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Peculiarities of photonic band gap width dependence upon concentration of the admixture layers randomly included in composite material

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Considered is a model of photonic crystalline superlattice as a set of macroscopically homogeneous layers with randomly included extrinsic (with respect to the ideal superlattice) layers of a variable thickness and composition. The polariton spectrum of such a non-ideal superlattice with an arbitrary number of layers per elementary cell obtained within the virtual crystal method is specified for the Si - diamond crystal system. The peculiarities of the band gap width dependence upon concentration of admixture layers and refractive index are considered. The study carried out shows that optical characteristics of a crystalline superlattice may vary significantly due to transformation of its polariton spectrum caused by the presence of admixture layers.

Рассмотрена модель фотонной кристаллической сверхрешетки как системы макроскопически однородных слоев с хаотически внедренными инородными (по отношению к идеальной сверхрешетке) слоями с переменным составом и толщиной. Полученный в приближении виртуального кристалла поляритонный спектр такой неидеальной сверхрешетки с произвольным числом слоев в элементарной ячейке конкретизирован для алмазно-кремниевой системы. Проанализированы особенности зависимости ширины запрещенной зоны и показателя преломления от концентрации примесных слоев. Проведенное исследование указывает на возможность значительных изменений оптических свойств кристаллической сверхрешетки, которые обусловлены трансформацией ее поляритонного спектра в результате присутствия инородных слоев.

Propagation of electromagnetic waves in layered crystalline media draws currently a close attention. In [1-3], the related researches are described carried out on magnetic photonic crystals, while in [4-6], on composite materials based on silicon and liquid crystal. The interest in those objects is due on the one hand to their significance for electronics, and on the other hand, to the advances in technology allowing growth of ultrathin films and periodic structures with controlled characteristics. The general theory of optical waves in anisotropic crystals, including those consisting of macroscopic layers, is well known [7]. A further development of the layered structure theory requires consideration of more complex model systems such as superlattices with layers of variable composition and thickness. The polariton excitation calculation procedure has much in common with consideration of other quasi-particle excitations (electron, phonon, etc.) in solids. A common calculation method of quasi-particle states in unordered media is the virtual crystal approximation (VCA), which consists in replacing the configuration-dependent parameters of the problem Hamiltonian by their configuration-averaged values [8]. It is convenient to study the polariton spectra and corresponding optical characteristics of imperfect superlattices using just that approximation, since it makes it possible to reveal the specific features and the transformations of the elementary excitation spectra due to a change in the concentration of defects in imperfect crystals.

In this work, a photonic crystalline superlattice is modeled as a set of macroscopically homogeneous layers with randomly included extrinsic (with respect to the ideal superlattice) layers of variable thickness and composition. The polariton spectrum of a non-ideal superlattice with an arbitrary number of layers per unit cell obtained within the VCA is concretized for the diamond-silicon crystal system. Dependence of the band gap width and refractive index peculiarities on concentration of admixture layers is analyzed.

Dielectric $\hat{\varepsilon}(\vec{r})$ and magnetic $\hat{\mu}(\vec{r})$ permeabilities which define optical characteristics of a periodic medium should satisfy the periodic boundary conditions:

$$\hat{\varepsilon}(x,y,z)=\hat{\varepsilon}(x,y,z+d),\ \hat{\mu}(x,y,z)=\hat{\mu}(x,y,z+d), \tag{1}$$

where $d=\sum_{j=1}^{\sigma}a_j$ is the superlattice period; σ, the number of layers per unit cell; a_j, the thickness values of the layers forming a one-dimensional chain of elements oriented along the z axis. The material tensors $\hat{\varepsilon}$ and $\hat{\mu}$ of a crystalline superlattice with an arbitrary number of layers σ have the following form in the coordinate representation:

$$\begin{pmatrix}\hat{\varepsilon}(z)\\ \hat{\mu}(z)\end{pmatrix}=\sum_{n,\alpha}\begin{pmatrix}\hat{\varepsilon}_{n\alpha}\\ \hat{\mu}_{n\alpha}\end{pmatrix}\left\{\theta\left[z-(n-1)d-\left(\sum_{j=1}^{\alpha}a_{nj}-a_{n\alpha}\right)\right]-\theta\left[z-(n-1)d-\sum_{j=1}^{\alpha}a_{nj}\right]\right\}. \tag{2}$$

In Eq. (2), $\theta(z)$ is the Heaviside function, $n=\pm1,\ \pm2,\ ...$ is the number of a one-dimensional crystal cell, index $\alpha=1,2,...,\sigma$ designates the cell elements. When a imperfect system is considered where the disordering is connected with variation of the composition (rather than of the thickness) of admixture layers, then $a_{n\alpha}\equiv a_\alpha$. Within our model, the configuration-dependent tensors $\hat{\varepsilon}_{n\alpha}$, $\hat{\mu}_{n\alpha}$ are expressed in terms of random quantities $\eta_{n\alpha}^{\nu}$ ($\eta_{n\alpha}^{\nu}$=1 if the $\nu(\alpha)$-th sort of layer is in the $(n\alpha)$-th site of the crystalline chain, $\eta_{n\alpha}^{\nu}$=0 otherwise):

$$\begin{pmatrix}\hat{\varepsilon}_{n\alpha}\\ \hat{\mu}_{n\alpha}\end{pmatrix}=\sum_{\nu(\alpha)}\begin{pmatrix}\hat{\varepsilon}_{\alpha}^{\nu(\alpha)}\\ \hat{\mu}_{\alpha}^{\nu(\alpha)}\end{pmatrix}\eta_{n\alpha}^{\nu(\alpha)}. \tag{3}$$

Calculation of a polariton spectrum for an imperfect superlattice is realized within the VCA (similarly to the solid quasi-particle approach) via the following replacement: $\hat{\varepsilon}\to\langle\hat{\varepsilon}\rangle$, $\hat{\mu}\to\langle\hat{\mu}\rangle$ (angular parentheses designate the procedure of configuration averaging). In this case, it follows from Eq. (3) and [8]:

$$\begin{pmatrix}\langle\hat{\varepsilon}_{n\alpha}\rangle\\ \langle\hat{\mu}_{n\alpha}\rangle\end{pmatrix}=\sum_{\alpha,\nu(\alpha)}\begin{pmatrix}\hat{\varepsilon}_{\alpha}^{\nu(\alpha)}\\ \hat{\mu}_{\alpha}^{\nu(\alpha)}\end{pmatrix}C_{\alpha}^{\nu(\alpha)}, \tag{4}$$

where $C_{\alpha}^{\nu(\alpha)}$ is the concentration of the $\nu(\alpha)$-th sort of admixture layer in the α-th sublattice; $\sum_{\nu(\alpha)}C_{\alpha}^{\nu(\alpha)}=1$, the normalization condition. It follows from Eq. (2) that the Fourier-amplitudes $\hat{\varepsilon}_l$, $\hat{\mu}_l$ and the averaged dielectric $\langle\hat{\varepsilon}_{n\alpha}\rangle$ and magnetic $\langle\hat{\mu}_{n\alpha}\rangle$ permeabilities of layers (4) are related as

$$\begin{pmatrix}\hat{\varepsilon}_l \\ \hat{\mu}_l\end{pmatrix} = -\frac{i}{2\pi l}\sum_{\alpha}\begin{pmatrix}\langle\hat{\varepsilon}_{n\alpha}\rangle \\ \langle\hat{\mu}_{n\alpha}\rangle\end{pmatrix}\left\{\exp\left(i\frac{2\pi}{d}l\sum_{j=1}^{\alpha}a_j\right)-\exp\left[i\frac{2\pi}{d}l\left(\sum_{j=1}^{\alpha}a_j-a_\alpha\right)\right]\right\}. \quad (5)$$

For an imperfect superlattice where the disordering is connected with variation of the thickness (rather than of the composition) of admixture layers, we have to use the following procedure of configuration averaging: $a_{n\alpha} \to a_\alpha\left\{C_\alpha^{\upsilon(\alpha)}\right\}$, $d \to d\left\{C_\alpha^{\upsilon(\alpha)}\right\}$ (here, $C_\alpha^{\upsilon(\alpha)}$ is the admixture layer concentration of the $\nu(\alpha)$-th sort thickness in the α-th sublattice) and $\hat{\varepsilon}_{n\alpha} \equiv \hat{\varepsilon}_\alpha$, $\hat{\mu}_{n\alpha} \equiv \hat{\mu}_\alpha$.

Since the configurational averaging "restores" the translational symmetry of a crystalline system, in the considered case of imperfect superlattice, the "acquired" translational invariance of the one-dimensional chain allows us to present the Maxwell equations (assuming the harmonic time dependence of the electric and magnetic field strengths $\vec{E}(\vec{r},\omega), \vec{H}(\vec{r},\omega)$) in the form:

$$\nabla\times\vec{E}(\vec{r},\omega) = \frac{i\omega}{c}\langle\hat{\mu}(z)\rangle\cdot\vec{H}(\vec{r},\omega),\ \nabla\times\vec{H}(\vec{r},\omega) = -\frac{i\omega}{c}\langle\hat{\varepsilon}(z)\rangle\cdot\vec{E}(\vec{r},\omega). \quad (6)$$

Hence, according to the Floquet theorem, the Fourier-amplitudes $\vec{f}_{K,p}^{(E,H)}$ of the electric and magnetic field strengths satisfy the following relation:

$$\left[\vec{\beta}+\left(K+p\frac{2\pi}{d}\right)\vec{e}_z\right]\times\begin{pmatrix}\vec{f}_{K,p}^{(H)} \\ \vec{f}_{K,p}^{(E)}\end{pmatrix} = \frac{\omega}{c}\begin{bmatrix}-\sum_l\hat{\varepsilon}_l\cdot\vec{f}_{K,p-l}^{(E)} \\ \sum_l\hat{\mu}_l\cdot\vec{f}_{K,p-l}^{(H)}\end{bmatrix}. \quad (7)$$

Here, $\vec{\beta}$ is an arbitrary planar (in the XOY plane) wave vector; $\vec{e}_z$, the unit vector along the z axis; $\vec{K} = (0,0,K)$ is the Bloch vector. The system (7) defines the normal modes of electromagnetic waves being propagated in the considered "periodic" medium. Furthermore, we assume (like in [6]) that K are close to the value defined by the Bragg's condition: $\left|K-\frac{2\pi}{d}\right| \approx K$, $c^2K^2 \approx \omega^2\varepsilon_0$. This case corresponds to a resonance between the plane wave components $\vec{f}_{K,p}^{(E,H)}$ at $p = 0, -1$ (these terms dominate in the system (7)). After eliminating the $\vec{f}^{(H)}$ variables, Eqs. (7) with respect to $\vec{f}^{(E)}$ take the form:

$$\begin{bmatrix}K^2-\frac{\omega^2}{c^2}\varepsilon^{(0)} & -\frac{\omega^2\varepsilon^{(1)}}{c^2} \\ -\frac{\omega^2\varepsilon^{(-1)}}{c^2} & \left(K-\frac{2\pi}{d}\right)^2-\frac{\omega^2}{c^2}\varepsilon^{(0)}\end{bmatrix}\begin{pmatrix}f_{K,0}^{(E)} \\ f_{K,-1}^{(E)}\end{pmatrix} = 0, \quad (8)$$

where $\varepsilon_{l=0} \equiv \varepsilon^{(0)}$, $\varepsilon_{l=-1} \equiv \varepsilon^{(-1)}$. Putting the determinant of the system (8) equal to zero, we obtain the dispersion relations $\omega_\pm = \omega\ (K)$. Two roots of this equation $\omega_\pm$ define the boundaries of the spectral band: at frequencies $\omega_-(K) < \omega < \omega_+(K)$ (band gap), the roots are complex and electromagnetic waves decay (Bragg's reflection); frequencies $\omega < \omega_-$, $\omega > \omega_+$ correspond to propagating waves.

For simplicity, we shall restrict our study to the case of light propagating along the z-axis ($\vec{\beta} = 0$) in a nonmagnetic Si - diamond crystal system ($\hat{\mu} = \hat{I}$ is the unit matrix). We consider the layers to be macroscopically homogeneous and isotropic ($\varepsilon_{ij} = \varepsilon\delta_{ij}$). Below, considered is the case of

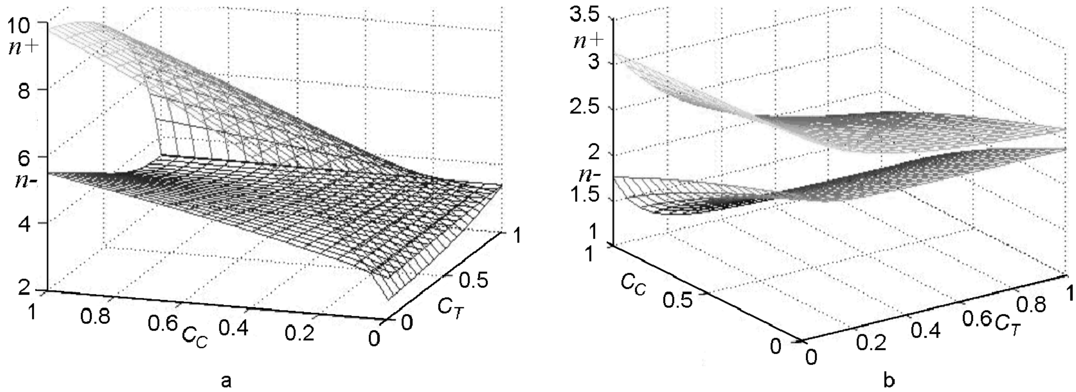

Fig.1. Refractive index $n_+, n_-\ (C_C, C_T)$ of the composite superlattice (with alternating silicon and diamond layers) vs. the concentrations of admixture layers of variable thickness and composition for $a_1^{(1)}/a_2 = 1$: (a) $a_1^{(2)}/a_1^{(1)} = 0.001$, $\varepsilon_1^{(2)}/\varepsilon_1^{(1)} = 20$; (b) $a_1^{(2)}/a_1^{(1)} = 10$, $\varepsilon_1^{(2)}/\varepsilon_1^{(1)} = 0.2$.

admixture layers of a variable thickness and composition only in Si-sublattice. The concentration, dielectric permeability, and thickness of the base material in the first and the second sublattice are denoted by $C_1^{(1)}, \varepsilon_1^{(1)}, a_1^{(1)}$ and $C_2^{(1)}, \varepsilon_2^{(1)}, a_2^{(1)}$ ($\varepsilon_1^{(1)} = 5.7$, $\varepsilon_2^{(1)} \equiv \varepsilon_2 = 11.7$), respectively. For admixture layers, those quantities are denoted by $C_{1C}^{(2)}$ (for the variable composition) and $C_{1T}^{(2)}$ (for the variable thickness) as well as $\varepsilon_1^{(2)}, a_1^{(2)}$ (there are no admixtures in the Si-sublattice). Simple transformations (taking into account that $\left|\varepsilon^{(-1)}\right| = \left|\varepsilon^{(1)}\right|$) result in the following relations for the refractive index $n_\pm \equiv cK/\omega_\pm$ of the studied system:

$$n_\pm^2\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right) = \varepsilon^{(0)}\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right) \pm \left|\varepsilon^{(1)}\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right)\right| \cong \varepsilon^{(0)}\left[1 \pm \frac{\Delta\omega_1\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right)}{\omega}\right]. \quad (9)$$

Here $\varepsilon^{(0)}$ and $\varepsilon^{(1)}$ can be expressed as:

$$\varepsilon^{(0)} = \varepsilon_2(1 + f_C f_T)/(1 + f_T) \quad (10)$$

$$\varepsilon^{(1)} = \frac{\varepsilon_2}{\pi}|1 - f_C| Sin\frac{\pi f_T}{1 + f_T}. \quad (11)$$

The functions $f_C = \left[1 - C_{1C}^{(2)}\left(1 - \varepsilon_1^{(2)}/\varepsilon_1^{(1)}\right)\right]\varepsilon_1^{(1)}/\varepsilon_2$ and $f_T = \left[1 - C_{1T}^{(2)}\left(1 - a_1^{(2)}/a_1^{(1)}\right)\right]a_1^{(1)}/a_2$ depend on the concentration of admixture layers, their relative thickness and dielectric permeability. Hence, the lowest photonic band gap width is $\Delta\omega_1 = |\omega_+ - \omega_-|$, $\Delta\omega_1/\omega \cong (n_+^2 - n_-^2)/2\varepsilon^{(0)}$. It follows from Eq. (9) that the quantity $\Delta\omega_1$ is determined by the corresponding coefficient of the Fourier expansion (5), which in this case is $\left|\varepsilon^{(1)}\right|$. In [6, 7], it was shown that the band gaps of higher orders are defined as well by corresponding Fourier-coefficients of the dielectric permeability.

Fig. 1 shows the concentration dependence of the refractive index $n_\pm \equiv cK/\omega_\pm$ for the studied composite superlattice. It is seen that the corresponding surfaces are of complex shape depending on the dielectric permeability of both admixture layers and its thicknesses. In Fig. 2, the lowest energy photonic gap width is plotted vs. the concentrations $C_{1C}^{(2)} \equiv C_C$, $C_{1T}^{(2)} \equiv C_T$ of admixture lay-

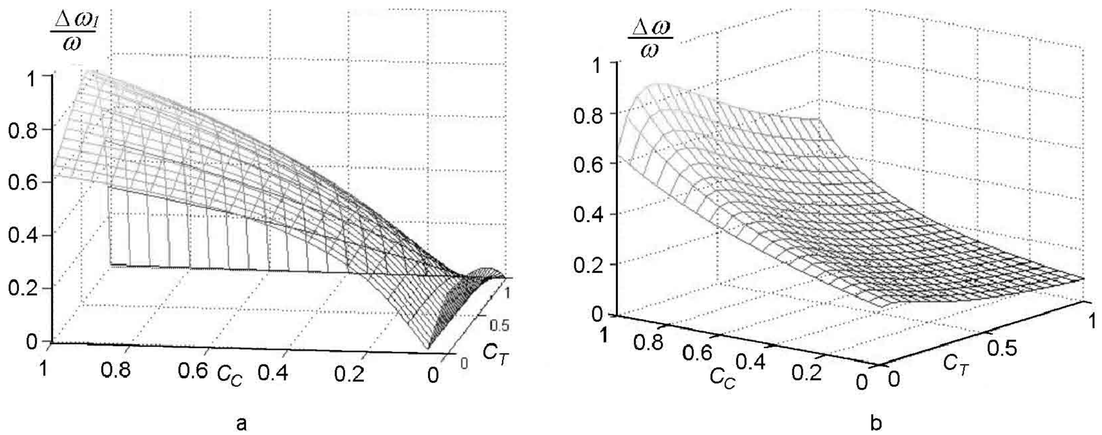

Fig. 2. Relative width of the lowest photonic band gap $\Delta\omega_1/\omega$ of the composite superlattice (with alternating silicon and diamond layers) vs. the concentrations of admixture layers of variable thickness and composition for $a_1^{(1)}/a_2 = 1$: (a) $a_1^{(2)}/a_1^{(1)} = 0.001$, $\varepsilon_1^{(2)}/\varepsilon_1^{(1)} = 20$; (b) $a_1^{(2)}/a_1^{(1)} = 10$, $\varepsilon_1^{(2)}/\varepsilon_1^{(1)} = 0.2$.

ers for a superlattice with alternating silicon and diamond layers. The energy gap $\Delta\omega_1$ is zeroed at $|1-f_C|Sin\frac{\pi f_T}{1+f_T} = 0$ for the case a in Fig. 2.

Thus, description of the polariton spectrum transformation in a sufficiently simple superlattice using VCA is the first step in the study of imperfect systems. Investigation of polariton spectra properties and the related physical quantities (density of elementary excitation states, characteristics of the normal electromagnetic waves, etc.) in more complex systems requires application of more complex methods, e.g., the method of coherent (one- or multi-site) potential [8], the averaged T-matrix method [9] and their numerous modifications used for various particular problems. As a whole, the study carried out in this work shows that optical characteristics of a crystalline superlattice specified by transformation of its polariton spectrum resulting from the presence of admixture layers, may be altered significantly.

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Особливості залежності величини фотонної енергетичної щілини композитного матеріалу від концентрації хаотично введених домішкових шарів

В.В.Румянцев, С.А.Федоров, Е.Я.Штаєрман

Розглянуто модель фотонної кристалічної супергратки як системи макроскопічно однорідних шарів з хаотично введеними чужорідними (відносно ідеальної супергратки) шарами змінного складу та товщини. Одержаний у наближенні віртуального кристалу поляритонний спектр такої неідеальної супергратки з довільною кількістю шарів в елементарній чарунці конкретизовано для алмазно-кремнієвої системи. Проаналізовано особливості особливості залежності ширини забороненої зони та показника заломлення світла від концентрації домішкових шарів. Проведене дослідження вказує на можливість значних змін оптичних властивостей кристалічної супергратки, які обумовлені трансформацією її поляритонного спектру внаслідок присутності чужорідних шарів.