ANALYSIS OF STATISTICAL CHARACTERISTICS OF QUASI-BREATHER WITH SOFT-TYPE OF NONLINEARITY IN THE CRYSTALS OF A_3B STOICHIOMETRY

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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.

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).

The simulation was being performed using the LAMMPS Molecular Dynamics Simulator molecular dynamics package. 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 was used for simulating the interatomic interaction. In computational chemistry, the embedded atom model is applied for approximate description of two atoms interaction energy (1). 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 rij – 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

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.

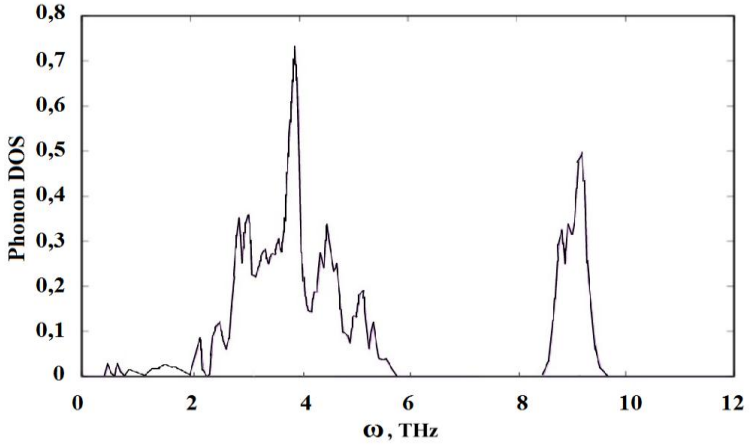

Fig. 1. Density of Pt_3Al crystal phonon states

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.

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