Introduction

The work is devoted to the study of nonlinear vibrations of the lattice of the CuPt and CuPt₇ crystals. The modeling parameters for a given crystal are considered, on the basis of which the basic properties of the material are calculated. Further, the characteristics of high-amplitude excitations are studied for various initial input values.

Crystal model

The model we are considering is a bulk FCC CuPt crystal containing up to $5 \cdot 10^4$ particles interacting via the potential obtained by the embedded atom method. Two variants of the lattice with orthogonal basis vectors and the trigonal configuration were considered. The model we are considering is a bulk CuPt crystal containing up to $1.2 \cdot 10^4$ particles interacting via the potential obtained by the embedded atom method.

Results

The results obtained do not indicate a rigid type of nonlinearity of vibrations for both crystal systems of CuPt, which does not allow the vibration frequency of the copper atom to fall into the band gap of the phonon spectrum for the trigonal crystal system. This eliminates the possibility of exciting discrete breathers with a soft type of nonlinearity. In this case, we note that at sufficiently large amplitudes, for these crystal structures, prolonged but damped vibrations of Cu atoms were observed. This was most clearly manifested in a cubic crystal, due to the higher order of symmetry. In this case, we can speak not about discrete breathers, but about nonlinear high-amplitude vibrations of lattice sites in a defect-free CuPt crystal.

Next, using the example of a cubic crystal, we consider the features of such nonlinear modes in CuPt. 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. The most stable oscillations of the copper atom were obtained for initial amplitudes of 0.96 Å.

Conclusion

Crystals CuPt and CuPt₇ were studied by the molecular dynamics method for the presence of discrete breathers with soft and hard types of nonlinearity and nonlinear long-lived modes. It is shown that, in the CuPt crystal, it is impossible to excite breathers with a hard type of nonlinearity. Moreover, at certain initial amplitudes, the lifetime of individual modes can be specified as the average lifetime of thermal signals of large amplitude. The carriers of such modes are Cu atoms. This is most clearly manifested for a crystal with a cubic system in the form of a higher order of symmetry.

Acknowledgments

This work was supported by the Russian Science Foundation grant No. 21-12-00275.