Abstract. Steady-state and non-stationary elastic wave propagation processes in nanostructures modeled by rectangular-cell and hexagonal-cell lattice sheets and tubes are investigated. The dispersion properties of nanostructures modeled by regular lattices are analytically analyzed, while computer simulations are conducted with the aim to reveal the development of unsteady state processes. Line-localized primitive waveforms in lattices are revealed. Intrinsic wave beaming phenomena arising under the action of vibration sources are discovered.

Introduction

Nowadays, nanotechnologies are rapidly progressing, and the necessity has arisen in obtaining predictable properties of nanostructures by processes using various mechanical actions exerted on starting systems. Among various physical properties of nanoparticles, nanofibers and nanotubes, their waveguide facilities are becoming increasingly important allowing dynamic strength state and fracture propagation to be theoretically predicted (see, e.g., [1-3]).

The main wave phenomenon inherent to periodic lattices modelling nanostructures is that free wave propagation takes place only within certain discrete bands of frequencies known also as pass-bands alternated with stop-bands, where the steady-state wave propagation is forbidden. In the field of waves in lattices or, more generally, waves in structured media, the monograph by Brillouin [4] has been basic for subsequent investigations of various theoretical and engineering aspects of wave propagation in periodic structures and composites (see, e.g., [5-10]).

During recent decades, this topic has got a second wind, when so-called “artificial crystals” as band-gap materials were discovered. Artificial phononic (or zonic) crystals are periodic lattices or composite structures designed to control waves of sound and vibration. Some important results related to band-gaps in phononic crystals can be found, e.g., in [9-15]. In the frequency spectrum of band-gap materials, there exist resonant frequencies, which usually demarcate pass- and stop-bands. In the 1D case, the wave group velocity equals zero at these frequencies: there is no steady-state solution corresponding to an external non-selfequilibrated excitation, and the wave energy flows from a source decelerating with time, like heat, and not as a wave [16]. In 2D/3D cases, a resonant point can also exist in the interior of pass bands [17]. Such resonant points differ from the 1D case by the fact that the group velocity is at zero only for some special wave orientations. Resonance processes excited in infinite rectangular-cell and triangular-cell lattices by harmonic sources are associated with intrinsic wave beaming phenomena [17-19]. Note that resonance points inside pass-bands can be found in more complicated discrete and continuous periodic structures (see, e.g., [9–15]). However, they were not fixed as special...
points, and their essence was not discussed. Equifrequency resonant contours in dispersion surfaces for material-bond lattices were considered, for example, in [21-24].

The study of transient response to various types of excitations can be found in many works dealing with periodic structures (see, e.g., [6-8,18] for 1D problems and [20-25] for 2D problems). To the best of the authors’ knowledge, [24] remains the only one (forestalling the mentioned work [17]), in which an unexpected beaming-like character of resonant wave propagation was detected. However, in that work, the spatial distribution of disturbances was not discovered (besides, an incorrect explanation of the obtained result was suggested).

The paper is partially aimed to describe some consequences of the existence the so-called Localized Primitive Waveforms (LPWs) initially discovered in [17]. The LPW is a “selfequilibrated” standing wave strictly localized on a line of a certain orientation. Any sinusoidal wave, and hence any wave at this frequency, can be represented as a set of the LPWs, and it bears evidence of the features of the LPW. In particular, the sinusoidal-wave group velocity orientation coincides with the LPW orientation nearest to the wave propagation direction, and this is why it is piece-wise constant at this frequency. A pronounced beam effect caused by the resonant excitation in a square-cell lattice was analytically described [17-19]. Note that the beam effect was considered in [21, 22, 25] beyond its connection with the specific LPW form and the resonant character of propagating waves.

Below we explore steady-state and time dependent elastic wave propagation processes in nanostructures modeled by rectangular-cell and hexagonal-cell lattice sheets and tubes. To compare waveguide properties in these two cases we use results obtained for rectangular-cell sheets obtained in [25]. The dispersion properties of lattice structures are analytically analyzed, while computer simulations are conducted with the aim to reveal the development the unsteady state pattern. We have obtained dispersion equations for anti-plane oscillations of nanostructures modeled by rectangular- and hexagonal-cell lattices, shown equifrequency resonant contours, LPWs, and corresponding parameters of energy fluxes. The presented numerical solutions (having an independent significance) are complementary of analytical results and together with latter allow a fairly complete picture of nanostructures dynamics to be analyzed. Note that results of purely computer simulations of wave processes in nanostructures obtained on the basis of the classical molecular dynamic models, corresponding advanced methods and tools can be found for example, in [26-30].

1. Rectangular-cell lattice. Dispersion pattern

Consider uniform rectangular-cell lattice RCL consisting on material particles at nodes \((m,n)\), \(m,n=0,\pm1,\pm2,\ldots\), linked by elastic massless bonds – see Fig. 1(a). We use discrete coordinates \(m\) and \(n\) together with continuous coordinates \(x\) and \(y\). The following nomenclature is used: \(M\) is the particle mass, \(g_x\) and \(g_y\) are out-plane normalized stiffnesses of \(x\)- and \(y\)-bond, respectively, \(l_x\) and \(l_y\) are their lengths. We will explore transversal oscillations of the lattice.

First, to explore the dispersion pattern, we are doing to obtain the dispersion equation of type \(\varphi(\omega, k_x, k_y) = 0\), where \(\omega\) is the frequency, \(k_x\) and \(k_y\) are wave numbers or
projections of the wave vector \( \mathbf{k}(k_x, k_y) \). Then we analyze dispersion surfaces \( \omega = \omega(k_x, k_y) \) and calculate group velocity vectors \( \mathbf{c}_g(k_x, k_y) \), \((c_{gx}, c_{gy})_x = (\omega_x', \omega_y') \).

\[
\text{(a)}
\]

\[
\text{(b)}
\]

Fig. 1: Rectangular-cell lattice layer (a), and (b) single-wall nano-tube

In a linear approximation, systems of homogeneous equations of the RSL dynamics can be written as follows:

\[
M \ddot{u}_{m,n} = g_x \left( u_{m,n+1} + u_{m-1,n} - 2u_{m,n} \right) + g_y \left( u_{m+1,n} + u_{m,n-1} - 2u_{m,n} \right)
\]

where \( u_{m,n} \) is the out-plane displacement of the \((m,n)\)-particle.

A general solution of the system (1) we have represented by a superposition of sinusoidal waves

\[
u_{m,n}(t) = U_{m,n} e^{i \sigma}, \quad U_{m,n} = U e^{i \left( k_x x + k_y y \right)} = U e^{i \left( k_x x + k_y y \right)} \left( |k_x| \leq \pi, |k_y| \leq \pi \right),
\]

where \( U \) is constant. Substituting (2) into (1), we obtain the dispersion surface

\[
\omega = \sqrt{\frac{2 \left[ g_x (1-\cos k_x) + g_y (1-\cos k_y) \right]}{M}}.
\]

(3)

If \( x \)- and \( y \)-bonds differ only by their lengths \( l_x \neq l_y \), then putting \( l = l_y \) and taking \( l_x \) and \( M \) as measurement units, we obtain a dispersion surface for a RCL with a single free parameter \( l \),

\[
\omega = \sqrt{\frac{2 \left[ 1-\cos k_x + (1-\cos k_y) l \right]}{M}}, \quad \left( |k_x| \leq \pi, |k_y| \leq \pi \right).
\]

(4)

This surface has a pass-band \( \omega \in [0, \omega_p] \) and stop-band \( \omega > \omega_p \), where \( \omega_p = \sqrt{2(2 + 2l)/M} \) is the resonance frequency at the bands interface.

In the case of a lattice with the same bonds \( (l=1) \), Eqn. (4) becomes a well-known dispersion relation for a square-cell lattice (SCL):
\[ \omega = \sqrt{2(1 - \cos k_x) + 2(1 - \cos k_y)} \left( |k_x| \leq \pi, \quad |k_y| \leq \pi \right). \quad (5) \]

with \( \omega_r = \sqrt{8} \) at the pass/stop-bands interface.

Together with the RCL, we introduce its special kind adopted as a simplified rectangular-cell lattice (SRCL), in which \( g_x = g_y, \quad l \neq 1 \). For a SRCL, the dispersion equation \( (4) \) turns into the following:

\[ \omega = \sqrt{2(1 - \cos k_x) + 2(1 - \cos k_y)} \left( |k_x| \leq \pi, \quad |k_y| \leq \pi \right). \quad (6) \]

Then, we reveal similarities and differences inherent to dispersion properties of well-studied in [17] SCLs and RCLs considered here. For a sinusoidal wave, the group velocity vector \( c_g \) (as well as the energy flux) is oriented along an external normal to the equifrequency contour \( \omega = \text{const} \). As shown in [17], the contour \( \omega = 2 \) is resonant for SCLs \( (5) \). Below we show that this contour is also resonant for SRCL \( (6) \).

In Fig. 2, dispersion surfaces, \( (a) \), and resonance contours at \( \omega = 2 \), \( (b) \), for SRCL are depicted. The contour is rhombic: \( k_x \pm l k_y = \pm \pi \), in contrast to the square one, \( k_x \pm k_y = \pm \pi \), in the SCL [17]. From \( (6) \) we obtain the following consequences in \( x \)- and \( y \)-projections of the group velocity \( c_g \) at \( \omega = 2 \):

\[ (c_g)_x = \frac{\sin k_x}{2}, \quad (c_g)_y = \frac{l \sin k_y}{2}. \quad (7) \]

**Fig. 2:** Dispersion pattern in a SRCL: \( (a) \) dispersion surface \( (6) \), \( (b) \) equifrequency contour at \( \omega = 2 \) in plane \( k_x, k_y \) (arrows show the energy flux orientation), \( (c) \) the three-particle-width band. Particles involved in anti-phase oscillations marked by hollow circles with \( \pm \), and immobile those – by black circles.
Here the energy flux along the axes \( x \) and \( y \) is absent: \( (c_\varepsilon)_x = 0 \) \( (q_x)_y = 0 \) and \( (c_\varepsilon)_y = 0 \) \( (k_x)_y = 0 \). As we show below, the group velocity orientation in \( q_x, q_y \)-plane (or, which is the same, in \( x, y \)-plane) coincides with orientation of Localized Primitive Waveforms (LPWs) initially discovered in [17]. It follows from (7) that for \( \omega = 2 \) the group wave velocity value \( g_c \) and its orientation \( \beta \) are

\[
|c_\varepsilon| = \frac{\sqrt{1 + l^2}}{2} \sin \frac{\pi}{1 + \tan \alpha} \left( \alpha = \arctan \frac{lk_y}{k_x}, \beta = \arctan \frac{(c_\varepsilon)_y}{(c_\varepsilon)_x} = \pm \arctan l, \right. \tag{8.1}
\]

where \( \alpha \) and \( \beta \) is the phase velocity and group velocity orientations, respectively.

If \( l = 1 \), we obtain results corresponding to a SCL [17]:

\[
|c_\varepsilon| = \frac{\sqrt{2}}{2} \sin \frac{\pi}{1 + \tan \alpha} \left( \alpha = \arctan \frac{k_y}{k_x}, \beta = \arctan \left( \frac{\partial \omega}{\partial k_y} / \frac{\partial \omega}{\partial k_x} \right) = \pm \frac{\pi}{4}, \right. \tag{8.2}
\]

As it can be seen from (8), the group velocity is zero in those and only in those four directions, \( \alpha = \pm 0 \) and \( \alpha = \pm \pi/2 \). Directions determining LPW (diagonal) orientations are associated with the angles \( \pm \beta \) and shown in Fig. 2 (b) by arrows. In Fig. 2 (c), for one of the above-mentioned angles, \( +\beta \), a three-particle-width band is shown, within of which we consider the diagonal \((m,m)\) and a neighboring particle (black circle) connected with two diagonal particles involved in anti-phase oscillations. Their actions on a near-diagonal particle are self-equilibrated, and thus, black particles can be at rest. So the existence of the LPW is a consequence of a certain symmetry of the lattice structure. One can see that \( \omega = \sqrt{2(g_x + g_y)/M} = 2 \) is the LPW one (measurement units are \( g_x = g_y = M = 1 \)) as in a SCL: indeed, in a SRCL, lengths of \( x \)- and \( y \)-bonds in a cell are different, but their stiffnesses are equal, \( g_x = g_y \).

Consider now a RSL possessing different lengths bonds and different stiffnesses, \( g_x = g_y \). A dispersion relation for such a lattice is expressed by (4). Note that LPWs are absent here, but, as shown below, the dispersion pattern has some common points with the above-considered in SCL (and SRCL).

Projections of the group velocity vector, its module and energy flux directions obtained from (4) are

\[
(c_\varepsilon)_x = \frac{\sin k_x}{\omega}, \ (c_\varepsilon)_y = \frac{\sin(lk_y)}{\omega},
\]

\[
|c_\varepsilon| = \frac{1}{\omega} \sqrt{\sin^2 k_x + \sin^2(lk_x)}, \beta = \arctan \left( \frac{\sin(lk_y)}{\sin k_x} \right), \tag{9}
\]

Below we also use the following expression for the group velocity direction \( \beta \) in terms of \( \omega \) and \( k_x \) obtained from (4):
\[ \beta = \arctan \frac{\sqrt{1 - \left[ 1 - l \left( \omega^2 / 2 + \cos(k_x) - 1 \right) \right]^2}}{l \sin(k_x)}. \] (10)

There exist four specific angular points in the dispersion surface: \( \omega = 2 (k_x = \pm \pi, \ k_y = 0) \) and \( \omega = 2/\sqrt{l} (k_x = 0, \ k_y = \pm \pi / l) \), in which the group velocity is equal to zero. Here, similarly to SCL (SRCL) cases, the directions coinciding with the axes \( x \) and \( y \) are forbidden for the energy flux.

In the upper row of Fig. 3, the first quarter of the plane \( k_x, k_y \) is shown with value and direction of group velocities expressed by the length and direction of the respective arrow. Besides, some equifrequency contours are depicted. Such contours in the entire Brillouin zone are presented in the lower row of Fig. 3. The value of \( l \) is taken equal to 1.5. We compare results for SRL, column \((a)\), and RCL, column \((b)\), in order to reveal their similarities and differences. Recall that in a SRCL, resonance frequency \( \omega = 2 \) determines a rhombic contour \( k_x \pm l k_y = \pm \pi \) (see Fig. 2). In the RCL case, equifrequency contours are curvilinear. Two such contours, \( C_1 \) and \( C_2 \), correspond to the frequencies \( \omega_1 = 2\sqrt{1.5} \approx 1.63 \) and \( \omega_2 = 2 \), respectively.

**Fig. 3:** Group velocity pattern (upper row) and equifrequency contours (lower row) in square-cell \((a)\) and \((b)\) rectangular-cell lattices. Dotted straight lines in the lower picture of \((b)\) are tangents to contours at angular points.
The analysis of relations (9) and (10) shows that for relatively low frequencies, there are no preferable directions of \( \mathbf{c}_g \), and values \(|\mathbf{c}_g|\) are practically constant. If the frequency increases, the dependence of \(|\mathbf{c}_g|\) and \(\beta\) on coordinates \(k_x\) and \(k_y\) becomes sensible.

First, consider the SRL case in Fig. 3(a). If the frequency tends to a resonant one, \(\omega = 2\), values of \(|\mathbf{c}_g|\) tend to zero in the vicinity of the above-mentioned angular points of the contour, \(k_x = \pm \pi, k_y = 0\) and \(k_x = 0, k_y = \pm \pi/2\). When \(\omega_0 = 2\), directions of \(\mathbf{c}_g\) with wave numbers \(k_x \sim 0\) \((k_y \sim 0)\) turn to the right (left) at an angle \(\pi/2\). Such behavior of the free wave pattern is related to the formation of caustics. In the RCL case, the caustic appears in the same angular points, which are located now in different contours, \(C_1\) and \(C_2\). Note that an analysis of caustics in the considered structure can be found in [21], but contours \(C_1\) and \(C_2\) containing angular points have not been discussed.

As shown in [23], sources with frequencies \(\omega_0 = \omega_1\) and \(\omega_0 = \omega_2\) excite resonance phenomena with a pronounced beaming character of the spatial wave pattern.

With increasing \(\omega_0\), the process of \(\mathbf{c}_g\) transition consists of two parts:

(i) If \(\omega_0\) tends to \(\omega_1 = 2/\sqrt{I} = 1.63\), the value of \(|\mathbf{c}_g|\) in the vicinity of \(q_x \sim 0\) decreases with increasing \(k_y\). It tends to zero if \(\omega_0 = \omega_1\) and \(k_y \rightarrow \pi/2\), and \(\mathbf{c}_g\) orientation (angle \(\beta\)) sharply turns from \(\beta = \pi/2\) to \(\beta = 0\). If \(k_x\) increases, the value of \(|\mathbf{c}_g|\) in the contour \(C_1\) also increases, while the change in \(\beta\) orientation obeys the requirement for the vector \(\mathbf{c}_g\) to be normal to \(C_1\).

(ii) With further increase in \(\omega\), when it approaches \(\omega_2 = 2\) (contour \(C_2\)) and passes through it, the group velocity pattern is similar to that described above in case (i), but it is realized now nearby the domain \((\omega = \omega_2, k_x \rightarrow \pi)\), and the vector \(\mathbf{c}_g\) turns from \(\beta = 0\) to \(\beta = \pi/2\).

The analysis of the dispersion pattern shows that most parts of the contours \(C_1\) and \(C_2\) can be approximated by tangents (which are parallel) at angular points. From (10) we have obtained \(\mathbf{c}_g\) orientation corresponding to these tangents:

\[
\beta = \beta_* = \arctan(1/\sqrt{I}).
\] (11)

This angle is prevalent for wave propagation from a local source with the frequencies \(\omega_1\) and \(\omega_2\) to the periphery. A certain part of the wave is scattered inside the interval \(0 < \beta < \beta_*\), while the interval \(\beta_* < \beta \leq \pi/2\) determines forbidden directions for the energy flux.
2. Hexagonal-cell lattice. Dispersion pattern
Consider uniform hexagonal-cell lattice HCL consisting on material particles at nodes $(m,n)$, $m,n=0,\pm 1,\pm 2,\ldots$, linked by elastic massless bonds – see Fig. 2(a). We use discrete rhombic Cartesian coordinates $m$ and $n$ together with continuous rectangular coordinates $x$ and $y$. As above, we consider out-plane oscillations of the lattice. The generating element of the lattice is rhombic, $[m,n]$-see Fig. 4(a)-is bounded by coordinate lines $m$ and $n$, while $u$-nodes are located at the intersection of coordinate lines $m$ and $n$, while $u$-nodes are located leftward the correspondent $v$-node. Each $v$-node is connected to three $u$-nodes, and vice versa, each $u$-node is connected to three $v$-nodes. Such a consideration results in the existing of two oscillating modes in the hexagonal-cell lattice.

Let the distance between two neighboring nodes, particle masses and stiffnesses of connecting bonds be measurement units, $m=g=a=1$. Then, with the cell geometry in mind, Newton's law for the transverse motion of particles arranged in a hexagonal lattice is,

\[
\ddot{u}_{m,n} = v_{m,n} + v_{m,n-1} + v_{m-1,n} - 3u_{m,n},
\]
\[
\ddot{v}_{m,n} = u_{m,n} + u_{m,n+1} + u_{m+1,n} - 3v_{m,n},
\]

(12)

Following to [1], assume the conventional harmonic solutions of the form of the plane wave (in $xy$-plane):

\[
(u_{m,n}, v_{m,n}) = (U, V) \exp \left(i \omega t + n\vec{a}_1 + m\vec{a}_2 \right),
\]

(13)

where $\vec{a}_1 = \sqrt{3}/2 \hat{x} + 1/2 \hat{y}$, $\vec{a}_2 = \sqrt{3}/2 \hat{x} - 1/2 \hat{y}$ ($\hat{x}$ and $\hat{y}$ are unit vectors).

After substituting (13) to (12) we obtain a system of two linear equations, the nontrivial solution of which determines the following dispersion equation:

\[
\omega_{LI} = \sqrt{3 + \sqrt{1 + 4 \cos (k_x/2) \left(\cos (k_x\sqrt{3}/2) + \cos (k_y/2)\right)}}
\]

(14)
where signs ‘−’ and ‘+’ correspond to first (acoustical) and second (optical) modes.

Eqn. (14) show that a complete stop-band between modes is absent: they are connected in only four points, the so-called conical points (CP), which are obtained by equating $\omega_1 = \omega_\Pi$. Their coordinates are $[k_x, k_y] = \left[\pm 2\pi/\sqrt{3}, \pm 2\pi/3\right]$, and $\omega_{CP} = \sqrt{3}$ is the CP frequency. The point $k_x = k_y = 0$, $\omega = \sqrt{6}$ determines the resonant frequency demarcated the pass band of mode II and the stop band $\omega > \sqrt{6}$. Below we show that LPWs are realized at the same contour $k_y = \pm \pi \cup k_y = \pm 2\pi \pm \sqrt{3}k_x$ corresponded to resonant frequencies $\omega = \sqrt{2}$ (the mode I) and $\omega = 2$ (the mode II).

In Fig. 5, dispersion surfaces of modes I and II are depicted together with sets of eigenfrequency contours for each mode.

![Dispersion surfaces and eigenfrequency contours](image)

**Fig. 5:** Dispersion surfaces and eigenfrequency contours for mode I (a) and II (b) of a hexagonal-cell cell lattice. Bold circles are angular points of contours, in which group velocities are zero. Hollow circles - CPs, in which surfaces of modes I and II are connected.

To evaluate parameters of the energy flux depending on the frequency and the wave vector we have obtained group velocities (their absolute values, x- and y-projections and directions, $\beta$) for modes I and II. Expression (14) gives:

$$
(c_{g,x})_{\Pi} = \frac{\sqrt{3} \cos(k_y/2) \sin\left(\sqrt{3}k_x/2\right)}{2\omega_{\Pi} \phi(k_x, k_y)},
(c_{g,y})_{\Pi} = \frac{\sin(k_y/2) \cos\left(\sqrt{3}k_x/2\right) + \sin(k_x)}{2\omega_{\Pi} \phi(k_x, k_y)},
$$

$$
\phi(k_x, k_y) = \sqrt{1 + 4 \cos(k_y/2) \left[\cos(k_x \sqrt{3}/2) + \cos(k_y/2)\right]},
\beta_{\Pi} = \arctan \frac{3 \cos^2(k_y/2) \sin^2\left(\sqrt{3}k_x/2\right)}{\sin(k_y/2) \cos\left(\sqrt{3}k_x/2\right) + \sin(k_x)}.
$$

(15)
Consider the eigenfrequency contour \[ k_y = ±\pi, k_x = ±2\pi ± \sqrt{3}k_y (−\pi ≤ k_x ≤ \pi) \] at \( \omega = \sqrt{2} \) (as was shown above it’s the same also at \( \omega = 2 \)), which is of special interest:

\[
\begin{align*}
    k_y = ±\pi & \quad \Rightarrow \quad |c_{g I, II}| = \frac{\alpha_{I, II} \cos \sqrt{3}k_y / 2}{4}, \quad \beta = ±\pi \frac{1}{2} \\
    k_y = ±2\pi ± \sqrt{3}k_x & \quad \Rightarrow \quad |c_{g I, II}| = \frac{\alpha_{I, II} \sin \sqrt{3}k_y}{4}, \quad \beta = ±\pi \frac{1}{6} \\
\end{align*}
\] (16)

The group velocity for the mode II have the contrary orientation to that for the mode I and their absolute value is less by \( \sqrt{2} \) times. As was mentioned above, the group velocity orientation in \( k_x, k_y \)-plane coincides with orientation of LPWs.

In the first row of Fig. 6, the first quarter of the plane \( xy \) is shown, value and direction of the group velocity expressed by the length and direction of the respective arrow. Besides, some parts of equifrequency contours can be seen. Such contours in the entire Brillouin zone are presented in the second row of Fig. 6. We compare results for the acoustic mode, column (a), and the optic mode, column (b), in order to reveal their differences. In the case of long waves \( k_x, k_y \to 0 \) the mode I has a maximal values: \( c_g = 1/2 \) while the mode II determines \( c_g = 0 \). The main difference is the opposite directions of velocities in these two cases. The group velocity in CP is \( c_g = 1/4 \) in both modes.

The LPW frequencies in HCLs can be obtained by the considerations similar to used above in the SRCL case. In Fig. 6, two-particle-width bands are depicted allowing LPW frequencies for mode I (a) and mode II (b) to be evaluated, direction \( \beta \) corresponds to one of three directions, in which the energy flux possesses the maximal value. First, consider a band shown in Fig. 7 (a). The particles in the generating cell, \( u \) and \( v \) (signed by circles with sign ‘+’), move in phase, in according with the oscillation form of mode I. The in-phase motion of particles but of the opposite sign (‘−’) is realized in a neighboring cell. In the considered case, the oscillation frequency of the cell is \( \omega_i = \sqrt{\frac{4g}{2M}} = \sqrt{2} \) (recall, \( g \) and \( M \) are measurement units). On the other hand, the similar consideration of anti-phase oscillations inherent to mode II, Fig. 7 (b), allows to obtain the corresponding LPW frequency as \( \omega_{II} = \sqrt{\frac{4g}{M}} = 2 \) (it is easy to see that the total stiffness in this case is equal to \( 4g \) consisting of \( 2g \), the sum of stiffnesses of two bonds linking a moving particle to immobile those, and \( 2g \), the stiffness of the bond half linking moving particles with each other. The LPW orientations are shown in Fig. 7 (c).

In addition to the LPWs special forms, there are CP frequency \( \omega = \sqrt{3} \) corresponding to the oscillation form, in which one of two particle families (named \( u \) or \( v \)) are immobile, and all neighboring particles oscillate in anti phase with the frequency at the pass/stop-bands boundary, \( \omega = \sqrt{6} \). The latter case is similar to the simplest antiphase resonant oscillations in the one-dimensional mass-spring chain with the frequency demarcated pass- and stop-bands.

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Fig. 6: Dispersion pattern in the HCL. Group velocities (the upper row) in first quarters of the plane $q_x, q_y$ and equifrequency contours in the Brillouin zone (the lower row). (a) – mode I, (b) – mode II. Relative values and directions of group velocities in current zone point (the upper row) are expressed by the length and direction of the respective arrow.

Fig. 7 The LPW forms, (a) and (b), and orientations, (c), in a HCL
3. Unsteady-state dynamics under harmonic excitations

4.1 RCL

We have analyzed wave patterns at kinematic excitation, \( u_{0,0} = U \sin \omega_0 t \cdot H(t) \), and/or force excitation, \( F_{0,0} = F \sin \omega_0 t \cdot H(t) \), applied to particle \( m = n = 0 \) at \( t = 0 \). Here \( H(t) \) is the Heaviside function, \( U \) and \( F \) are excited amplitudes (below we set \( U = 1 \) and \( F = 1 \)). In computer simulations we use Eqn. (1) with zero initial conditions and external loadings (*) and (**).

An explicit finite-difference scheme has been developed for computer simulations in a finite domain, the time step is taken two orders less than the time measurement unit, which (as calculations show) allows the accuracy level \( \sim 10^{-4} \) to be satisfied. Boundaries of the calculation domain are chosen at such a long distance from the source that their influence on the space region of interest was not detected.

![Fig. 8: Distributions of displacements along three directions: \( n = m \), \( n = m/2 \) and \( n = 0 \) at the force excitation with \( \omega_0 = 2 \). A pronounced beaming pattern of wave propagation along the direction \( n = m \) is detected.](image)

First we consider a SCL, as a partial case of the RCL. At the resonant force excitation, \( \omega_0 = 2 \), a phenomenon of “spatial wave separation” is shown in Fig. 8. As can be seen, a sufficiently large part of the source energy is captured by the diagonal line \( n = m \) (\( \beta_s = \pi/4 \)). In accordance with the dispersion analysis and relations (8.2) speed of its propagation is \( c_g = \sqrt{2} \). At the same time, oscillations along directions \( n = m/2 \) and \( n = 0 \) are practically locked in the source vicinity. As calculations show there are no any noticeable differences in kinematic and force excitations.

Examples of the wave beaming phenomenon are presented in Figs. 9(a) and (b) for SCL and SRCL (with \( l = 1.5 \)), respectively. The structures are subjected to a local kinematic excitation with the resonance frequency \( \omega_0 = 2 \). Points in the mentioned figures represent nodes, in which amplitudes \( |U_{m,n}| \) of envelopes of \( u_{m,n} \) are higher than 10\% of the source amplitude. One can see an star-like beaming, which, as was said above, is realized in accordance with the LPW orientations.
In Fig. 10, we present examples of the same perturbation pattern in a RCL (parameter of the cell form is $l = 1.5$) at $t = 250$. The kinematic excitations with several values of $\omega_0$ were applied. Here spatial wave patterns are more saturated than in the SCL-SRCL case (compare with Fig. 9). First, in accordance with the orientation (11), a star-like pattern appears for two frequencies $\omega_0 = \omega_1 = 1.63$ and $\omega_0 = \omega_2 = 2$. Calculations show that for these frequencies a resonant character of oscillations is realized, similar to that in SCLs.

![Fig. 9: Star-like beaming pattern at the resonant frequency $\omega_0 = 2$ in square-cell – (a) and simplified rectangular-cell – (b) lattices at $t = 200$ in the case of kinematic excitation. Outside the stars, displacements of nodes remain less than 10% of the maximal value in the source.](image)

![Fig. 10: Beaming wave patterns in the rectangular-cell lattice at $t = 250$ (kinematic excitation). Points represent particles with $|U_{m,n}| \geq 0.1$;](image)

The spatial character of wave propagation with frequencies within the interval $(\omega_1, \omega_2)$ is restricted by forbidden directions in compliance with (10) and the above-
Presented dispersion analysis. Obtained in [17] unsteady-state asymptotical \( t \to \infty \) solutions and conducted in [19, 23] computer simulations show that in the case of local monochromatic excitations a logarithmic growth with time is realized in SCLs \( \omega_0 = 2 \) and RCLs \( \omega_0 = 1.63 \) and \( \omega_0 = 2 \).

Finally, we have to compare the results of computer simulations conducted in the case of the resonance frequency located at the interface of pass- and stop-bands: \( \omega_0 = \omega_r = \sqrt{2(2 + 2/l)} \) (the force source). In Fig. 11, modules of envelopes, \( |U_{m,n}| \), in diverse nodes \((m,n)\) are depicted vs. time for several values of \( l \).

\[ \omega_0 = \omega_r = \sqrt{2(2 + 2/l)} \]

\[ \omega_0 = 1.2, \sqrt{2}, \sqrt{3}, 2, 2.2, \sqrt{6} \]

\[ (x, y) \approx (35, 20) \text{ and } (x, y) \approx (16.5, -35.5) \]

The main difference of the response in the considered case from that discussed above for frequencies within the pass-band is that in the former case there are no preferable directions of wave propagation. Besides, resonant growth of perturbations with time is relatively slower.

**4.1 HCL**

Some results of computer simulations of the wave propagation pattern in HCLs are presented below in Figs. 12-13. Calculations conducted in the case of the force excitation of particle \( u_{0,0} \), its location is associated with the origin of rectangular coordinates \( x = y = 0 \). Depicted in Figs. 12 envelopes of \( u_{m,n} \) and \( v_{m,n} \) in two cells: \( 1 - (m,n) = (23, 0) \) and \( 2 - (m,n) = (-15, 26) \), are obtained at various frequencies \( \omega_0 \): \( \omega_0 = 1.2, \sqrt{2}, \sqrt{3}, 2, 2.2, \sqrt{6} \). Cells 1 and 2, \( (x, y) \approx (35, 20) \) and \( (x, y) \approx (16.5, -35.5) \), respectively are located in practically the same distance \( d \approx 40 \) from the source. Cell 1 is located in the resonant ray \( (\beta = \pi/6) \), while cell 2 is located approximately in the middle between two resonant rays \( \beta = \pi/6 \) and \( \beta = \pi/2 \). The shown dependences are realized also in symmetric points (with respect to lattice structure). The presented results and results of additional calculations allow the following conclusions to be formulated:
1. Relatively long waves up to values close to the first resonance, $\omega = \sqrt{2}$, have no preferred directions of propagation: the influence of lattice structure does not appear and waves propagate as in the corresponding homogeneous solid.

2. The wave pattern is drastically changed at the resonant frequency for mode I, $\omega = \sqrt{2}$: the detectable growth of amplitudes in the star rays and a weak response in intermediate regions are detected.

3. At the frequency of the conical point, $\omega = \sqrt{3}$, the wave energy practically does not leak to the periphery.

4. The resonance for mode II, $\omega = 2$, results in the practically the same response that was considered above for mode I. In accordance with the dispersion analysis (16), the main perturbations arrive at the observation points with delay (in comparison with this process for mode I).

5. A frequency $\omega = 2.2$ located between two resonances $2 < \omega < \sqrt{6}$ results in the same qualitative process realized in the case a low-frequency excitation: the wave has no preferred directions of propagation.

6. Amplitudes of low-frequency long-wavelength resonance at $\omega = \sqrt{6}$, the frequency demarcated pass- and stop-bands, are relatively small, but a resonant character of perturbations is detected.

In Fig. 13 a star-like distribution of the main part of disturbances is shown calculated at resonant excitations.
Fig 12: Envelopes of displacements in diverse nodes at a set of frequencies $\omega_b$.
4.2 Nano-tubes

In this Subsection, some results are presented of computer simulations of the wave propagation pattern in square-cell (Fig. 1b) and hexagonal-cell single-wall nano-tubes (Fig. 4b). A simplified statement of the problem is used, in which the casing curvature is not taken into account. By another words, particles remain in out-plane motion, while closed-loop casing is modeled by equating the boundary conditions on x-edges of SCL/HCL sheets of the width equal to $2\pi R$, where $R$ is the casing radius.

Examples of the wave beaming phenomenon in nano-tubes are presented in Figs. 14 and 15 for SCL and HCL, respectively. The structures are subjected to a local kinematic excitation with the resonance frequency $\omega_0 = 2$ (SCL) and $\omega_0 = \sqrt{2}$, 2 (HCL) Circumference of tubes is considered to be $2\pi R = 100$ nodes (while the length is infinite for any practical reason). The presented results show, the periodicity condition has an irrelevant influence on the wave beaming structure, it remains in tubes

![Fig. 13: Star-like beaming pattern in square-cell tube at the resonant frequency $\omega_0 = 2$ at $t = 500$ (kinematic excitation). Outside the stars, maximal displacements of nodes remain less than (a) 7% and (b) 10% of the maximal value in the source](image_url)
**Fig. 14:** Star-like beaming pattern in hexagonal-cell tube at the resonant frequencies: $\omega_0 = \sqrt{2}$, (a) and (b), and $\omega_0 = 2$, (c) and (d), at $t = 500$ (kinematic excitation). Outside the stars, maximal displacements of nodes remain less than 7% (a, c) and 10% (b, d) of the maximal value in the source.

The numbers on Fig. 14 are referring to unit cells (which is consist of two particles $u$ and $v$), therefore total number of nodes with considered displacements is twice over the presented number.

4. **Hexagonal-cell lattice with non-local connections of particles**

Consider the uniform hexagonal-cell lattice depicted in Fig. 4 with additional links resulting in non-local connections of particles. New links are shown by thin lines in Fig. 15. As above we consider out-plane oscillations of the lattice and use discrete rhombic Cartesian coordinates $m$ and $n$ together with continuous rectangular coordinates $x$ and $y$. The rhombic cell $[m,n]$ remains the same that presented in Fig. 4.

In the considered model each particle of $u(v)$-family is additionally connected to six neighboring particles of the same family (see. Fig. 15). Let as above, the distance between two neighboring nodes, particle masses and stiffnesses of bonds linking neighboring $u$- and $v$-particles are measurement units, $M = g = a = 1$. Then, with the cell geometry in mind, the free transverse motion of the system is the follows:
As above, assume the conventional harmonic solutions of the form of the plane wave (in xy-plane):

\[
(u_{m,n}, v_{m,n}) = (U, V) \exp \left( i \omega t + nk \cdot \vec{a}_1 + mk \cdot \vec{a}_2 \right),
\]

where \( \vec{a}_1 = \sqrt{3}/2 \hat{x} + 1/2 \hat{y} \), \( \vec{a}_2 = \sqrt{3}/2 \hat{x} - 1/2 \hat{y} \) (\( \hat{x} \) and \( \hat{y} \) are unit vectors).

After substituting (18) to (17) we obtain a system of two linear equations, the nontrivial solution of which determines the following dispersion equation:

\[
\omega_{I,II} \sqrt{3 + 6 \gamma - 2\Psi} = \sqrt{3 + \Psi}, \quad \Psi = \sqrt{2\cos(ky) + 4\cos(k_x/2)\cos(\sqrt{3}k_x/2)}
\]

where signs ‘−’ and ‘+’ correspond to first (acoustical) and second (optical) modes.

Eqn. (19) show that a complete stop-band between modes is absent: they are connected in four CP. Their coordinates are \( [k_x, k_y] = [\pm 2\pi/\sqrt{3}, \pm 2\pi/3] \), and \( \omega_{CP} = \sqrt{9\gamma + 3} \) is the CP frequency. We can show that in the considered structure, LPWs are realized at the same contour \( k_y = \pm \pi \cup k_y = \pm 2\pi \pm \sqrt{3}k_x \) that was pointed above (formula), but new resonant frequencies are revealed now: \( \omega = \sqrt{8\gamma + 2} \) (the mode I) and \( \omega = \sqrt{8\gamma + 4} \) (the mode II).

In Fig. 16, dispersion surfaces of modes I and II are depicted together with sets of eigenfrequency contours for each mode.
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**REFERENCES**


