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NUMERICAL MODELING OF THE ACOUSTIC ACTIVITY OF NON-IDEAL 1D CRYSTALLINE SUPERLATTICE

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ АКУСТИЧЕСКОЙ АКТИВНОСТИ НЕИДЕАЛЬНОЙ 1D КРИСТАЛЛИЧЕСКОЙ СВЕРХРЕШЕТКИ

The paper studies propagation of acoustic excitations through a non-ideal (defect containing) one-dimensional superlattice. The virtual crystal approximation is employed to perform a numerical modeling of the dependence of specific rotation angle of elastic wave polarization plane on structural defect concentrations in a two-sublattice one-dimensional phononic crystal disordered in its composition and constituent layer widths.
Key words: acoustic excitations, non-ideal one-dimensional phononic crystal, acoustically active medium, virtual crystal approximation

В статье исследуется распространение акустических возбуждений через неидеальную (содержащую дефекты) одномерную сверхрешетку. Для численного моделирования зависимости удельного угла поворота плоскости поляризации упругой волны от концентрации структурных дефектов в двухподрешеточном одномерном фононном кристалле, неупорядоченном по своему составу и ширине составляющих слоев, используется. приближение виртуального кристалла
Ключевые слова: акустические возбуждения, неидеальный одномерный фотонный кристалл, акустически активная среда, приближение виртуального кристалла

1. INTRODUCTION

The studies of propagation of sound in matter on both macroscopic and microscopic levels constitute the subject of physical acoustics [1], [2]. At the present time they draw attention in the context of solving of various applied problems such as e.g. the elimination of undesirable sounds (noise reduction), the search for methods of enhancement of useful sounds and the purposes of acoustic detection (involving echo-sounding devices). A special importance is attached to development and perfection of acoustic technologies capable of measuring various physical characteristics in media with the help of sound and creation of novel acoustic metamaterials, which allow controlling propagation of acoustic waves in a medium. Refinement of experimental techniques along with the development of theoretical concepts widens the frequency range of acoustic excitations amenable to investigation and renders acoustic methods indispensable for the study of solid state structures.

Nowadays there is a considerable amount of studies [3-8] devoted to calculation electromagnetic and acoustic spectra in superlattices. They are based on the use of T-matrix method, and solution of system of equations for Fourier-expansion coefficients of corresponding fields. The finding of specific physical properties (such as e.g. the transmission coefficients of electromagnetic irradiation, the energy-band structure etc.) usually poses an extremely difficult computational problem, wpich requires the use of approximate methods.

For instance, in Ref. [9] it is shown that in the vicinity of the first Brillouin zone one can approximately express the corresponding frequencies as analytical functions of the Bloch wave vector. Let us note that real-life acoustic superlattices are always non-ideal [10-12]. A widely used method of calculation of normal modes in disordered superlattices with random volumetric distribution of structural defects is the virtual crystal approximation [13-15], which is based on replacement of configurationally dependent parameters of Hamiltonian with their configurationally averaged values. We have studied electromagnetic excitations [7], [8] using the approach developed previously for ideal superlattices [9] and utilizing the virtual crystal approximation to obtain the desired optical characteristics of non-ideal superlattices. Below we adopt the assumption of a rigid constraint to study acoustic excitations in a layered system, which is justified for small oscillations and the absence of intralayer slip.

When examining propagation of acoustic excitations in crystalline structures particular interest lies in manifestations of spatial dispersion, which is responsible for acoustical activity e.g. in noncentro-symmetrical media (similarly to optical activity [16]).

Let us remind that the problem of finding of normal elastic waves which are required for calculation of characteristics of spatially dispersive one-dimensional superlattices has not yet been solved. However, it is quite obvious that in the case of a layer width much exceeding the characteristic scale of spatial dispersion the corresponding quantities can be calculated approximately provided that each layer's contribution into acoustical activity is regarded as independent. That means that in order to find the specific rotation angle $\varphi(\omega)$ of polarization plane it is sufficient to know the layerwise specific rotation angles $\varphi(\omega)$ (ω being the acoustic excitation frequency, n being the number of elementary cell, α being the layer number in a cell) and concentrations of foreign layers (if any).

In the present paper we employ the previously developed approach [16] to consider acoustic excitations in a defect-containing one-dimensional phononic crystal comprised by plane-parallel layers with anisotropic (in contrast to Ref. [17]) impurity layers, whose elastic properties differ from those of the “matrix” layers. The obtained expression expression for $\varphi(\omega)$ is indispensable for the numerical modeling of defect concentration dependence of acoustical activity of complex one-dimensional superlattices.

2. THEORETICAL MODEL

To make our discussion more specific let us consider acoustic excitation in a one-dimensional inhomogeneous (along the z-axis) layers medium, where certain of the “matrix” layers have been randomly replaced by uniform uniaxial impurity layers. Elementary cells of the so-transformed structure would differ from those of the initial structure both in their composition and thickness. Strictly speaking in such a case one cannot speak of elementary cells in the conventional sense at all (due to the broken translation invariance). However there remains a preserved one-to-one correspondence between layers of the ideal and non-ideal systems. Let us now investigate the propagation of linearly polarized transversal acoustic excitation along the layerwise acoustic axis (perpendicular to the layers’ surfaces) within the described model, where all acoustic axes are collinear. In accordance with the phenomenological approach [18-20], the rotation angle of polarization plane of acoustic wave in a defect containing topologically ordered one-dimensional superlattice composed of N elementary cells is given by the following expression:

$$\phi(\omega)=\sum_{n=1}^{N}\sum_{\alpha=1}^{\sigma}\phi_{n\alpha}(\omega)\,a_{n\alpha} \tag{1}$$

It is assumed that the number of cells N is sufficiently big to justify the procedure of configurational averaging. In (1) $a_{n\alpha}$ and $\varphi_{n\alpha}(\omega)$ are correspondingly the configurationally dependent width of the α-th layer of the n-th elementary cell and the specific rotation angle of polarization plane of acoustic wave with frequency ω. σ is the number of layers in elementary cell. By analogy with [21], we arrive at the following expressions for configurationally dependent quantities $\varphi_{n\alpha}(\omega)$ and $a_{n\alpha}$:

$$\varphi_{n\alpha}(\omega)=\sum_{\mu(\alpha)}^{r(\alpha)}\varphi_{\alpha}^{\mu(\alpha)}(\omega)\eta_{Cn\alpha}^{\mu(\alpha)},\qquad a_{n\alpha}=\sum_{\nu(\alpha)}^{s(\alpha)}a_{\alpha}^{\nu(\alpha)}\eta_{Tn\alpha}^{\nu(\alpha)} \tag{2}$$

Configurational averaging yields the following expression for the rotation angle of elastic wave polarization plane:

$$\langle\varphi(\omega)\rangle = N\left[\sum_{\alpha=1}^{\sigma}\varphi_{\alpha}^{(1)}(\omega)a_{\alpha}^{(1)}+a_{\alpha}^{(1)}\sum_{\mu(\alpha)=1}^{r(\alpha)}\Delta\varphi_{\alpha}^{\mu(\alpha)}(\omega)C_{C\alpha}^{\mu(\alpha)}+\varphi_{\alpha}^{(1)}\sum_{\nu(\alpha)=1}^{s(\alpha)}\Delta a_{\alpha}^{\nu(\alpha)}C_{T\alpha}^{\nu(\alpha)}+\right.$$
$$\left.+\sum_{\mu(\alpha)=1}^{r(\alpha)}\sum_{\nu(\alpha)=1}^{s(\alpha)}\Delta\varphi_{\alpha}^{\mu(\alpha)}(\omega)\Delta a_{\alpha}^{\nu(\alpha)}C_{C\alpha}^{\mu(\alpha)}C_{T\alpha}^{\nu(\alpha)}\right] \tag{3}$$

$\Delta\phi_{\alpha}^{\mu(\alpha)}=\phi_{\alpha}^{\mu(\alpha)}-\phi_{\alpha}^{(1)}$, $\Delta a_{\alpha}^{\nu(\alpha)}=a_{\alpha}^{\nu(\alpha)}-a_{\alpha}^{(1)}$. $C_{C\alpha}^{\mu(\alpha)}$, $C_{T\alpha}^{\nu(\alpha)}$ are, correspondingly, concentrations of defect layers differing from the “matrix” substance in their composition and thickness. The first term in Eq. (3) corresponds to rotation angle of polarization plane of acoustic wave of an ideal one-dimensional superlattice composed of layers of the (1)-st type (this substance is assumed to be the “matrix” one). The second term is due to compositional disordering of the superlattice. It turns to zero in the case when composition remains unchanged. The third term reflects disordering in thickness (and turns to zero if the latter is absent). The last term is due to disordering of the superlattice both in composition and layers' thickness. Absence of at least one type of disordering results in the fourth term of Eq. (3) turning to zero. Each of the four terms in Eq. (3) has the physical meaning of rotation angle per one elementary cell. Unlike the specific angle $\varphi_{n\alpha}^{\mu(\alpha),\nu(\alpha)}$, which is measured in degrees per length unit these angles are measured in degrees.

3. RESULTS AND DISCUSSION

In this section it is our goal to apply the above theory to examine a two-sublattice system consisting of paratellurite (1st sublattice) and α-quartz (2nd sublattice) layers. Elements of the second sublattice are randomly replaced by defect layers of two types, the first being layers of a different substance (paratellurite) and the same width, and the second being layers of the same substance (α-quartz) and different width. The corresponding concentrations of impurity layers are denoted as C_C and C_T. Thicknesses of layers in the two sublattices are assumed to be equal. Specific rotation of polarization plane of elastic wave $\varphi_1^{(1)} = \varphi_2^{(2)}$ in the direction of acoustic axis in paratellurite layers is 913 deg/cm at a frequency 30 MHz, which is 8000 higher than in α-quartz [22, 23]. This is explained by a stronger anisotropy of elastic properties and lesser velocity of elastic waves in paratellurite crystal as compared to α-quartz [22]. Hence follows that in expression (3) $\Delta\varphi_1^{(1)} = 0,\ \Delta\varphi_2^{(1)} = 0,\ \Delta\varphi_2^{(2)} = \varphi_2^{(2)} - \varphi_2^{(1)} \approx \varphi_2^{(2)}$. Simple calculations yield the concentration dependence of rotation angle of polarization plane of elastic wave in the considered one-dimensional superlattice:

$$\Phi(\omega, C_C, C_T) \equiv \langle \varphi(\omega) \rangle / N a_1^{(1)} = \varphi_1^{(1)}(\omega)\left[1 + C_C a_2^{(1)}/a_1^{(1)} + C_C C_T \left(a_2^{(2)}/a_1^{(1)} - a_2^{(1)}/a_1^{(1)}\right)\right]. \quad (4)$$

Fig. 1 shows three examples of concentration dependence $\Phi(C_C, C_T)$ for $a_2^{(2)}/a_1^{(1)} = 1$ and a number of different values of relation $a_2^{(1)}/a_1^{(1)}$, namely $a_2^{(1)}/a_1^{(1)} = 3$ for the 1st surface plot, $a_2^{(1)}/a_1^{(1)} = 1$ for the 2nd surface plot, and $a_2^{(1)}/a_1^{(1)} = 0,1$ for the 3D surface plot.

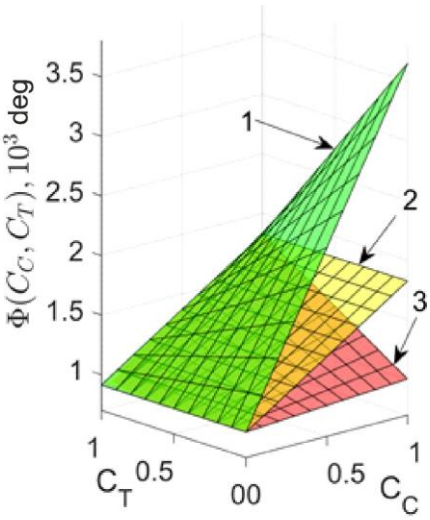

Fig. 1. Concentration dependence of the rotation angle of polarization plane $\Phi(C_C, C_T)$ of elastic wave in a non-ideal one-dimensional superlattice for $a_2^{(2)}/a_1^{(1)} = 1$. The 1st surface corresponds to $a_2^{(1)}/a_1^{(1)} = 3$, the second - to $a_2^{(1)}/a_1^{(1)} = 1$, the 3d - to $a_2^{(1)}/a_1^{(1)} = 0,1$.

The obtained functional dependence $\Phi(C_C, C_T)$ indicates the possibility of controlling the rotation angle of polarization plane by changing composition and widths of constituent layers in the phononic structure. In particular the surface plots of function $\Phi\left(C_C, C_T\right)$ shown in Fig. 1 by and large indicate an increase of the rotation angle with increasing defect concentrations C_C, C_T. It follows from the above calculations that in order to assess the effect of structural defects it is necessary to take into account the dimensional parameters $a_2^{(2)}/a_1^{(1)}$ and $a_2^{(1)}/a_1^{(1)}$.

CONCLUSION

The paper examines the dependence of rotation angle $\Phi\left(\omega\right)$ of elastic wave polarization plane in a one-dimensional superlattice on concentrations C_C, C_T of structural defects formed by random substitutions of the matrix layers with impurity layers of altered compositions (substance) and widths. It is shown that the behavior of $\Phi\left(\omega\right)$ depends on the specific superlattice parameters, on polarization of acoustic waves, as well as on relations of structural parameters $a_2^{(2)}/a_1^{(1)}$, $a_2^{(1)}/a_1^{(1)}$, $a_2^{(1)}/a_1^{(1)}$, which on the whole define the acoustic activity of the overall structure. Our results can serve as a sound theoretical basis for construction of acoustic composite materials suitable for various operative conditions.

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RESUME

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Numerical modeling of the acoustic activity of non-ideal 1D crystalline superlattice

Background: The results obtained earlier by the authors of the study of acoustic excitations in an imperfect 1D superlattice are transferred to similar calculations of the characteristics of the acoustic activity of a phonon crystal of a system of plane-parallel layers with anisotropic impurity layers differing in elastic characteristics.

Materials and methods: Numerical modeling.

Results: The expression found in the work for the specific rotation angle of the plane of polarization of an elastic wave in a non-ideal 1D phonon crystal allows numerical modeling of the concentration dependence of the acoustic activity of complex one-dimensional non-ideal superlattices.

Conclusion: In this paper, within the framework of the virtual crystal approximation, mathematical modeling of the dependence of the specific rotation angle of the plane of polarization of an elastic wave in a non-ideal 1D phonon crystal on the concentration of structural defects with variations in the layers of the model system both in composition and thickness is performed.

The obtained results may be useful in the design of acoustic composite materials used in various operating modes.

РЕЗЮМЕ

Ю. А. Безус, В. В. Румянцев, С. А. Федоров

Численное моделирование акустической активности в неидеальной
1D *кристаллической сверхрешетке*

Предыстория: Полученные авторами ранее результаты исследования акустических возбуждений в несовершенной 1D сверхрешетке перенесены на аналогичные расчеты характеристик акустической активности фононного кристалла - системы плоскопараллельных слоев с анизотропными примесными слоями, отличающимися упругими характеристиками.

Материалы и методы: Численное моделирование.

Результаты: Найденное в работе выражение для удельного угла вращения плоскости поляризации упругой волны в неидеальном 1D фононном кристалле позволяет осуществлять численное моделирование концентрационной зависимости акустической активности сложных одномерных неидеальных сверхрешеток.

Заключение. В работе в рамках приближения виртуального кристалла выполнено математическое моделирование зависимости удельного угла вращения плоскости поляризации упругой волны в неидеальном 1D фононном кристалле от концентрации структурных дефектов при вариации слоев модельной системы как по составу, так и толщине.

Полученные результаты могут оказаться полезными при конструировании акустических композитных материалов, используемых при различных режимах эксплуатации.

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