

## Calculation 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 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 (EAM) was used for simulating the interatomic interaction. In computational chemistry, the embedded atom model is applied for approximate description of two atoms interaction energy.

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.

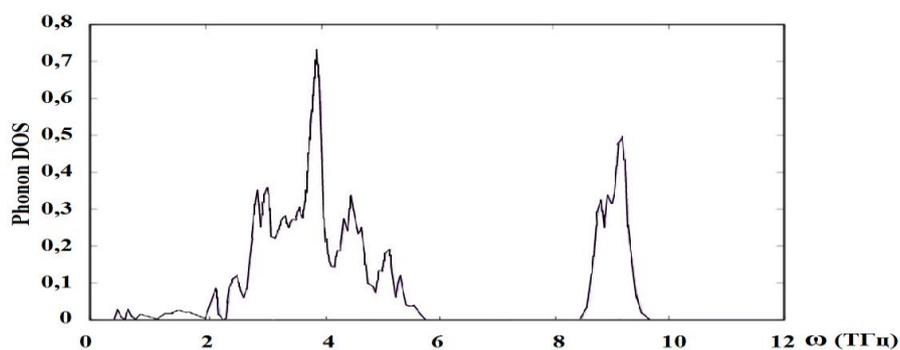


Fig. 1. Density of  $Pt_3Al$  crystal phonon states

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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