Nonlinear high-amplitude excitations of the $CuPt_7$ crystal lattice: a molecular dynamics study

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Abstract. This article analyzes the structure and properties of the $CuPt_7$ crystal for the possible existence of non-linear high-amplitude oscillations of the light alloy component. The densities of the phonon states of a crystal are calculated and analyzed for its different structures. It is demonstrated that the phonon system of a crystal has a narrow forbidden zone. The dependences of the possibility of the existence of high-amplitude oscillations on the initial conditions are revealed. It is shown that such oscillations are possible with the initial deviation of the Cu atom from the equilibrium position by more than 0.95 Å for FCC $CuPt_7$. For such oscillators, their lifetime, the amount of stored energy, and other characteristics were obtained, which make it possible to characterize nonlinear high-amplitude lattice vibrations.

1. Introduction

The concept of energy localization at the nodes of ideal crystals began to actively develop from [1, 2], and later this direction grew into the theory of discrete breathers and related directions [3]. Objects such as discrete breathers can be the basis for the implementation of a number of ideas, in particular, the ideas of a thermal transistor proposed by manly in [4], or radio-frequency filters, magnetometers, etc. [5-9]. The concept of a discrete breather is closely related to the concept of a nonlinear localized mode; in earlier works, they were often used as synonyms. Here we consider both of these terms as applied to high-amplitude lattice vibrations of the $CuPt_7$ crystal.

The choice of the object of study in the form of an alloy of $CuPt_7$ is due to a number of factors. First of all, Pt-based alloys have a number of interesting properties. These include corrosion resistance and high melting point, which makes them promising for use in space. However, intense external exposure in the form of irradiation can lead to the excitation of such objects as discrete breathers with a soft type of nonlinearity [10-12]. They can contribute to the properties of these crystals. Discrete breathers are spatially localized high-amplitude excitations of the crystal lattice, caused by the anharmonicity of the interatomic forces, which leads to the dependence of the oscillation frequency of atoms on their amplitudes. For the existence of such objects in crystals, the crystal must meet a number of requirements: this is the presence of a band gap in the phonon spectrum of the crystal, and also, in the case of biatomic crystals, a significant difference in the masses of the alloy components. At the same time, it is worth

noting that there may exist so-called immersed discrete breathers, the frequency of which may be included in the phonon spectrum of the crystal [3] breathers with a rigid type of nonlinearity.

Unlike discrete breathers, nonlinear localized modes have a relatively small lifetime, on the order of several tens of lattice oscillation periods. They quickly dissipate their energy in the form of thermal lattice vibrations to neighboring atoms. However, their existence time is an order of magnitude greater than the usual thermal oscillations, which is caused by the anharmonicity of the interatomic forces.

2. The model and the experimental technique

The models considered by us are a bulk FCC $CuPt_7$ crystal, which contained 23328 particles (Figure 1), interacting through the potential obtained by the embedded atom method (EAM potential) [13]. Two variants of the lattice with orthogonal basis vectors (Figure 1a) and the trigonal configuration (Figure 1b) [14] were considered.

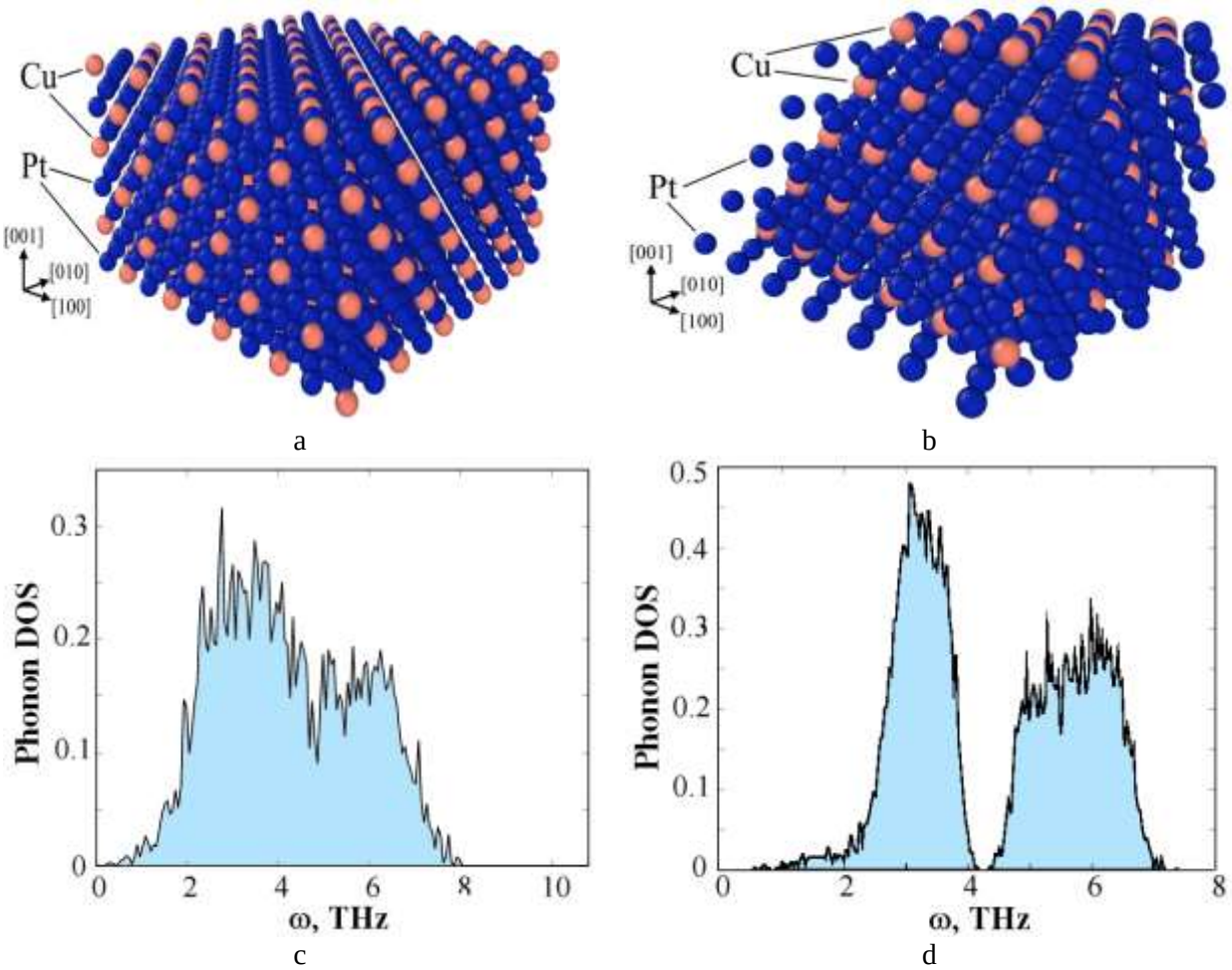


Figure 1. The structure of a $CuPt_7$ crystal, a) with orthogonal basis vectors, b) a trigonal structure [13] c), d) The corresponding density of phonon states of crystal models.

The choice of potential and the validity of its use for a specific task is an important step in modeling. The total energy E of a crystal can be expressed as: $E = \frac{1}{2}\sum_{i,j,i\neq j}\varphi_{ij}(r_{ij}) + \sum_i F_i(\rho_i)$, where φ_{ij} represents the pair energy between atoms i and j separated from each other by the distance r_{ij}, a Fi–nesting energy associated with nested atom i in a local location with electron density ρ_i. The electron density 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 the site

of atom i, located at a distance r_{ij} from atom j. The simulation was carried out using the LAMMPS package [15]. The equations of motion of atoms were integrated using a fourth-order numerical scheme of accuracy with an integration step of 0.5 fs.

For calculating the density of phonon states, the LAMMPS software package was also used, which includes the necessary procedures for these purposes, based on the Fourier transform of the autocorrelation functions of atom displacements with time. The results for a lattice with orthogonal basis vectors are shown in Figure 1c, for the trigonal structure in Figure 1d.

3. The results and the discussions

An analysis of the crystal structure and the calculated phonon spectrum suggests a possible existence of such objects as a discrete breather with a soft type of nonlinearity in $CuPt_7$. So in the crystal presented in fig. 1b, there is a forbidden zone, which is a necessary condition for the existence of a discrete breather. In addition, lighter copper atoms are surrounded by heavy platinum atoms, which should also have a beneficial effect on the localization of vibrations of the light sublattice. However, the mass of copper is less than 3 times the mass of platinum, which is often not enough to form the condition for the existence of a discrete breather.

Further, the dependence of the oscillation frequency of Cu atoms on the amplitude was obtained for both of the above types of crystal syngonies. As an example, consider oscillations along the <001> direction.

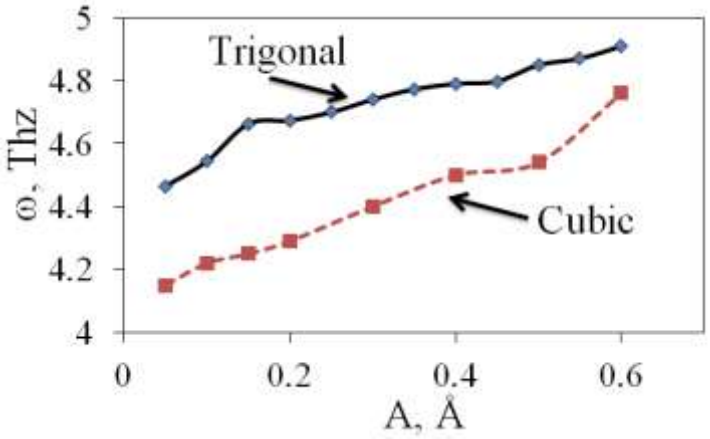
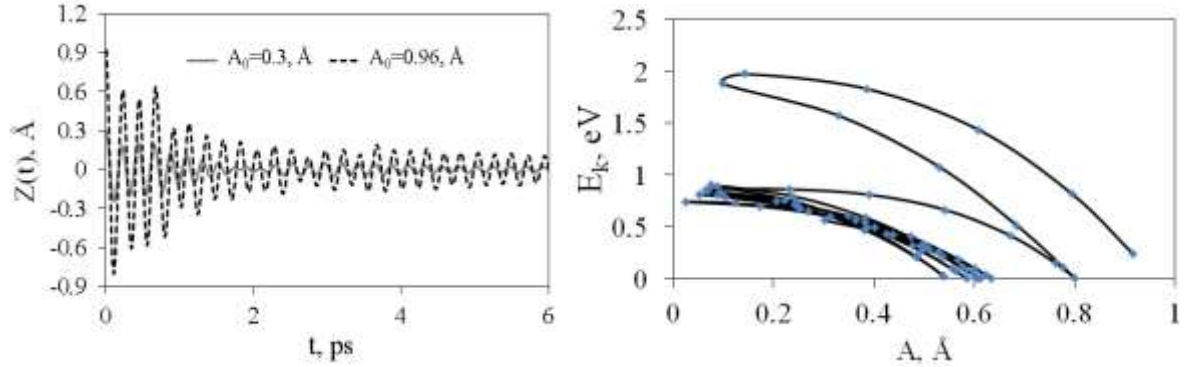


Figure 2. The dependence of the oscillation frequency of the Cu atom in the $CuPt_7$ crystal on the amplitude for the trigonal and cubic syngonies of the $CuPt_7$ lattices.

The results obtained in Figure 2 speak of a hard type of nonlinearity of oscillations for both $CuPt_7$ crystal syngonies, which does not allow the oscillation frequency of the copper atom to fall into the band gap of the phonon spectrum for the trigonal crystal syngony. This eliminates the possibility of excitation of discrete breathers with a soft type of nonlinearity. In this case, we note that for sufficiently large amplitudes, for these structures of crystals, long but damped oscillations of Cu atoms were observed. This was most pronounced in a cubic crystal, due to a higher order of symmetry. In this case, we can speak not about discrete breathers, but about nonlinear high-amplitude oscillations of lattice sites in a defect-free $CuPt_7$ crystal.

Next, using the example of a cubic crystal, we consider the features of such nonlinear modes in $CuPt_7$. The frequency of their oscillations lies in the spectrum of the crystal; therefore, energy is rapidly dissipated into neighboring atoms and further throughout the crystal. In figure 3a shows the dependence of the atomic coordinate on time, along the direction <001>. The most stable oscillations of the copper atom were obtained for initial amplitudes of 0.96 Å. For comparison, this dependence is also given for the initial amplitude of 0.3 Å. In this case, the oscillations decay much faster and are not restored further.



a) b)

Figure 3. a) the change in the coordinate of the Cu atom from time relative to the equilibrium position for the initial amplitudes of 0.3 and 0.96 Å; b) the dependence of the energy of an atom on the modulus of the deviation of an atom from its equilibrium position for the first three periods of oscillations for an initial amplitude of 0.96 Å.

According to the simulation results, such nonlinear modes can localize energy of the order of 1 eV. In figure 3b shows the dependence of the energy of the atom on its deviation from the equilibrium position. It is important to note that in the first two periods of oscillations a kind of hysteresis is observed. This is caused by the displacement of neighboring Pt atoms from the lattice sites. Further relaxation of the structure leads to consistent oscillations and such a phenomenon is not observed.

4. Conclusion

Thus, the $CuPt_7$ crystal was studied by the molecular dynamics method for the existence of discrete breathers in it with a soft type of nonlinearity and nonlinear long-lived modes. It is shown that excitation of breathers with a soft type of nonlinearity is not possible in this crystal. Moreover, for certain initial amplitudes, the lifetime of individual modes can significantly exceed the average time for the existence of high-amplitude thermal oscillations of atoms. The carriers of such modes are Cu atoms; this is most pronounced for a crystal with a cubic system in the form of a higher order of symmetry.

Acknowledgements

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