Acoustic excitations in a non-ideal one-dimensional superlattice with anisotropic impurity layers

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Abstract. The virtual crystal approximation is used to study the specifics of propagation of acoustic excitations through a non-ideal one-dimensional superlattice. Numerical modeling is performed to evaluate the dependence of the lowermost acoustic band gap in a two-sublattice phonon crystal (disordered in composition and widths of constituent layers) on impurity layer concentration.

1. Introduction
Investigations into propagation of sound in matter, which constitute the subject matter of physical acoustics [1, 2] come to the forefront in numerous applied problems, such as the elimination of extraneous sounds (noise abatement), the search for extraction methods of useful acoustic signals, as well as the problem of acoustic object detection through the use of a sonic depth finder. In this connection, a significant attention is devoted to development and enhancement of acoustic devices intended for sound-measuring of physical properties of various media, as well as to fabrication of novel meta-materials for the purpose of controllable propagation of acoustic waves. Perfection of experimental techniques along with the broadening of theoretical perspectives result in expansion of the studied frequency ranges and make acoustic methods an indispensable tool for structural investigations of solids.

At present, there is a significant number of works [3–8] devoted to calculation of electromagnetic and acoustic excitations in superlattices based on the T-matrix method, which ultimately involve a solution of a system of equations for the Fourier-expansion coefficients of corresponding fields. The problem of finding of certain specific physical characteristics (such as e.g. the transmission coefficients of electromagnetic excitation, the band spectrum etc.) requires in the general case an expensive and often unfeasible calculation, which compels one to resort to some approximation methods. For instance, it is shown in reference [9] that in the vicinity of the Brillouin zone the dependence of the corresponding frequencies on Bloch wave vector can be approximated by a certain analytical expression. It is worthwhile reminding that the real-life acoustic superlattices are non-ideal systems [10–12]. A widely used method of calculation of normal modes in disordered superlattices with randomly distributed (over an entire volume) structural defects is the virtual crystal approximation, whose essence consists [13–15] in replacing the configurationally dependent Hamiltonian parameters by their configurationally averaged values. In references [7, 8] we have utilized an approach (initially developed for ideal superlattices [9]) to study electromagnetic excitations in non-ideal one-dimensional systems with impurity (defect) layers randomly distributed...
over a superlattice volume. The virtual crystal approximation enabled us in references [7, 8] to obtain the desired optical characteristics of non-ideal superlattices.

In the present work (which continues the lines of reference [8]) this approach is extended to investigation of the specifics of propagation of acoustic excitations through a non-ideal one-dimensional phonon crystal constituted by a system of plane-parallel layers containing anisotropic impurity layers with different elastic characteristics (in contrast to reference [16] devoted to arrays of isotropic layers).

2. Elastic waves in non-ideal one-dimensional superlattices

In the general case of a non-uniform medium the matter density $\rho(r)$ and the elastic moduli $\Lambda(r)$ are functions of coordinates, whereas the field of elastic displacements $u(r,t)$ is described by a system of equations [1, 17]:

$$\ddot{u}_i(r,t) = \left[ \hat{L}(r) \right]_{im} u_m(r,t),$$

where $\hat{L}(r)$ is a differential operator of the form

$$\left[ \hat{L}(r) \right]_{im} = \frac{1}{\rho(r)} \left[ \frac{\partial \Lambda_{\alpha\beta\mu\nu}(r)}{\partial x_{\alpha}} \frac{\partial}{\partial x_{\beta}} + \Lambda_{\alpha\beta\mu\nu}(r) \frac{\partial^2}{\partial x_{\beta} \partial x_{\nu}} \right],$$

corresponding to Lagrange function density $\frac{1}{2} \rho(r) \left( \frac{\partial u}{\partial t} \right)^2 - \frac{1}{2} \Lambda_{\alpha\beta\mu\nu}(r) \frac{\partial^2 u}{\partial x_{\mu} \partial x_{\nu}}$ [17].

It follows from (1) that once the study is confined to monochromatic elastic excitations $u(r,t) = u(r) \exp(-i\omega t)$ the equation for displacement amplitudes $u(r)$ assumes the form

$$\hat{L}(r)u(r) = -\omega^2 u(r),$$

Let us consider acoustic excitations in a one-dimensional inhomogeneous (along the z-axis) layered medium. It is assumed to be comprised by an array of plane-parallel uniform layers obtained by a random replacement of layers of a certain given one-dimensional superlattice with extrinsic uniform uniaxial impurity layers. The structural “cells” of the so transformed “superlattice” differ from the corresponding cells of an ideal system both in widths and composition. Strictly speaking, such a system does not allow invoking the concept of a cell due to the broken translation invariance. Nevertheless a one-to-one correspondence is preserved between the layers of the non-ideal and ideal systems. In the frames of the constructed model the matter density $\rho(z)$ and the elastic moduli $\Lambda(z)$ can be represented through the use of $\theta$-function:

$$\rho(z) = \sum_{n,\alpha} \rho_{n\alpha} \theta_{n\alpha}(z), \quad \Lambda(z) = \sum_{n,\alpha} \Lambda_{n\alpha} \theta_{n\alpha}(z).$$

In what follows we can conveniently use the quantity $\hat{B}(z) = \hat{\Lambda}(z)/\rho(z)$, which by analogy with equation (4) can be written as

$$\hat{B}(z) = \sum_{n,\alpha} \hat{B}_{n\alpha} \theta_{n\alpha}(z), \quad \hat{B}_{n\alpha} = \frac{\Lambda_{n\alpha}}{\rho_{n\alpha}}$$

where
\[ \theta_{n\alpha}(z) = \theta \left[ z - (n-1)d - \left( \sum_{j=1}^{\alpha} a_{n\alpha} - a_{n\alpha} \right) \right] - \theta \left[ z - (n-1)d - \sum_{j=1}^{\alpha} a_{n\alpha} \right]. \tag{6} \]

\( \rho_{n\alpha} \), \( \hat{\Lambda}_{n\alpha} \) and \( a_{n\alpha} \) denote, correspondingly, the layerwise characteristics (matter density and elastic moduli) and layer widths. \( n \) numerates the “cells”, and \( \alpha \) numerates elements in a “cell”.

A simplest approximation, which allows examination of transformation of elementary excitation spectrum (caused by the presence of foreign layers) is the virtual crystal approximation. It permits (through configurational averaging of relevant parameters entering the problem’s Hamiltonian) to obtain the acoustic excitation spectrum as a function of impurity concentration. The averaging procedure “transforms” the considered non-ideal system into the so-called “virtual crystal”, where the translation symmetry is restored.

Unlike in the case of an ideal superlattice, in an imperfect one-dimensional phonon crystal of varied composition and layer widths, tensor \( \hat{B}_{n\alpha} \) and quantity \( a_{n\alpha} \) are configurationally dependent. In terms of random variables \( \eta^{x\mu}_{n\alpha} \) they can be written as

\[
\hat{B}_{n\alpha} = \sum_{v(a)=1}^{r(a)} \hat{B}_{a}^{v(a)} \eta_{n\alpha}^{v(a)}, \quad a_{n\alpha} = \sum_{\mu(a)=1}^{r(a)} a_{a}^{\mu(a)} \eta_{n\alpha}^{\mu(a)},
\]

where \( \eta^{x\mu}_{n\alpha} = 1 \), if the \( n\alpha \)-th node of the one-dimensional crystal is occupied by a layer of the \( v(\alpha) \)-th type (and/or by a layer of the \( \mu(\alpha) \)-th width), and \( \eta^{x\mu}_{n\alpha} = 0 \) otherwise. It is assumed below that these factors of disorderliness are independent of each other. The configurational averaging procedure (denoted by angular brackets) applied to equation (7) in accordance with the VCA (and by analogy with the quasi-particle approach [8, 14]) yields

\[
\langle \hat{B}_{n\alpha} \rangle = \sum_{v(a)=1}^{r(a)} \hat{B}_{a}^{v(a)} C_{Ca}^{v(a)} , \quad \langle a_{n\alpha} \rangle = \sum_{\mu(a)=1}^{r(a)} a_{a}^{\mu(a)} C_{Ta}^{\mu(a)} ,
\]

(8)

Here \( C_{Ca}^{v(a)} \) and \( C_{Ta}^{v(a)} \) are concentrations of impurity layers of the \( v \)-th and \( \mu \)-th types of composition (lower index “C”) and width (lower index “T”) contained in the \( \alpha \)-th sublattice. An obvious condition must hold \( \sum_{v(a)=1}^{r(a)} C_{Ca}^{v(a)} = 1 \), \( \sum_{\mu(a)=1}^{r(a)} C_{Ta}^{\mu(a)} = 1 \). Similarly to the case of a non-ideal superlattice, the problem of finding phonon-polarit characteristics is reduced to a corresponding problem formulated for the “virtual crystal”, whose layerwise characteristics are described by quantities \( \hat{B}_{a}^{v(a)} \), layer widths \( a_{a}(\{ C_{Ta}^{\mu(a)} \}) \) and cell periods \( d(\{ C_{Ta}^{\mu(a)} \}) \) (curly brackets contain the set of variables \( C_{Ca}^{v(a)} \), \( C_{Ta}^{\mu(a)} \) for different values of \( v, \mu \)). For this reason within the VCA the corresponding quantities (the spectrum, the band gap etc.) are the functions of extrinsic layer concentrations \( C_{Ca(Ta)}^{v(\mu)} \).

Let us consider propagation of elastic monochromatic wave with Bloch vector \( \mathbf{K} = (0,0,K) \) in a one-dimensional phonon “virtual crystal”, which is an ideal system with lattice period \( d \) obtained as a result of configurational averaging. We shall have then \( \rho(z) = \rho(z + d) \), \( a_{n\alpha} = a_{\alpha} \), \( \rho_{n\alpha} = \rho_{\alpha} \) (analogous equalities hold for tensor \( \hat{\Lambda} \)). Straightforward calculations with the use of equation (3) yield the following system for Fourier-amplitudes \( U_k^{m}(g) \) of the elastic displacements field \( \mathbf{u}(r,t) \):

\[
a^{\mu}U_k^{m}(g) = \sum_{g'} B_{0\mu\mu}(g - g')(K + g')^2 - iA_{0\mu\mu}(g - g')(K + g')U_k^{m}(g').
\]

(9)
where \( g = \frac{2\pi}{d} p \) (\( p = 0, \pm 1, \pm 2, \ldots \)) are vectors of the corresponding reciprocal lattice. It can be easily shown that in the case of a one-dimensional superlattice whose layerwise characteristics obey condition (9) tensor \( A_{mn} (g) \) turns to zero. Fourier-transform of tensor \( \hat{B} \), obtained with the use of expression (9) has the form

\[
\hat{B}(p) = -\frac{i}{2\pi p} \sum_{\alpha} \hat{B}_\alpha^{(e)} C_\alpha^{(a)} \times \\
\times \left\{ \exp \left[ i \frac{2\pi}{d} \left( C_{Tm}^{(a)} \right) p \sum_{j=1}^{g} a_j \left( \left( C_{Ta}^{(a)} \right) ^{-1} \right) \right] - \exp \left[ i \frac{2\pi}{d} \left( C_{Tm}^{(a)} \right) p \sum_{j=1}^{g} a_j \left( \left( C_{Ta}^{(a)} \right) ^{-1} \right) \right] \right\}
\]

(10)

For anisotropic layers of a one-dimensional phonon crystal tensor components of \( \hat{A} \) (and, correspondingly of \( \hat{B} \)) are given in [18], whereas for uniform layers of a one-dimensional phonon crystal tensor components of \( \hat{A} \) (and \( \hat{B} \)) have the form specified in reference [19]:

\[
A_{ikm} = \lambda \delta_{ik} \delta_{lm} + \mu \left( \delta_{ik} \delta_{ml} + \delta_{im} \delta_{kl} \right),
\]

(11)

where \( \lambda, \mu \) are Lamé coefficients. In an arbitrary case expression (11) is no longer valid. Under the presence of foreign uniaxial layers for \( K \) chosen along the symmetry axis \( K = (0, 0, K) \) non-zero are the following components of tensor отлилы от нуля \( \hat{B}(p) \) [18]:

\[
B_{zzz}(p), B_{xz}(p) = B_{zyz}(p).
\]

In such a case occurs a longitudinal-transverse splitting of the phonon excitation and the system of equations (9) breaks up into two independent subsystems, first of which contains only quantities \( B_{zzz} \), and describes propagation of longitudinal acoustic excitations, whereas the second one describes transverse excitations and contains \( B_{zzz} = B_{zyz} \). Such splitting is obviously possible due to a clever choice of the problem’s geometry.

The dispersion laws of the corresponding acoustic excitations are defined by the infinite system of equations (6), which in the general case (for arbitrary \( K \)’s) is solved with the use of approximation methods (similarly to calculation of exciton-polariton excitations in dielectric superlattices [3]). Nevertheless (as demonstrated below) for the values of wave vector \( K \) close to the Brillouin zone boundary \( K - \frac{2\pi}{d} \approx K \), the dependence \( \omega = \omega(K) \) can be written as an analytic expression.

Indeed, it can be seen from (6) that in that case the largest-magnitude quantities are \( U'_x (g) \) for \( g \) with \( p = 0, -1 \) under fulfillment of condition \( \omega^2 \approx K^2 B_{zzz}^{(0)} \) (similarly to (11) in reference [7]). Here \( B_{zzz}^{(0)} = B_{zzz,zzz}(p = 0) \), \( B_{zzz}^{(-1)} = B_{zzz,zzz}(p = -1) \) are the Fourier coefficients [18]. Retaining in system (9) only the terms corresponding to resonance of the specified plane waves \( p = 0, -1 \), we arrive at the following dispersion law of acoustic excitations:

\[
\omega_{z,\pm}^2 = \left( C_{Cz}^{(a)} \right) \rightarrow K^2 \left| B_{zzz}^{(0)} \left( \left( C_{Cz}^{(a)} \right) \right) \right| = K^2 \left| B_{zzz}^{(-1)} \left( \left( C_{Cz}^{(a)} \right) \right) \right|. 
\]

(12)

3. Results and discussion

In real-world applications of all the various quantities, which can be obtained from theoretical examinations of propagation of acoustic excitations a special role is played by the band-gap width \( \Delta \omega = |\omega_+ - \omega_-| \). \( \omega_+ \), \( \omega_- \) are the roots of equation (12) which define the boundaries of the spectral band.
Under frequencies $\omega \, (K) < \omega < \omega_{s} \,(K)$ the roots are complex (forbidden band), and correspond to damped acoustic waves (Bragg reflection). Waves with frequencies falling into range $\omega < \omega_{s}, \, \omega > \omega_{s}$ are undamped. According to equation (12) in the considered case the lowermost band gap width equals to

$$\Delta \omega\left(\left\{ C_{Ca}^{(a)} \right\}, \left\{ C_{Ta}^{(d)} \right\} \right) = \sqrt{1 + \frac{B_{h}^{(c)}}{B_{h}^{(d)}} \left( \left\{ C_{Ca}^{(a)} \right\}, \left\{ C_{Ta}^{(d)} \right\} \right) / B_{h}^{(d)} \left( \left\{ C_{Ca}^{(c)} \right\}, \left\{ C_{Ta}^{(d)} \right\} \right) - \frac{1}{\left( \left\{ C_{Ca}^{(c)} \right\}, \left\{ C_{Ta}^{(d)} \right\} \right) / B_{h}^{(d)} \left( \left\{ C_{Ca}^{(c)} \right\}, \left\{ C_{Ta}^{(d)} \right\} \right)}}. (13)$$

Quantities $B_{h}^{(c)} \left( \left\{ C_{Ca}^{(a)} \right\}, \left\{ C_{Ta}^{(d)} \right\} \right)$, which depend on concentration on extrinsic (as compared to an ideal superlattice) layers, are defined by the number of sublattices as well as by material characteristics such as the Lame coefficients $\lambda$, $\mu$ (for homogeneous systems), the matter density $\rho$ and the coefficients of elasticity (for a uniaxial subsystem). For this reason under various problem’s parameters the band gap width can demonstrate diverse types of concentration dependences.

We have performed numerical modeling for the specific case of disordered (in composition and layer widths) two-sublattice one-dimensional phonon crystal. The first sublattice is assumed to be comprised by duraluminium layers (with Young modulus $E_{1} = 70 \, GPa$, Poisson’s ratio $\sigma_{1} = 0.31$ and density $\rho_{1} = 2800 \, kg/m^{3}$), the second lattice is comprised by celluloid layers (Young modulus $E_{2} = 1.9 \, GPa$, Poisson’s ratio $\sigma_{2}^{(1)} = 0.39$ and density $\rho_{2}^{(1)} = 1400 \, kg/m^{3}$). The second sublattice contains impurity layers of $\alpha$-quartz whose concentration is $C_{C}$. Since the second sublattice is also varied in layer widths the averaged period of the considered one-dimensional phonon crystal equals has the form

$$d(C_{T}) = a_{t} \left[ 1 + \frac{a_{1}^{(1)}}{a_{t}} + \left( \frac{a_{2}^{(2)}}{a_{t}} - \frac{a_{1}^{(1)}}{a_{t}} \right) C_{T} \right], \quad (14)$$

where $a_{t}$ is the layer width of the first sublattice, $a_{1}^{(1)}$ is the layer width of the second lattice of the ideal superlattice, $a_{2}^{(1)}$ is the width of foreign layer in the second sublattice, whose concentration is $C_{T}$.

Detailed calculation based on equation (10) yields the following expressions:

$$B_{h}^{(0)} = \frac{a_{t}}{d(C_{T})} \left[ B_{h}^{(0)} - B_{h}^{(1)} \left( C_{C}^{(2)} \right) \right]$$

$$B_{h}^{(c)} = \frac{1}{\pi} \left[ B_{h}^{(0)} + \left( B_{h}^{(1)} - B_{h}^{(2)} \right) C_{C}^{(2)} \right]^{2} - \frac{2 B^{(2)}}{B_{h}^{(0)}} \left( B_{h}^{(1)} - B_{h}^{(2)} \right)^{2} \left( C_{C}^{(2)} \right)^{2} \sin \frac{\pi a_{t}}{d(C_{T})}. \quad (15)$$
Here, according to reference [18],

\[ B_{(2)}^{(1)} = \frac{E_2^{(1)}(1-\sigma_2^{(1)})}{\rho_2^{(1)}(1+\sigma_2^{(1)})(1-2\sigma_2^{(1)})}, \quad B_{(1)}^{(1)} = \frac{E_1}{2\rho_1(1+\sigma_1)} \]

and for uniaxial impurity layers, according to

\[ B_{(2)}^{(2)} = \frac{E_2^{(2)}(1-\sigma_2^{(2)})}{\rho_2^{(2)}(1+\sigma_2^{(2)})(1-2\sigma_2^{(2)})}, \quad B_{(1)}^{(2)} = \frac{E_1}{2\rho_1(1+\sigma_1)} \]

Let us examine the specifics of variation of the band gap \( \Delta\omega/\omega \) of the superlattice under changing concentration, composition and widths of impurity layers. The dependence \( \Delta\omega/\omega(C_c, C_r) \) is plotted in figure 1.

\[ \frac{\Delta\omega}{\omega} = \frac{\Delta f}{f} \]

\[ a) \quad b) \]

**Figure 1.** Dependence of the band gap width \( \Delta\omega/\omega \) of the considered superlattice (constituted by duraluminium and celluloid layers) on concentrations of impurity \( \alpha \)-quartz layers \( C_c, C_r \). Surfaces 1 and 2 correspond to longitudinal and transverse modes, respectively. Figure a) corresponds to \( a_1^{(1)}/a_1 = 5, a_2^{(1)}/a_1 = 0.1 \). Figure b) corresponds to \( a_1^{(2)}/a_1 = 10, a_2^{(2)}/a_1 = 0.5 \).

Examination of the behavior of surface plots \( \Delta\omega/\omega(C_c, C_r) \) shows that the values of \( \Delta\omega \) may substantially differ depending on the specifically chosen problem’s parameters as well as on foreign layer concentration. Under certain \( C_c, C_r \) the band gap \( \Delta\omega \) can be quite large (and so the considered multi-layer system would be weakly permeable for acoustic waves), whereas for other values of impurity concentration the band gap \( \Delta\omega \) may become rather small. As can be seen from figure 1, the band gap can turn to zero at a certain value of \( C_c \), and as this takes place \( C_r \) may assume any arbitrary value. Once the zero value of \( \Delta\omega \) is attained, acoustic excitations would pass unhindered through the layered material with corresponding characteristics.

**4. Conclusion**

From the above numerical modeling follows a natural conclusion that the band gap width depends on parameters of the considered superlattice as well as on polarization of propagating acoustic waves. It is shown that concentration dependence \( \Delta\omega/\omega(C_c, C_r) \) is substantially affected by the ratios \( \frac{a_2^{(2)}}{a_1}, \frac{a_2^{(2)}}{a_1} \).
Also it should be noted that for a given superlattice at a certain specific acoustic wave frequency there won’t be necessary values of $C_{C}, C_{T}$ such that the transverse and/or longitudinal modes would satisfy the condition $\Delta \omega = 0$ (see figure 1). As can be evidently seen in the figure this condition holds only at a certain domain of $C_{C}$ values. Investigation of the dependence of the lowermost acoustic band gap width on impurity layer concentration carried out in the present work may prove useful for fabrication of acoustic composite materials intended for various operative conditions.

References
[1] Brekhovskikh L M 1980 Waves in Layered Media (Academic Press) p 503
[2] Shu Zhang, Chunting Xua and Nicholas Fang 2011 Phys. Rev. Lett. 106 024301(1)
[3] Joannopoulos J D, Johnson S G, Winn J N and Meade R D 2008 Photonic Crystals. Molding the Flow of Light (Second Edition Princeton: Princeton University Press) p 305
[4] Shabanov V F, Vetrov S Ya and Shabanov A V 2005 Optics of real photonic crystals. Liquid crystal defects, irregularities [In Russian] (RAS Publisher, Siberian Branch) p 239
[5] Kosevich A M 2001 JETP Letters 74 559
[6] Pendry J B and Li Jensen 2008 New Journal of Physics 10 1115032(1)
[7] Rumyantsev V V, Fedorov S A and Shtaerman E Ya 2010 Superlattices and Microstructures 47 29
[8] Rumyantsev V V, Fedorov S A and Gumennik K V 2011 Photonic Crystals: Optical Properties, Fabrication and Applications Chapter 8 / ed. William L Dahl (NY: Nova Science Publishers Inc.) p 34
[9] Yariv A and Yeh P 1984 Optical Waves in Crystals: Propagation and Control of Laser Radiation (Wiley: New York) p 604
[10] Feng-Ming Li and Yue-Sheng Wang 2005 Int. J. Solids Struct. 42 6457
[11] A-Li Chen and Yue-Sheng Wang 2007 Physica B: Condensed Matter 392 369
[12] Zhi-Zhong Yan, Chuanzeng Zhang and Yue-Sheng Wang 2010 Wave Motion 47 409
[13] Parmenter R H 1955 Phys. Rev. 97 587
[14] Ziman J M 1979 Models of Disorder (London: Cambridge Univ. Press) p 480
[15] Dargan T G, Capaz R B and Koiler Belita 1997 Brazilian J. of Phys. 27/A 299
[16] Rumyantsev V V, Fedorov S A and Gumennik K V 2014 Acoustical Physics 60 348
[17] Kosevich A M 1981 Physical mechanics of real crystals [In Russian] (Kiev: Naukova Dumka; translated into Polish: Wroclaw, Wydawnictwo Universitetu Wroclawskiego, 2000) p 327
[18] Sirotin Yu I and Shaskolskaya M P 1983 Fundamentals of Crystal Physics (Chicago: Imported Publications) p 654
[19] Nye J F 1985 Physical Properties of Crystals: Their Representation by Tensors and Matrices (Oxford University Press) p 352