Energy transport in an A\textsubscript{3}B crystal with intense external exposure at frequencies outside the crystal spectrum

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Abstract. The molecular dynamics method is used to consider the effect of energy transport in an A\textsubscript{3}B stoichiometry crystal, using Pt\textsubscript{3}Al as an example, which consists in the transfer of energy at frequencies outside the phonon spectrum of the crystal. This effect is called the effect of nonlinear supratransmission. The model was a bulk face-centered cubic crystal, the atoms of which interacted through a multi-particle potential, obtained by the immersed atom method. Different forms of oscillation of the region of external influence are considered. The possibility of transporting energy from the crystal surface into the depths by means of excitation of quasi-breathers near the impact area and their subsequent destruction in a crystal and dissipation of energy, stored on them, is shown. The quasi-breathers most intensely occurred near the impact region with a sinusoidal waveform. The results obtained indicate that the contribution of quasi-breathers to the energy transfer through the crystal, increases with increasing exposure amplitude. The minimum amplitude of the external influence, at which this effect was observed, is established. The results of the study can be useful in creating materials with predetermined properties, through various intensive external influences.

Introduction
The methods for modifying near-surface layers of the materials are often based on surface treatment with high-intensity external influences in the form of a plasma discharge, annealing, current pulses, etc. The energy fluxes from the surface of the crystals affect the structural and energy transformations of materials, thus providing modification of the surface layers of matter.

In this article, we consider the effect of energy transfer when a stoichiometric composition A\textsubscript{3}B, which has a forbidden zone in the phonon spectrum of a crystal, is periodically exposed to a crystal surface. The impact was carried out in a wide range of frequencies, both within the phonon spectrum and outside the phonon spectrum of the crystal. The effect of energy transfer at frequencies outside the phonon spectrum of a crystal is called nonlinear supratransmission [1]. The interest in this effect is not extinguished both for relatively simple nonlinear systems [2], and for more complex systems and materials [3-6]. In the classical approach to supratransmission there is an initial magnitude of the amplitude at which this effect occurs. However, in [3], by the example of deformed graphene, the possibility of energy transport through non-linear super-transmission without restrictions on the minimum value of the amplitude of the impact was shown. This motivates the study of this effect for various crystals and the search for mechanisms of energy transfer in nonlinear systems.
This mechanism is interpreted by the excitation of nonlinear localized modes of large amplitude near the zone of action - discrete breathers. Strictly speaking, such objects should be called quasi-breathers [7-9], due to the fact that they have a finite lifetime and are not strictly periodic in time.

The paper considers the model of a Pt$_3$Al crystal. Interest in this alloy is due to the prospect of its use in the composition of superalloys, as well as its resistance to high temperatures. In addition, the possibility of excitation of discrete breathers in this material by a stream of particles and at thermodynamic equilibrium was shown in [8].

The model and the experimental technique

The model under consideration is a bulk FCC crystal of A$_3$B stoichiometry, using Pt$_3$Al as an example, which contains $80 \cdot 10^3$ particles (figure 1), interacting through the potential obtained by the immersed atom method (EAM potential) [10]. In computational chemistry, the model of a submerged atom is used to approximate the description of the interaction energy between two atoms. 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:

$$E = \frac{1}{2} \sum_{i,j,i \neq j} \varphi_{ij}(r_{ij}) + \sum_i F_i(\rho_i), \quad (1)$$

where $\varphi_{ij}$ represents the pair energy between atoms $i$ and $j$ separated from each other by the distance $r_{ij}$, and $F_i$ is the energy of the attachment associated with the inserted atom $i$ in the local location with the electron density $\rho_i$. Electronic density can be calculated by the formula:

$$\rho_i = \sum_{j,j \neq i} f_j(r_{ij}). \quad (2)$$

where $f_j(r_{ij})$ is the electron density of the region of atom $i$ located at a distance $r_{ij}$ from the atom $j$.

The modelling was carried out using the LAMMPS package [11]. Periodic boundary conditions were imposed on the FCC crystal model along the X and Y axes, and free boundary conditions along the Z axis. The resulting model was divided into 3 blocks. Block I consisted of 3-4 layers of atoms that oscillated according to the harmonic law in accordance with the ranges of frequencies and amplitudes of atomic vibrations. Periodic effects were applied to all atoms from block I. Next, block II was located - an energy absorber by which the estimated absorbed energy was estimated by the crystal. In part III of the computational cell, a block of 4-5 layers of atoms was settled, rigidly fixed, acting as a damper. This
ensured the absence of movement of the entire Pt3Al crystal model, and made the model closer to the real crystal. In figure 1 (b) shows the density of phonon states of the crystal model under consideration. Two variants of the direction of external influence on the crystal were considered. In the first case, the crystal was oriented so that the Z axis corresponded to the crystallographic direction <110>, in the second case the direction <111>.

During the calculations, the integration step was 1 fs, and the estimated time of each launch was 1 ps, the initial temperature of the computational cell was 0 K. For all cases, the NVE ensemble was considered.

Periodic impact was carried out according to the following harmonic laws:

\[ Q_{1Z}(t)=A_0 \sin(2\pi \nu t+\varphi) \] (3)
\[ Q_{2Z}(t)=A_0(1-\cos^2(2\pi \nu t+\varphi)) \] (4)
\[ Q_{3Z}(t)=A_0|\sin(2\pi \nu t+\varphi)| \] (5)

where for all cases \(A_0\) is the amplitude of the external action, \(\varphi\) – phase, \(2\pi \nu=\omega\) is the frequency of the oscillations of the region I in figure 1 (a). Oscillations were made along the Z axis with frequencies from 0.2 to 15 THz, and with the different amplitudes from 0.05 to 0.5 Å, which was ensured by running the script 52 times for each value of amplitude. Such a range makes it possible to cover the entire spectrum of low-amplitude atomic vibrations for the crystal under consideration. Figure 2 shows the impact forms for each equation.

![Figure 2](image_url)

**Figure 2.** Type of external influences by means of equations (3), (4), (5), for the parameters \(A_0=0.3\) Å, \(\omega=3\) THz.

The absorbed energy for the atoms of zone II was calculated by calculating the kinetic energy of the atoms of this block, then the value obtained was divided by the number of atoms in this block, followed by averaging. Such calculations were performed for each frequency value and for both directions of action.

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**The results and the discussions**

The absorbed energy was fixed depending on the frequency of exposure and amplitude. The results obtained for the impact of the law (3) are presented in figure 3 (a) and (b). On the basis of this graph, it can be noted that for amplitudes less than 0.2 Å the effect of energy transfer to the crystal was absent in the forbidden zone of the phonon spectrum (figure 1 (b)). For amplitudes of 0.2 angstroms and more, energy is transferred to the crystal, including at frequencies in the band gap of the phonon spectrum. With increasing amplitude, the absorption peak shifts deeper into the forbidden frequencies of the
phonon spectrum of the crystal, which indicates an increase in the fraction of nonlinear modes in the process of energy transfer. The active excitation of breathers occurs in close proximity to the area of impact; we obtained similar results earlier for two-dimensional models of this alloy [8]. Note that there is a threshold value of the amplitude of the impact from which this effect begins to manifest itself, which is typical of the classical interpretation of the effect of supratransmission.

**Figure 3.** The dependence of the absorbed energy of the computational cell per atom per picosecond on the frequency of external influence and amplitude. For (a) and (b) the impact of the formula (3), for (c) and (d) according to the formula (4), for (e) and (f) according to the formula (5). For (a), (c) and (e), exposure was carried out along the crystallographic direction <110>, for (b), (d) and (f), exposure was carried out along the crystallographic direction <111>.

In figure 3 (c) and (d) the results of actions are shown according to the harmonic law (4), in figure 2 (e) and (f) by the formula (5). It is evident from the graphs that the amount of energy transferred to the crystal is an order of magnitude smaller than when exposed to the formula (3). The reason for the discrepancies in the results is that the excitation of quasi-breathers near the area of influence occurs more slowly in these cases, since the form of action differs from the excitation parameters of quasi-
breathers. In this case, the directions under consideration differ from those at which the breathers are excited in the bulk of the crystal and near the surface [12]. Thus, the imposition of two factors leads to a decrease in the energy absorbed.

Since the results obtained for equations (3)-(5) have differences, then the behavior of the first layer of atoms near the action area is analyzed. For this purpose, one Pt and Al atoms were selected in this layer and their dynamics was tracked over time for the entire frequency range. For frequencies close to the optical branch of the phonon spectrum, according to the harmonic law (3), vibrations on the Al atom are more actively excited, which indicates the excitation of discrete breathers, while for expressions (4) and (5), such activity is not observed. In this case, for Eq. (3), a local expansion occurs near the region of influence, which indicates the excitation of discrete breathers.

Conclusion
The molecular dynamics method for a Pt3Al crystal is used to consider the mechanism of nonlinear supratransmission for various forms and directions of external influence. It was shown that the transport of energy through this mechanism is possible along the directions corresponding to the crystallographic directions of the existence of a quasi-breather in a crystal and under sinusoidal influence; otherwise, the effect was minimized. The data obtained indicate that the contribution of quasi-breathers to the energy transfer through the crystal increases with increasing amplitude of the effect. The results of the study can be useful in creating materials with predetermined properties, through various intensive external influences.

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