Gap discrete breathers in two- and three-dimensional diatomic crystals with Morse interactions

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In this talk, gap discrete breathers (DBs)[1-4] in two- and three-dimensional diatomic crystals with Morse interatomic interactions are analyzed. Three-dimensional lattices has the $L1_2$ structure with A_3B stoichiometry while in the two-dimensional case a (111) plane of this structure is considered preserving the A_3B stoichiometry. Parameters of the potential reproduce main properties of Ni_3Al intermetallide. In both cases we study the effect of the atomic weight ratio (M_A/M_B) on the phonon spectra and on the conditions of existence and properties of the gap DBs. It was found that the gap DBs can be easily excited in the presence of wide gap in the phonon spectrum, which appears for sufficiently large mass ratio ($M_A/M_B > 3.5$ in our study). We have also found that the DB frequency decreases with increase in its amplitude so that the Morse potentials result in soft anharmonicity, which suggests that it is unlikely to find DBs with the frequencies above the phonon spectrum. Thus, the DBs in Morse crystals can be expected only in the lattices with a gap in the phonon spectrum and this may happen for the crystals with a complex structure.
Then we study numerically the dynamics of a modulationally unstable Brillouin-zone-boundary phonon mode and demonstrate that the so-called anti-Fermi-Pasta-Ulam mechanism of energy localization [5] gives rise to formation of the gap DBs with the lifetime much greater than the period of their oscillations. The smaller the amplitude of the phonon mode, the longer is the lifetime of DBs. Slow radiation of energy by the DBs results in the subsequent thermal equilibrium of the system.

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