EFFECT OF RANDOM VARIATIONS OF BOTH COMPOSITION AND THICKNESS OF 1D PHOTONIC CRYSTAL WITH ADMIXTURE PLASMA LAYERS ON PHOTONIC BAND GAP

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Propagation of an electromagnetic excitation in composite materials - nonideal 1D photonic crystals (such as a Si/liquid crystal and SiO_2/Si) which are a topologically ordered sets of layers with a random number of admixture plasma layers - is numerically simulated within the virtual crystal approximation. Peculiarities of the dependence of photonic band gap width on admixture plasma layers concentration have been studied. The results are the evidence of substantial photon mode spectrum reconstruction caused by presence of defect layers in nonideal superlattices which differ from the basic ones in both the composition and thickness.

Introduction

Propagation of electromagnetic waves in layered crystalline ambiences is currently drawing a close attention. Ref. [1] gives the account of the related research carried out for photonic crystals based on silicon and liquid crystal (LC), Ref. [2] - for composite materials containing the plasma layers. The interest towards these objects is on one hand due to their significance for electronics, and on the other hand due to the advance of technology allowing growth of ultrathin films and periodic structures with controlled characteristics.

There are numerous theoretical and experimental studies exciton-like excitations in ideal dielectric superlattices. A general theory of optical waves in anisotropic crystals, including those, formed of macroscopic layers, is discussed in Ref. [3]. The further development of the theory of layered structures requires considering more complex models like superlattices with randomly included admixture layers. A better understanding of how the optical properties of such systems depend on concentration of admixture layers gives basis for modeling and constructing the layered materials with prescribed characteristics.

The method applied for calculating polariton excitation spectra is rather similar to the ones, used in cases of other quasiparticle excitations, like electronic, phononic etc. In the present work we employ the virtual crystal approximation (VCA) [4], based on configurational averaging, for description of polariton excitations in a *macroscopically* inhomogeneous medium. It is a well-known method; however its use up to now [5] has been limited to *microscopic* calculating the quasiparticles excitations spectra in disordered systems. Mathematical posing of the problem is similar in these two cases. Within VCA the configurationally dependent parameters of the Hamiltonian are replaced with their configurationally averaged values. Description of transformation of a polariton spectrum in a sufficiently simple superlattice, using this approximation, is the first step towards the study of imperfect systems. However investigation of properties of polariton spectra and the related physical quantities (density of elementary excitation states, characteristics of the normal electromagnetic waves etc.) in less simple systems requires application of more complex method (such are the method of the coherent potential or the averaged T-matrix method).

In the paper a superlattice is modeled as a set of macroscopically homogeneous layers with randomly included extrinsic (with respect to the ideal superlattice) layers of variable composition and thickness. Corresponding configuration-dependent material tensors in our model of an imperfect superlattice are represented in terms of random quantities. After configuration-averaging the translational symmetry of a considered system is "restored" that allows us obtain the system of equations which define normal modes of electromagnetic waves, propagating in one-dimensional “periodic” medium.

Investigation of disorder effects in an imperfect superlattice allowing modeling the properties of photonic crystal containing the plasma layers is still of a great interest [2]. Development of the theory of photonic structures requires consideration of model systems such as photonic superlattice with plasma layers. Within the VCA we study a model of 1D-superlattice as a macroscopically homogeneous layered system, which is a topologically ordered ensemble (such as a Si/liquid crystal or SiO_2/Si system) with randomly included admixture plasma layers.

Theoretical fundamentals

Dielectric $\hat{\varepsilon}(\vec{r})$ and magnetic $\hat{\mu}(\vec{r})$ permeability, which determine optical characteristics of a periodic medium, must satisfy the periodic boundary conditions:

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

where $d=\sum_{j=1}^{\sigma}a_j$ is the period of the superlattice, σ is the number of layers per elementary cell, a_j are the thicknesses of the layers which form 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:

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

In Eq. (1) $\theta(z)$ is the Heaviside function, $n=\pm1,\ \pm2,\ ...$ is the number of a one-dimensional crystal cell, index $\alpha=1,2,...,\sigma$ designates the elements of the cell. Within our model, the configurationally dependent tensors $\hat{\varepsilon}_{n\alpha},\ \hat{\mu}_{n\alpha}$ are expressed through the random quantities $\eta^{\nu}_{n\alpha}$ ($\eta^{\nu}_{n\alpha}$=1 if the $\nu(\alpha)$-th sort of layer is in the $(n\alpha)$-th site of the crystalline chain, $\eta^{\nu}_{n\alpha}$=0 otherwise):

$$\begin{pmatrix}\hat{\varepsilon}_{n\alpha}\\ \hat{\mu}_{n\alpha}\end{pmatrix}=\sum_{\nu(\alpha)}\begin{pmatrix}\hat{\varepsilon}^{\nu(\alpha)}_{\alpha}\\ \hat{\mu}^{\nu(\alpha)}_{\alpha}\end{pmatrix}\eta^{\nu(\alpha)}_{n\alpha} \qquad (2)$$

Calculation of a polariton spectrum for the imperfect superlattice is realized within the VCA (similarly to the solid quasi-particle approach) through the following replacement: $\hat{\varepsilon}\to\langle\hat{\varepsilon}\rangle,\ \hat{\mu}\to\langle\hat{\mu}\rangle$ (in the case of the variable layer thickness replacement is $d\to\langle d\rangle$ and $a_{n\alpha}\to\langle a_{\alpha}\rangle$). Angular parentheses designate the procedure of configuration averaging. In addition, from Eq. (2) we have:

$$\begin{pmatrix}\langle\hat{\varepsilon}_{n\alpha}\rangle\\ \langle\hat{\mu}_{n\alpha}\rangle\end{pmatrix}=\sum_{\alpha,\nu(\alpha)}\begin{pmatrix}\hat{\varepsilon}^{\nu(\alpha)}_{\alpha}\\ \hat{\mu}^{\nu(\alpha)}_{\alpha}\end{pmatrix}C^{\nu(\alpha)}_{\alpha}, \qquad \langle a_{n\alpha}\rangle=\sum_{\upsilon(\alpha)=1}^{r(\alpha)}a^{\upsilon(\alpha)}_{\alpha}C^{\upsilon(\alpha)}_{\alpha} \qquad (3)$$

where $C^{\nu(\alpha)}_{\alpha}$ is the concentration of the $\nu(\alpha)$-th sort of admixture layer in the α-th sublattice. There is a normalization condition $\sum_{\nu(\alpha)}C^{\nu(\alpha)}_{\alpha}=1$. It follows from Eq. (1) that the Fourier-amplitudes $\hat{\varepsilon}_l,\ \hat{\mu}_l$ and the averaged dielectric $\langle\hat{\varepsilon}_{n\alpha}\rangle$ and magnetic $\langle\hat{\mu}_{n\alpha}\rangle$ permeability of layers (3) are related as

$$\begin{pmatrix}\hat{\varepsilon}_l\\ \hat{\mu}_l\end{pmatrix}=-\frac{i}{2\pi l}\sum_{\alpha}\begin{pmatrix}\langle\hat{\varepsilon}_{n\alpha}\rangle\\ \langle\hat{\mu}_{n\alpha}\rangle\end{pmatrix}\left\{\exp\left(i\frac{2\pi}{d}l\sum_{j=1}^{\alpha}a_j\right)-\exp\left[i\frac{2\pi}{d}l\left(\sum_{j=1}^{\alpha}a_j-a_{\alpha}\right)\right]\right\} \qquad (4)$$

Since the configurationally 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 write Maxwell equations for harmonic dependency of the electric and magnetic field strengths $\vec{E}(\vec{r},\omega),\ \vec{H}(\vec{r},\omega)$ on a time. Hence, according to the Floquet theorem, Fourier-amplitudes $\vec{f}_{K,p}^{\,(E,H)}$ of the electric and magnetic field strengths satisfy the following relation:

$$\left[\vec{\beta}+\left(K+p\frac{2\pi}{d}\right)\vec{e}_z\right]\times\begin{pmatrix}\vec{f}_{K,p}^{\,(H)}\\ \vec{f}_{K,p}^{\,(E)}\end{pmatrix}=\frac{\omega}{c}\begin{bmatrix}-\sum_l \hat{\varepsilon}_l\cdot\vec{f}_{K,p-l}^{\,(E)}\\ \sum_l \hat{\mu}_l\cdot\vec{f}_{K,p-l}^{\,(H)}\end{bmatrix}. \qquad (5)$$

Here $\vec{\beta}$ is an arbitrary planar (in the XOY plane) wave vector, $\vec{e}_z$ is a unit vector along the *z*-axis, $\vec{K}=(0,0,K)$ is the Bloch vector. The system (5) defines normal modes of electromagnetic waves, propagating in the considered "periodic" medium. Below, for simplicity, we shall restrict our study to the case of light, propagating along the *z*-axis ($\vec{\beta}=0$) in a nonmagnetic lattice ($\hat{\mu}=\hat{I}$ is a unit matrix); the liquid-crystal layers we shall treat as uniaxial ($\varepsilon_{ij}=\varepsilon_{xx}\delta_{xi}\delta_{jx}+\varepsilon_{yy}\delta_{yi}\delta_{jy}+\varepsilon_{zz}\delta_{zi}\delta_{jz}$; obviously, that for $\vec{K}\parallel z$, *zz*-components of the tensor $\hat{\varepsilon}$ do not appear in final formulas, and $\varepsilon_{xx}=\varepsilon_{yy}\equiv\varepsilon$). Furthermore, we shall (like in Ref. [3]) assume, that K is close to the value, defined by the Bragg's condition: $\left|K-\frac{2\pi}{d}\right|\approx K$, $\quad c^2K^2\approx\omega^2\varepsilon_0$. This case corresponds to a resonance of plane waves between the components $\vec{f}_{K,p}^{\,(E,H)}$ at $p=0,\,-1$ (these terms dominate in the system (6)). After eliminating the $\vec{f}^{\,(H)}$ variables, Eqs. (5) with respect to $\vec{f}^{\,(E)}$ take the form:

$$\begin{bmatrix}K^2-\frac{\omega^2}{c^2}\varepsilon^{(0)} & -\frac{\omega^2\varepsilon^{(1)}}{c^2}\\ -\frac{\omega^2\varepsilon^{(-1)}}{c^2} & \left(K-\frac{2\pi}{d}\right)^2-\frac{\omega^2}{c^2}\varepsilon^{(0)}\end{bmatrix}\begin{pmatrix}f_{K,0}^{(E)}\\ f_{K,-1}^{(E)}\end{pmatrix}=0, \qquad (6)$$

where $\varepsilon_{l=0}\equiv\varepsilon^{(0)}$, $\varepsilon_{l=\pm1}\equiv\varepsilon^{(\pm1)}$. Putting the determinant of the system (6) 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.

Results

To specify the results, let's firstly consider the propagation of electromagnetic excitation in an imperfect Si/LC 1D superlattice with two elements (layers) in the cell, namely, with the first layer of silicon ($\varepsilon_1=11.7$) and the second layer of liquid crystal ($\varepsilon_2^{(1)}=5.5$).Then we study SiO_2/Si 1D superlattice (with $\varepsilon_1=3.7$). The concentration, thickness and permittivity of the basic material layer in the first and second sublattices are denoted as $C_1^{(1)}$, $a_1^{(1)}=a_1$, $\varepsilon_1^{(1)}\equiv\varepsilon_1$ and $C_2^{(1)},a_2^{(1)},\varepsilon_2^{(1)}\equiv\varepsilon_2$, and the corresponding parameters of impurity layers with a different composition $C_{2C}^{(2)}\equiv C_C$ and thickness $C_{1T}^{(2)}\equiv C_T$, as well as $a_2^{(2)},\varepsilon_2^{(2)}$. Note that the permittivity profile for inhomogeneous plasma is $\varepsilon_2^{(2)}(z)=1-\omega_e^2(z)/\omega^2$. For considered model plasma frequency is $\omega_e<<\omega$ (collisions in plasma are neglected) and plasma density for $a_{n\alpha}$-th layer varies exponentially:

$$n(z)=n_{cr}\left\{\exp\left[-\delta\left[z-(n-1)d-\sum_{j=1}^{\alpha}a_{nj}+a_{n\alpha}\right]/a_{n\alpha}\right]+\exp\left[-\delta\left(-z+(n-1)d+\sum_{j=1}^{\alpha}a_{nj}\right)/a_{n\alpha}\right]\right\}/2, \qquad (7)$$

gradation parameter δ corresponds to the volume average plasma permittivity $<\varepsilon_2^{(2)}>=0.9$. Below we are considered the case of admixture plasma layers only in LC-sublattice for Si/LC superlattice and in Si-sublattice for SiO_2/Si system. Simple calculations taking into account (3)-(7), yield the dependence the lowest photonic band gap width $\Delta\omega = |\omega_+ - \omega_-|$ on plasma concentration of the systems studied:

$$\Delta\omega_1/\omega = (\varepsilon_1 - f_d f_{1C})^{-1}\sqrt{f_{1C}^2 f_{1T} + f_{2C} f_{2T} + f_{3C} f_{3T}}\,, \tag{8}$$

$$f_d = a_2\left[a_1 + a_2 + C_T\left(a_1^{(2)} - a_1\right)\right]^{-1},\ f_{1T} = \pi^{-2} Sin^2\pi\ f_d\,,\quad f_{2T} = f_d\,\frac{\pi^{-1}\delta\ Sin2\pi\ f_d + 4 f_d Sin^2\pi\ f_d}{\delta^2 + (2\pi\ f_d)^2}\,,$$

$$f_{3T} = f_d^2\,\frac{Sin^2\pi\ f_d}{\delta^2 + (2\pi\ f_d)^2}\,,\quad f_{1C}^2 = \left[C_C(\varepsilon_2 - 1) + \varepsilon_1 - \varepsilon_2\right]^2,\quad f_{2C} = C_C f_{1C}\,,\quad f_{3C} \equiv C_C\,.$$

The dependence $\Delta\omega(C_C\,, C_T)$ is shown in Fig. 1 for Si/LC superlattice and in Fig. 2 for SiO_2/Si system for different relative both composition and thickness of layers. Surface 1 in Fig. 1 refers the case of $a_1/a_2 = 0.1$ and $a_1^{(2)}/a_2 = 0.5$, surface 2 corresponds to the case of $a_1/a_2 = 0.5$ and $a_1^{(2)}/a_2 = 0.1$. In Fig. 2 photonic band gap $\Delta\omega_1/\omega$ corresponds to the values $a_1^{(2)}/a_2$ and a_1/a_2 that are equal to 0,1; 10 (surface 1) and 10; 0,1(surface 2).

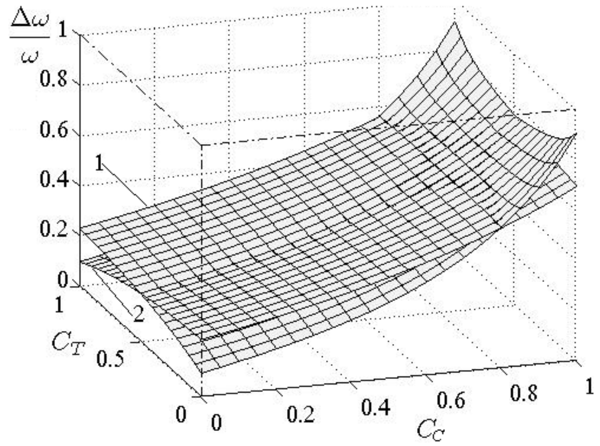

Fig. 1. Concentration dependence for a nonideal Si/LC 1D superlattice which contains plasma layers in LC-sublattice.

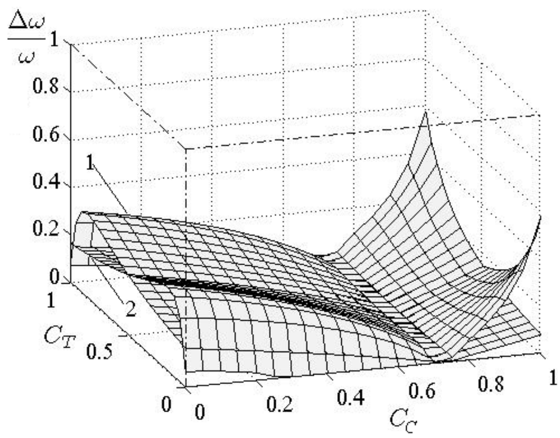

Fig. 2. Concentration dependence for a nonideal SiO_2/Si 1D superlattice which contains plasma layers in Si-sublattice.

Conclusions

Our results show that the optical characteristics of imperfect 1D superlattice may be significantly altered owing to transformation of their photon mode spectrum resulting a presence of admixture layers. Graphic representation $\Delta\omega(C_C, C_T)$ proves that the concentration dependence for the binary systems considered above differs for different relative composition of plasma layers. The case of nonideal multilayered systems with a larger number of sublattices and components of alien layers 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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