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# NONLINEAR OSCILLATIONS IN CRYSTAL LATTICES OF METALS UNDER FORCED ACTIONS AT TERAHERTZ FREQUENCIES

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**Keywords:** molecular dynamics modeling, nonlinear oscillations, modulation instability, terahertz frequencies, interaction potential.

**Abstract.** In this work, we analyze the phenomenon of modulation instability of short-wavelength modes for a number of model nonlinear lattices and metals under high-amplitude periodic actions at terahertz frequencies outside the phonon spectrum of crystals. Such influences lead to the transfer and transport of energy not by phonons, but by other collective modes of large amplitude. Chaotic discrete breathers spontaneously arising as a result of the modulation instability of delocalized nonlinear vibrational modes in a triangular lattice with a β-FPU interaction potential are studied.

# НЕЛИНЕЙНЫЕ КОЛЕБАНИЯ В КРИСТАЛЛИЧЕСКИХ РЕШЕТКАХ МЕТАЛЛОВ ПРИ ВЫНУЖДЕННЫХ ВОЗДЕЙСТВИЯХ НА ТЕРАГЕРЦОВЫХ ЧАСТОТАХ

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**Ключевые слова:** молекулярно-динамическое моделирование, нелинейные колебания, модуляционная неустойчивость, терагерцовые частоты, потенциал взаимодействия.

**Аннотация.** В настоящей работе осуществлен анализ явления модуляционной неустойчивости коротковолновых мод для ряда модельных нелинейных решеток и металлов при высокоамплитудных периодических воздействиях на терагерцовых частотах вне фононного спектра кристаллов. Такие воздействия приводят к передаче и транспорту энергии не фононами, а иными коллективными модами большой амплитуды. Изучены хаотические дискретные бризеры, спонтанно возникающие в результате модуляционной неустойчивости делокализованных нелинейных колебальных мод в треугольной решетке с потенциалом взаимодействия β-ФПУ.

Nonlinear excitations of the crystal lattice at frequencies outside the phonon spectrum lead to the transfer and transport of energy not by phonons, but by other large-amplitude collective modes, among which one can note delocalized nonlinear vibrational modes (DNVM), discrete breathers (DB), waves soliton type, crowdions [1].

In [2], Burlakov et al. discovered an important effect consisting in the development of instability of short-wavelength nonlinear delocalized modes, leading to spontaneous localization of energy on discrete breathers, which, in the context of this phenomenon, were called chaotic. The emerging discrete breathers slowly radiate their energy, and the system inevitably comes to thermal equilibrium, but this transition occurs through long-lived spatially localized vibrational modes. This phenomenon is also devoted to a very large number of studies, where it was shown that it can be observed in gratings of different dimensions and different types (with and without a gap in the spectrum) [3].

We have studied chaotic discrete breathers spontaneously arising as a result of the modulation instability of DNM with frequencies above the phonon spectrum. As was established in [4], there are three triangular-lattice DNVM with frequencies above the phonon spectrum, these are single-component DNVM 2 and 4, as well as two-component DNVM γ2 (Fig. 1).

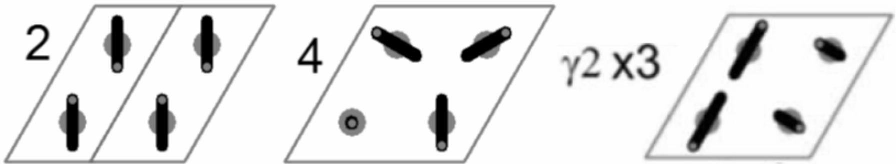

Fig. 1. Triangular DNVM obtained by Ryabov using the theory developed by Chechin and Sakhnenko

The potential energy of the bond between two nearest particles of the triangular lattice is determined by the β-FPU potential:

$$\varphi(r)=\frac{k}{2}\cdot(r-h)^2+\frac{\beta}{4}\cdot(r-h)^4.$$

To study the evolution of energy localization in the lattice, we will follow the change in the localization parameter:

$$L=N\frac{\sum_{n=1}^{N}e_n^2}{\left(\sum_{n=1}^{N}e_n\right)^2},$$

where $e_n$ – is the total energy of one particle, averaged over the period of the DNM oscillation, and the summation is carried out over all $N$ particles in the computational cell. Note that if all the energy is localized on one particle, then we have $L=N$. With an equal distribution of energy over all particles, we have $L=1$.

As expected, all three DNVM under consideration are destroyed with the formation of DB, as evidenced by the sharp increase in the energy localization parameter in Fig. 2 (a). DB exist in the system for quite a long time, slowly radiating energy, and as a result, the system comes to thermal equilibrium. On Fig. 2 (b) shows the energy distribution over the computational cell at the initial moment of localization (on the left) and at the moment of maximum localization (on the right) for all three DNVM. Light areas - the energy is maximum, dark - is minimal. Despite the existing differences at the initial stage of energy localization, the result is the same – chaotic discrete breathers are formed in the system.

It is interesting to trace the evolution of the macroscopic characteristics of the lattice during the transition from the DB regime to thermal equilibrium. One can observe the change in time of the value $C_V=H/K$ and $<p>=(\sigma_{xx}+\sigma_{yy})/2$. The first is the ratio of the total energy of the system to the kinetic one and characterizes the heat capacity of the lattice at constant volume, and the second is the pressure in the lattice averaged over the period of the DNVM oscillation. A clear correlation of these macroscopic quantities with a change in the localization parameter shown in Fig. 2 (a) is seen. When $L$ is maximum, $C_V$ and $<p>$ are minimum. Note that the pressure drop at constant volume indicates a negative contribution of the DB to the thermal expansion of the lattice. Similar results were also obtained for the lattice rigidity defined as $C=(C_{11}+C_{22})/2$.

We conclude that DB reduce the heat capacity, thermal expansion, and stiffness of a lattice with a hard type of nonlinearity.

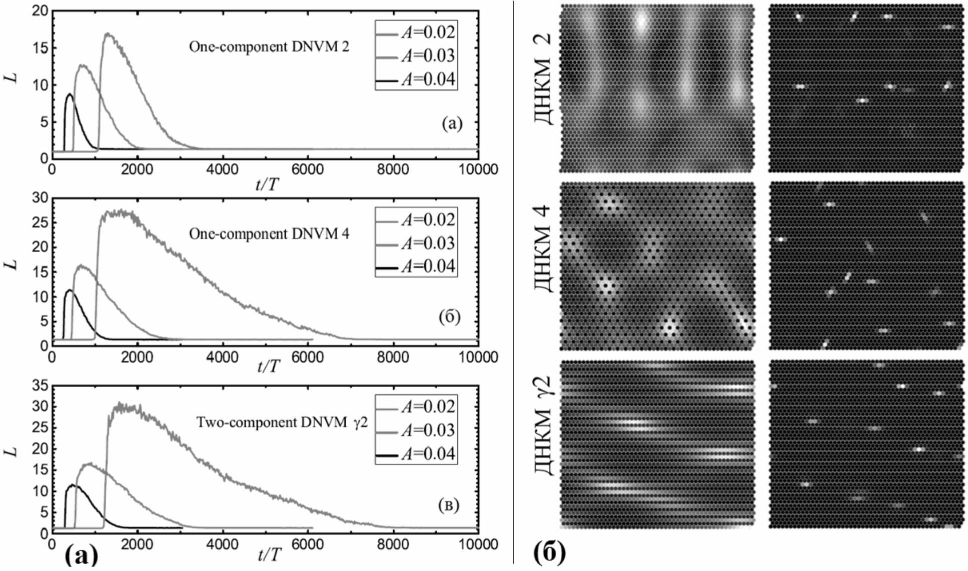

Fig. 2. Change of localization parameter from time (a). Energy distribution over the lattice, showing the development of modulation instability (b)

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