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Peculiarities of band gap width dependence upon concentration of the admixture strips randomly included in quasi-two-dimensional photonic crystal

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The propagation peculiarities of an electromagnetic excitation localized in a nonideal quasi-two-dimensional $Si/SiO_2/GaAs$ photonic crystal that constitutes a topologically ordered set of strips with a random number of defect strips is numerically simulated within the virtual crystal approximation. The defect strips differ from the basic ones (for an ideal periodic structure) in the composition. The peculiarities of the lowest photonic band gap dependence upon concentration of admixture strips are considered. The study has shown that optical characteristics of the nonideal $Si/SiO_2/GaAs$ striped film may vary due to transformation of its polariton spectrum caused by the presence of admixture strips.

В рамках приближения виртуального кристалла численно моделируются особенности распространения электромагнитного возбуждения, локализованного в неидеальном квазидвумерном $Si/SiO_2/GaAs$ фотонном кристалле, который представляет собой топологически упорядоченную совокупность полос, содержащую произвольное число полос-дефектов. Дефектные страйпы отличаются от базисных страйпов (идеальной периодической структуры) по составу. Рассматриваются особенности зависимости ширины нижайшей фотонной щели от концентрации примесных страйпов. Выполненное исследование показывает, что оптические характеристики неидеальной полосчатой $Si/SiO_2/GaAs$ пленки могут изменяться вследствие трансформации поляритонного спектра из-за наличия примесных страйпов.

1. Introduction

The investigations in electromagnetic excitation propagation in thin films and layered crystalline systems are topical due to the needs of semiconductor electronics in quasi-two-dimensional objects with specified structure and by the advance in quasi-two-dimensional electrodynamics [1-6]. There is a considerable success in the study of multilayer systems, in particular, of magnetic photonic crystals [3, 4] and composite materials based on silicon and liquid crystals (see [1, 2, 7] and references therein). Before [6, 8], we have studied the propagation of electromagnetic waves localized in a thin homogeneous film and derived the dispersion laws that determine the relevant integral optical characteristics. At the same time, the recent progress in nanotechnology and photonics [7-12] as well as the need in ultrathin composite materials stimulate the investigation of more complex quasi-two-dimensional structures than those studied in [6, 8]. This investigation can be most easily performed for thin films that consist of strips that differ from each other both in the composition and in the thickness. In this case, the calculation methods developed previously in [13] for the concentration dependence of polariton spectra can be used directly to calculate the corresponding excitations. In this work, we have studied the propagation of electromagnetic excitation localized in a nonideal quasi-two-dimensional system which, in a general case, is a topologically ordered ensemble of strips with a random number of defect strips. In these systems, the defect strips may differ from the basic ones (for an ideal periodic structure) in both the composition and thickness. These systems can be numerically simulated in some approximations; in this study, we use the virtual crystal approximation (VCA). The VCA [14] consists in the replacement of the configuration-dependent parameters of the problem Hamiltonian by their configuration-averaged values. The nonideal Si/SiO_2 film with randomly included admixture strips of variable thickness was studied in [15]. In this work, we study the concentration dependence of the lowest photonic band gap of a striped quasi-two-dimensional $Si/SiO_2/GaAs$ film (the 1D-superlattice having three elements per unit cell) which contains defect strips of variable composition.

2. Model

Interaction of an electromagnetic field with the film of thickness d can only be macroscopically described basing on modeling concepts, as in [6], for example. Let us consider the propagation of a plane electromagnetic wave with a frequency ω and a wave vector $\vec{q}$ in the plane of a thin plate according to the phenomenological approach [15] without concretization of the material microscopic structure. The long-wavelength field of wavelength $\lambda \sim d$ outside the film is independent of the crystal structure characteristics and on the polarization distribution along the film thickness. As is shown in [15], it is described by the D'Alembert equation, and the sole nontrivial information on the the film effect on the electromagnetic field consists in the boundary conditions which couple the field amplitudes at both film sides. The latter circumstance allows us to use the continuous approximation to find the exciting field $\vec{E}_{in}$ and the field-induced polarization of the plane layer. The material relations take the form

$$\begin{pmatrix} \vec{\Pi} \\ \vec{m} \end{pmatrix} = \hat{\chi}^{E,H} \cdot \begin{pmatrix} \vec{E}_{in} \\ \vec{H}_{in} \end{pmatrix} . \quad (1)$$

Here, $\vec{\Pi}$ and $\vec{m}$ are the surface densities of the electric and magnetic dipole moments, respectively. The tensor function of the film response in our quasi-two-dimensional case is

$$\chi_{ij}^{E,H}(\omega,\vec{q}) = \left(\delta_{ij} - n_i n_j\right)\chi_t^{E,H}(\omega,\vec{q}) + n_i n_j \chi_n^{E,H}(\omega,\vec{q}) .$$

It has the dimensionality of length.

The joint solution for the system of equations relating to the boundary conditions and the material relations (1) yields the dispersion laws of exciton polaritons of the α, β and n polarizations localized in the film. Here $\vec{n} \parallel z$ is the vector normal to the film, $\vec{\beta} = \vec{q}/q$ ($\vec{\beta} \mid\mid x$) and $\vec{\alpha} = \vec{n} \times \vec{\beta}$ (see Fig. 1).

Let us consider the propagation of an electromagnetic wave of the n polarization in the field frequency region far from magnetic dipole transitions. This limitation allows us to make the redesignation $\hat{\chi}^{E,H} \to \hat{\chi}^{E} \equiv \hat{\chi}$. Thus, in a general case of an inhomogeneous film, the material relation takes the form

$$\vec{E}_{in}(\vec{q},\omega) = \int d\vec{k}\,\hat{\chi}^{-1}\left(\vec{q}-\vec{k}\right)\cdot\vec{\Pi}\left(\vec{k},\omega\right) = S_n(\vec{q},\omega)\cdot\vec{\Pi}(\vec{q},\omega) . \quad (2)$$

As shown in [6], $S_n(\vec{q},\omega) = q^2\left(q^2 - \omega^2/c^2\right)^{-1/2}$.

We consider the film as a topologically ordered (periodic) set of strips, i.e., a one-dimensional superlattice composed of compositionally homogeneous elements (strips). A cell s of the 1D super-

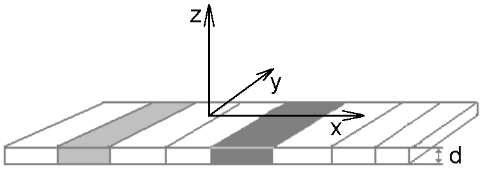

Fig. 1. 1D superlattice composed of compositionally homogeneous elements (strips).

lattice may include an arbitrary number of elements α of thickness $a_{s\alpha}$, each being oriented perpendicular to the *x* axis (Fig. 1).

Assuming that the polarizability of the ($s\alpha$) strip is $\chi_{s\alpha}$, we can write the film polarizability in the coordinate representation:

$$\chi(x) = \sum_{s,\alpha} \chi_{s\alpha} \left\{ \theta\left[x - (s-1)L - \left(\sum_{j=1}^{\alpha} a_{sj} - a_{s\alpha} \right) \right] - \theta\left[x - (s-1)L - \sum_{j=1}^{\alpha} a_{sj} \right] \right\}. \quad (3)$$

In Eq. (3), $\theta(x)$ is the Heaviside function, $s = \pm 1, \pm 2, ...$ is the number of a one-dimensional crystal cell, index $\alpha = 1,2,...,\sigma$ designates the elements of the cell. Here, *L* is the lattice constant; for the ideal 1D structure, $\chi(x) = \chi(x+L)$. The latter allows us to describe the surface density vector of the electric dipole moment using the Floquet theorem

$$\Pi(x) = f_K(x)\exp(-iKx) = \exp(-iKx)\sum_p f_{K,p} \exp\left(ip\frac{2\pi}{L}x \right), \quad (4)$$

the Bloch vector $\vec{K} = (K,0,0)$ being directed along the *x* axis. Thus, since the Fourier representation $\Pi(x)$, due to (4), has the form $\Pi(q) = \sum_p f_{K,p}\delta\left(q + K - \frac{2\pi}{L}p \right)$, we obtain from (2) the following system of equations with respect to the Fourier amplitude $f_{K,p}$:

$$S_n(K,\omega) f_{K,p} = \sum_l \left(\chi^{-1} \right)_l f_{K,p-l} \,. \quad (5)$$

The object of this study is a nonideal 1D superlattice. The imperfection in our case may be caused by variations in the composition of strips. We will determine the configuration disorder of strips using the random value $\eta_{s\alpha}^{\nu}$: $\eta_{s\alpha}^{\nu} = 1$ if the $\nu(\alpha)$-type of strips lies in the $s\alpha$ site and the value $\eta_{s\alpha}^{\nu} = 0$ in the opposite case. In this case, the configuration-dependent value is the film polarizability

$$\chi_{s\alpha} = \sum_{\nu(\alpha)} \chi_{\alpha}^{\nu(\alpha)} \eta_{s\alpha}^{\nu(\alpha)} \,. \quad (6)$$

Similarly to the solid quasi-particle approach, calculation of a polariton spectrum for the imperfect superlattice is realized within the VCA which is implemented through the replacement $\chi \to \langle \chi \rangle$, where angular parentheses mean the configurational averaging procedure. In addition, from Eq. (6) we have the relation

$$\langle \chi_{s\alpha} \rangle = \sum_{\alpha,\nu(\alpha)} \chi_{\alpha}^{\nu(\alpha)} C_{\alpha}^{\nu(\alpha)} , \quad (7)$$

where $C_{\alpha}^{\nu(\alpha)}$ is the concentration of the $\nu(\alpha)$-th kind of admixture strip in the α-th sublattice. Here a simple normalization condition $\sum_{\nu(\alpha)} C_{\alpha}^{\nu(\alpha)} = 1$ holds true. It follows from Eq. (3) that the Fourier amplitudes of the inverse polarizability $\left(\chi^{-1} \right)_l$ and the averaged value $\left\langle \left(\chi^{-1} \right)_{s\alpha} \right\rangle$ of strips (7) are related as

$$\left(\chi^{-1} \right)_l = -\frac{i}{2\pi l} \sum_{\alpha} \left\langle \left(\chi^{-1} \right)_{s\alpha} \right\rangle \left\{ \exp\left(i\frac{2\pi}{L} l \sum_{j=1}^{\alpha} a_j \right) - \exp\left[i\frac{2\pi}{L} l \left(\sum_{j=1}^{\alpha} a_j - a_{\alpha} \right) \right] \right\}. \quad (8)$$

The configurational averaging "restores" the translational symmetry of the crystalline system. The normal modes of electromagnetic waves propagating in this "periodic" structure are defined by the system of Eqs. (5). For simplicity, we assume from here on that the Bloch vector K value is close to the values defined by the Bragg condition [16]. In this case, when the main terms of (5) are $f_{K,p}$ at p = 0, –1, which corresponds to the resonance between these components of the plane waves, the system of equations takes the form

$$\begin{bmatrix} S_n(\omega,K)-\left(\chi^{-1}\right)_0 & -\left(\chi^{-1}\right)_1 \\ -\left(\chi^{-1}\right)_{-1} & S_n(\omega,K-2\pi/L)-\left(\chi^{-1}\right)_0 \end{bmatrix}\cdot\begin{pmatrix} f_{K,0} \\ f_{K,-1}\end{pmatrix}=0\,. \tag{9}$$

The dispersion relations $\omega_{\pm}=\omega(K)$ follow from the equality of the system (9) determinant to zero.

3. Results and discussion

To specify the results, let us consider the propagation of an electromagnetic excitation in an imperfect quasi-two-dimensional 1D superlattice with three elements (strips) per cell, namely, with the first strip of silicon ($\varepsilon_1=11{,}7$), second strip of SiO_2 ($\varepsilon_2=3{,}7$) and the third strip of GaAs ($\varepsilon_3=11$). Note that the approximation of the film as a thin isotropic plate of the thickness d makes it possible to describe the relation between $\chi_{nn}\equiv\chi$ components of the polarizability tensor and the plate permittivity ε as

$$\chi=d\frac{\varepsilon-1}{4\pi\varepsilon}\,. \tag{10}$$

We denote the concentration and thickness of the basic material layer in the first, second and third sublattices as $C_1^{(1)},a_1,\varepsilon_1^{(1)}\equiv\varepsilon_1$; $C_2^{(1)},a_2,\varepsilon_2^{(1)}\equiv\varepsilon_2$ and $C_3^{(1)},a_3,\varepsilon_3^{(1)}\equiv\varepsilon_3$, respectively, while the corresponding parameters of impurity strips (strips of a different composition), as $C_2^{(2)},\varepsilon_2^{(2)}$ and $C_3^{(2)},\varepsilon_3^{(2)}$ ($C_1^{(2)}=0$). Simple calculations taking into account (8)-(9) and the equality $\left|\left(\chi^{-1}\right)_{-1}\right|=\left|\left(\chi^{-1}\right)_1\right|$ yield the following expression for the lowest photonic band gap width $\Delta\omega$ of the system studied:

$$\Delta\omega=\left|\omega_+(K_{\min})-\omega_-(K_{\max})\right|\cong c\frac{\left|\left(\chi^{-1}\right)_1+\left(\chi^{-1}\right)_0\right|}{2\pi} \tag{11}$$

($|K|\le\pi/L$) and allow us to plot the dependences $\Delta\omega\left(C_2^{(2)},C_3^{(2)}\right)$ (Fig. 2). Here the values of $\left(\chi^{-1}\right)_0$ and $\left(\chi^{-1}\right)_1$ are found from the relations:

$$\varepsilon_{(0)}=(\varepsilon_1a_1+\varepsilon_2a_2f_2+\varepsilon_3a_3f_3)/L\,,$$

$$\begin{aligned}|\varepsilon_{(1)}|=\frac{1}{\pi\sqrt{2}}\{[\varepsilon_1]^2\left(1-Cos\frac{2\pi a_1}{L}\right)+[\varepsilon_2f_2]^2\left(1-Cos\frac{2\pi a_2}{L}\right)+\\ +[\varepsilon_3f_3]^2\left(1-Cos\frac{2\pi a_3}{L}\right)+\varepsilon_1\varepsilon_2f_2\left(-1+Cos\frac{2\pi a_1}{L}+Cos\frac{2\pi a_2}{L}-Cos\frac{2\pi a_3}{L}\right)+\\ +\varepsilon_1\varepsilon_3f_3\left(-1+Cos\frac{2\pi a_1}{L}+Cos\frac{2\pi a_3}{L}-Cos\frac{2\pi a_2}{L}\right)+\\ +\varepsilon_2\varepsilon_3f_2f_3\left(-1+Cos\frac{2\pi a_2}{L}+Cos\frac{2\pi a_3}{L}-Cos\frac{2\pi a_1}{L}\right)\}^{1/2}\end{aligned} \tag{12}$$

using Eq. (10) and the following expressions:

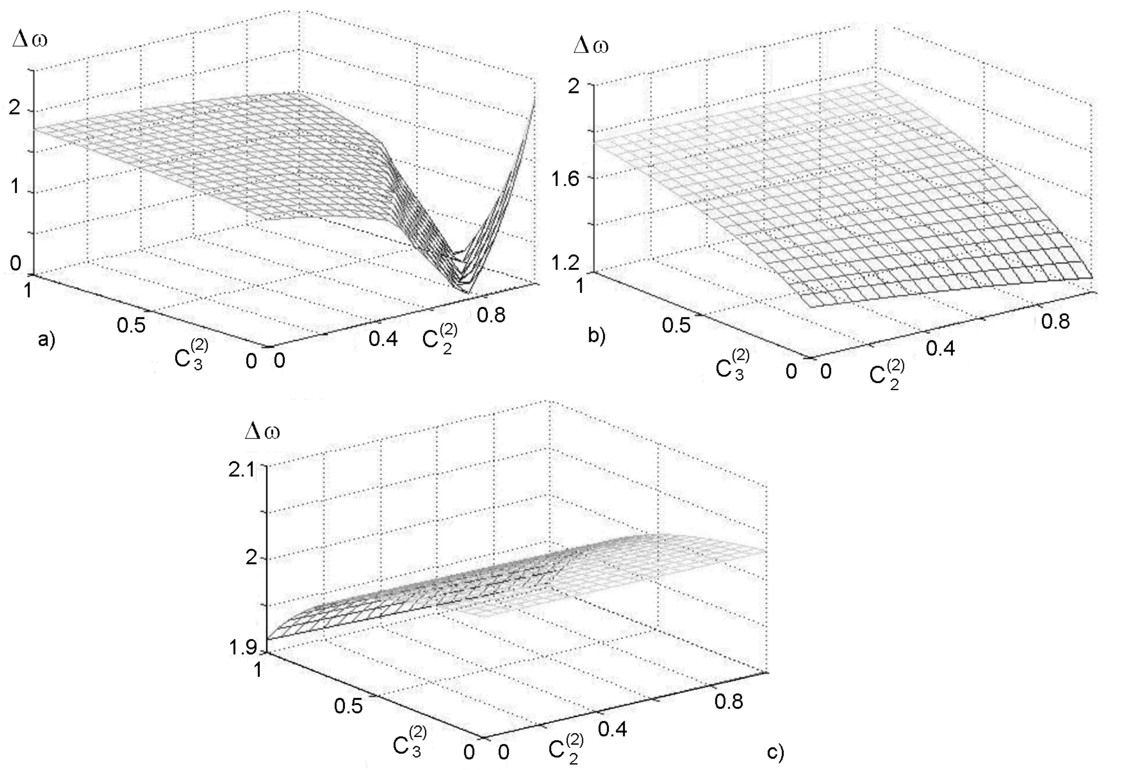

Fig. 2. Concentration dependences $\Delta\omega\left(C_2^{(2)}, C_3^{(2)}\right)$ of imperfect quasi-two-dimensional $Si/SiO_2/GaAs$ superlattice for different relative thickness of strips and composition of randomly included admixture strips:
a) $a_1/L = 0.5,\ a_2/L = 0.28, a_3/L = 0.22,\ \varepsilon_2^{(2)}/\varepsilon_2^{(1)} = 0.7,\ \varepsilon_3^{(2)}/\varepsilon_3^{(1)} = 1.1$;
b) $a_1/L = 0.8,\ a_2/L = 0.1, a_3/L = 0.1,\ \varepsilon_2^{(2)}/\varepsilon_2^{(1)} = 0.7,\ \varepsilon_3^{(2)}/\varepsilon_3^{(1)} = 1.3$;
c) $a_1/L = 0.49,\ a_2/L = 0.1, a_3/L = 0.41,\ \varepsilon_2^{(2)}/\varepsilon_2^{(1)} = 0.7,\ \varepsilon_3^{(2)}/\varepsilon_3^{(1)} = 0.7$;
$\Delta\omega$ is given in units of $2c/d$ (c is the speed of light and d is the film thickness).

$$a_1 + a_2 + a_3 = L\ ,$$

$$f_2 = 1 - C_2^{(2)}\left(1 - \frac{\varepsilon_2^{(2)}}{\varepsilon_2^{(1)}}\right),\ f_3 = 1 - C_3^{(2)}\left(1 - \frac{\varepsilon_3^{(2)}}{\varepsilon_3^{(1)}}\right). \tag{13}$$

Fig. 2 (cases a-c) shows the concentration dependence $\Delta\omega\left(C_2^{(2)}, C_3^{(2)}\right)$ of the studied nonideal quasi-two-dimensional $Si/SiO_2/GaAs$ composite superlattice for different relative thickness and compositions of strips. It is clearly seen that the shape of corresponding surfaces depends considerably both on thickness of strips and composition of randomly included admixture strips. For some parameter values, the energy gap of a quasi-two-dimensional $Si/SiO_2/GaAs$ photonic crystal may be equal to zero (case a), but for another ones, it changes monotonously (cases b and c).

4. Conclusion

Our results show that the optical characteristics of an imperfect quasi-two-dimensional 1D superlattice may be altered significantly owing to transformation of their polariton spectrum resulted a presence of admixture strips. The propagation of electromagnetic excitation in a nonideal 1D superlattice has been studied using a rather simple model within the virtual crystal approximation. To study the specific features of the polariton spectrum (and the physical values defined by this spectrum, for example, the density of elementary excitation states and the characteristics of normal electromagnetic waves) of more complex objects, it is necessary (depending on the problem stated) to invoke more complex methods, namely, the coherent (one- or many-site) potential method [17], the averaged T-matrix method, and their modifications.

The plotted dependence $\Delta\omega\left(C_2^{(2)}, C_3^{(2)}\right)$ (Fig. 2) proves that the concentration dependence for the ternary systems considered above differs for different relative composition of strips. The case of nonideal multistriped quasi-two-dimensional systems with a larger number of sublattices and components of alien strips supposes a wide variety of specific behaviors of the photonic gap width. This circumstance extends considerably the promises of modeling composite materials with predetermined properties.

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Особливості залежності ширини забороненої зони квазідвовимірного фотонного кристала від концентрації хаотично впроваджених домішкових страйпів

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

В рамках наближення віртуального кристала виконано чисельне моделювання особливостей поширення електромагнітного збудження, локалізованого у неідеальному квазідвовимірному фотонному кристалі $Si/SiO_2/GaAs$, який являє собою топологічно впорядковану сукупність смуг (страйпів), яка містить довільне число смуг-дефектів. Дефектні страйпи відрізняються від базових страйпів (ідеальної періодичної структури) своїм складом. Розглянуто особливості залежності ширини найнижчої фотонної щілини від концентрації домішкових страйпів. Виконане дослідження свідчить, що оптичні характеристики неідеальної смужкуватої плівки $Si/SiO_2/GaAs$ можуть змінюватися внаслідок трансформації поляритонного спектра, спричиненої присутністю домішкових страйпів.