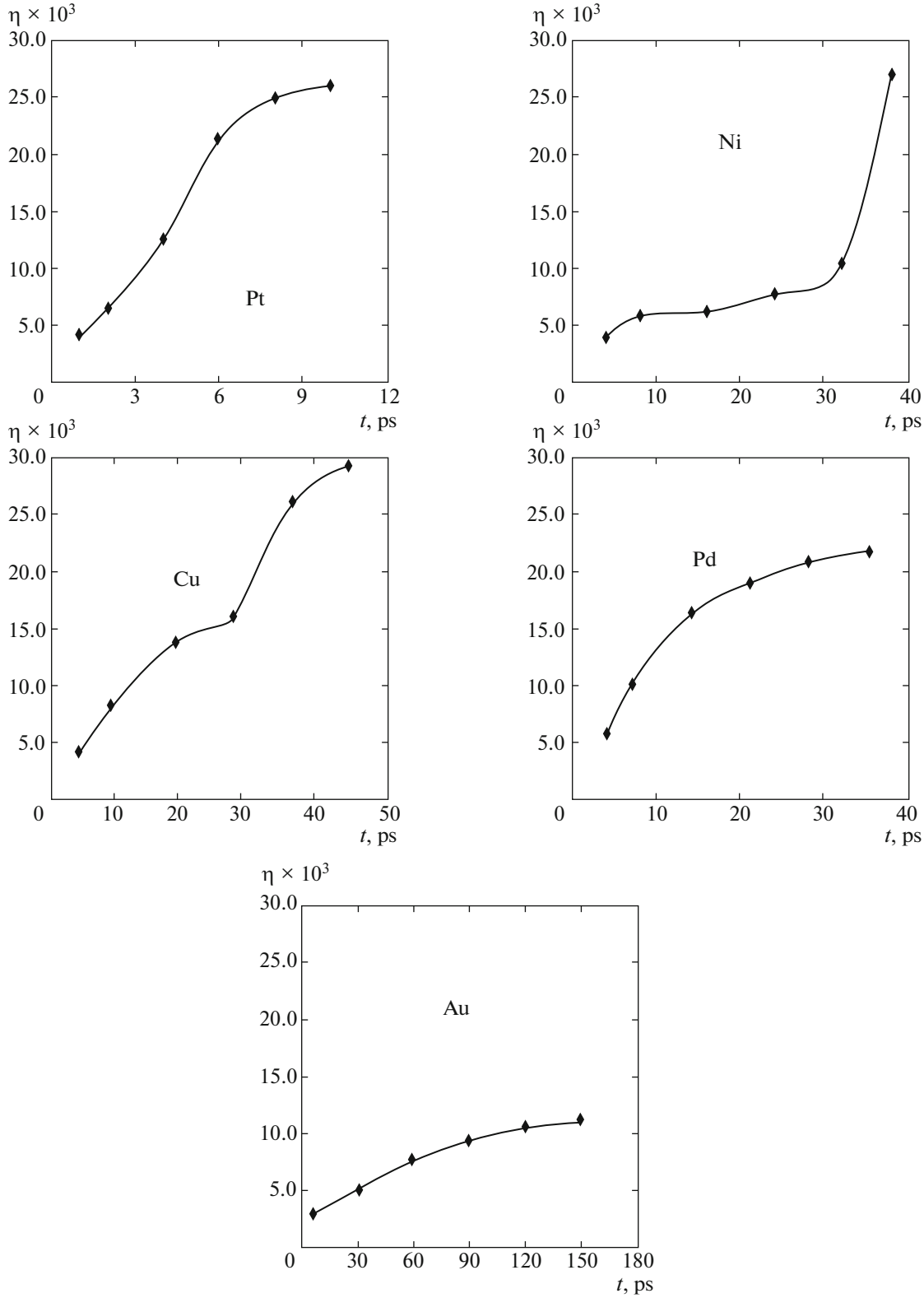

Fig. 5. Dependences of the standard deviation η of a quasi-breather on its lifetime for different metals.

As noted above, in contrast to conventional DBs, quasi-breathers are not strictly time-periodic dynamic objects and have a finite lifetime. For the metals considered in this study, the maximal lifetime of quasi-breathers constitutes dozens and hundreds of periods of vibrations. It should be noted that large-amplitude

thermal fluctuations, which are not quasi-breathers, attenuate after 2–3 periods. Thus, quasi-breathers have a lifetime exceeding the thermal fluctuation lifetime by several orders of magnitude, which allows us to treat them as independent physical objects that make a certain contribution to the formation of the properties of the systems under investigation. The maximal amplitude of oscillations of quasi-breathers attains significant values (about 0.4–0.6 Å in our case).

To characterize the closeness of a quasi-breather to a DB, we calculated the frequencies of vibrations on a certain time interval near $t = t_k$ for all atoms in the quasi-breather core. As expected, the values of frequencies were not strictly identical. In this connection, we find the standard deviations $\eta(t_k)$ of the vibrational frequencies of different atoms from the average frequency $\bar{\omega}$ of a breather:

$$\bar{\omega}(t_k) = \frac{1}{N}\sum_{i=1}^{N}\omega_i(t_k), \tag{4}$$

$$\eta(t_k) = \sqrt{\frac{\sum_{i=1}^{N}(\omega_i(t_k) - \bar{\omega}(t_k))^2}{N(N-1)}}. \tag{5}$$

The larger the value of $\eta(t_k)$, the stronger the difference between the quasi-breather solution and the exact solution for which $\eta(t_k) = 0$ at any instant t_k. Further, we considered a group of eight particles constituting the breather core.

The resultant dependences (Fig. 5) show that the higher the rate of the increase in the standard deviation in the group of atoms under investigation, the sooner the breather breaks. Not only the rate of increase, but also the absolute value of this quantity is important. Breakdown of a breather occurs at the instant when the difference between the fundamental frequency and the upper boundary of the phonon spectrum becomes smaller than the standard deviation. At this instant, the breather begins actively dissipate energy to the phonon subsystem of the crystal and breaks during a few periods of vibrations.

4. CONCLUSIONS

In this study, we have analyzed the static characteristics of steady-state quasi-breathers with the hard-type nonlinearity using the molecular dynamics methods for the following metals: Pt, Ni, Cu, Pd, and Au. We have obtained the dependences of the standard deviation of the group of atoms constituting the breather core on its lifetime. It is found that the breakdown of a breather occurs when the standard deviation exceeds the width of the gap between the fundamental frequency of a discrete breather and the upper boundary of the phonon spectrum for a given crystal. A quasi-breather can be characterized not only by static quantities, but directly by its lifetime in the crystal.

The results obtained in this work extend our knowledge about the properties of quasi-breathers in pure fcc metals; these results can be useful in staging experiments on indirect observation of quasi-breathers in real crystals, as well as for explaining energy dissipation effects under intense external actions on metallic objects.

ACKNOWLEDGMENTS

The research of S.V. Dmitriev and P.V. Zakharov was supported by the Russian Science Foundation (project no. 16-12-10175); the work of M.D. Starostenkov was supported by the Ministry of Education and Science of the Russian Federation in the frame of the basic part of state contract (project no. 3.4820.2017/BCh); the work of E.A. Korznikova was supported by the Russian Foundation for Basic Research (project no. 17-02-00984-A).

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Translated by N. Wadhwa