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PECULIARITIES OF BAND GAP WIDTH DEPENDENCE UPON CONCENTRATION OF ADMIXTURES RANDOMLY INCLUDED IN 1D PHOTONIC CRYSTAL

V.V. RUMYANTSEV
S.A. FEDOROV
K.V. GUMENNYK

400 Oser Avenue, Suite 1600
Hauppauge, N. Y. 11788-3619
Phone (631) 231-7269
Fax (631) 231-8175
E-mail: main@novapublishers.com
www.novapublishers.com

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CONTENTS

PREFACE

1D photonic crystalline superlattice is modeled as both a layered crystal and striped thin film. These 1D systems are sets of elements (layers or strips) with randomly included extrinsic (with respect to the ideal superlattices) elements (layers or strips) of a variable thickness or composition. The photon modes spectrum of a non-ideal superlattice with an arbitrary number of layers (strips) per elementary cell, obtained within the virtual crystal approximation, is concretized for the Si – diamond layered system, Si-liquid crystal and $Si/SiO_2/GaAs$ striped film. Dependence of the band gap width upon concentration of admixture elements and refractive index peculiarities is analyzed. The study carried out shows that optical characteristics of the nonideal photonic crystals may vary due to transformation of its photon modes spectrum caused by the presence of admixture elements (layers or strips).

Chapter 1

INTRODUCTION

At present, propagation of electromagnetic waves in thin films and layered crystal media (see [1-4] and references therein), in particular, in photonic magnetic crystals [5-7] and composite crystals based on silicon and liquid crystal [8-12], are being investigated extensively. Interest in investigation of these objects is motivated, on the one hand, by the demand for different layered structures with given properties in solid-state electronics and, on the other hand, by achievements in technologies providing the possibility of growing such films and periodic structures with controlled characteristics by the molecular-beam epitaxial method. A large number of works ([13-15] and references therein) have been devoted to theoretical and experimental investigation of exciton-type excitations in dielectric ideal superlattices. The general theory of optical waves in anisotropic crystals, including those composed of macroscopic layers, is considered in [16]. In [11], the forbidden photonic bands of a crystal made of alternating silicon and liquid crystal layers are calculated. 1D photonic band gap structures attract lot of attention of researches due to their omnifarious using for optical filtering [17], sensing [18] and so on. The logic of further development of the theory of layered structures requires consideration of more complex systems - superlattices with impurity layers, as well as with layers of variable composition and thickness. In [6], the dispersion of polaritons in a superlattice with a single impurity layer has been studied. At the same time, of considerable interest are investigations of nonideal superlattices with an arbitrary number of impurity layers and of the dependence of the polariton

spectrum on the concentration of corresponding defects, which make it possible to expand the capabilities of modeling the properties of such systems and to create layered materials with given characteristics.

The method of calculation of polariton excitations has much in common with methods of finding other quasiparticle excitations (electron, phonon, etc.) in solids. In the present chapter authors offer for description of photon modes in macroscopically heterogeneous ambience approach, based on configuration averaging (it specifically is new in this case), which was used before [19] for the microscopic calculation of disordered systems quasiparticles spectra. A relatively simple approximation in framework of this approach for calculation polariton spectra and corresponding optical characteristics of disordered ambiences is the virtual-crystal approximation (VCA) [19-21]. VCA (first it was used by L. Nordheim and R.H. Parmenter [19]) consist of replacing of correct one-electron potential (appropriate to a given configuration of atoms of the alloy) by its average which is taken over all possible random configurations. The approximation is a widely used for study of disordered structures. For example, based on the pseudopotential scheme under the VCA in which the effect of compositional disorder is involved, the dependence of optoelectronic properties of $GaAs_{x}Sb_{1-x}$ on alloy composition x have been studied in [22]. Within this approximation 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 VCA, 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 methods. Such are the method of the coherent (one- or many-site) potential [21], the averaged T-matrix method [23] and their numerous modifications used for various particular problems.

In the chapter a superlattice is modeled as a set of macroscopically homogeneous layers with randomly included extrinsic (with respect to the ideal superlattice) layers. 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 (1D) “periodic” medium. Within the VCA we study of peculiarities of the dependence of the band gap width and refractive index upon concentration of admixture layers for the non-ideal photonic crystalline system (that is layered crystal or striped thin film).

Chapter 2

PROPAGATION OF ELECTROMAGNETIC WAVES IN INHOMOGENEOUS STRUCTURES

Since the optical properties of a periodic medium are defined by the corresponding material tensors - the dielectric permittivity $\hat{\varepsilon}(\vec{r})$ and the magnetic permeability $\hat{\mu}(\vec{r})$ the following equalities are satisfied for the above ideal systems:

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

Here, $d=\sum_{j=1}^{\sigma} a_j$ is the period of the superlattice, σ is the number of layers in the unit cell, and a_j is the thicknesses of the *j*-th layer of the one-dimensional chain of elements on the *z* axis. Propagation of electromagnetic waves in inhomogeneous structures is described by the Maxwell equations, which take the following form in the $(\vec{k},\omega)$ representation:

$$\begin{cases} \vec{k}\times\vec{H}\left(\vec{k},\omega\right)=-\dfrac{\omega}{c}\int d\vec{q}\,\hat{\varepsilon}\left(q,\vec{k}-\vec{q}\right)\cdot\vec{E}\left(\vec{q},\omega\right) \\ \vec{k}\times\vec{E}\left(\vec{k},\omega\right)=\dfrac{\omega}{c}\int d\vec{q}\,\hat{\mu}\left(q,\vec{k}-\vec{q}\right)\cdot\vec{H}\left(\vec{q},\omega\right) \end{cases}, \qquad (2)$$

where $\vec{E}\left(\vec{k},\omega\right)$, $\vec{H}\left(\vec{k},\omega\right)$ are the Fourier amplitudes of the electric and magnetic field strengths. In the coordinate representation, the material tensors $\hat{\varepsilon}$ and $\hat{\mu}$ of the crystal superlattice with an arbitrary number σ of layers perpendicular to the z axis are expressed as follows:

$$\begin{pmatrix}\hat{\varepsilon}(z)\\ \hat{\mu}(z)\end{pmatrix}=\sum_{n,\alpha}\begin{pmatrix}\hat{\varepsilon}_{n\alpha}\\ \hat{\mu}_{n\alpha}\end{pmatrix}\left\{\theta\left[z-(n-1)d-\left(\sum_{j=1}^{\alpha}a_{nj}-a_{n\alpha}\right)\right]-\theta\left[z-(n-1)d-\sum_{j=1}^{\alpha}a_{nj}\right]\right\} \qquad (3)$$

In (3), $\theta(z)$ is the Heaviside function; $n=\pm1,\pm2,...$ is the cell number in the one-dimensional crystal; and the index $\alpha=1,2,...,\sigma$ enumerates the elements of the cell. It can be easily shown that the Fourier images of the material tensors $\hat{\varepsilon}\left(\vec{k}-\vec{q}\right)$, $\hat{\mu}\left(\vec{k}-\vec{q}\right)$ in system (2) for the case of the superlattice under study have the form

$$\begin{bmatrix}\hat{\varepsilon}\left(\vec{k}-\vec{q}\right)\\ \hat{\mu}\left(\vec{k}-\vec{q}\right)\end{bmatrix}=(2\pi)^2\delta(k_x-q_x)\delta(k_y-q_y)\sum_{\alpha}F_{\alpha}(k_z-q_z)\sum_{n}\begin{pmatrix}\hat{\varepsilon}_{n\alpha}\\ \hat{\mu}_{n\alpha}\end{pmatrix}\exp\left[i(k_z-q_z)nd\right] \qquad (5)$$

where the function $F_{\alpha}(k_z-q_z)$ is defined by the expression

$$F_{\alpha}(k_z-q_z)=\theta(k_z-q_z)\left\{\exp\left[-i(k_z-q_z)a_{\alpha}\right]-1\right\}\exp\left[i(k_z-q_z)\left(\sum_{j=1}^{\alpha}a_j-d\right)\right]\cdot$$

Here, $\theta(k_z)$ is the Fourier image of the Heaviside function $\theta(z)$. For an ideal superlattice,

$$\begin{pmatrix} \hat{\varepsilon}^{(0)}\left(\vec{k}-\vec{q}\right) \\ \hat{\mu}^{(0)}\left(\vec{k}-\vec{q}\right) \end{pmatrix} = (2\pi)^2 \delta\left(k_x - q_x\right)\left(k_y - q_y\right) \times$$
$$\times \sum_{\alpha} F_{\alpha}\left(k_z - q_z\right) \begin{pmatrix} \hat{\varepsilon}_{\alpha}^{(0)} \\ \hat{\mu}_{\alpha}^{(0)} \end{pmatrix} \left\{ \sum_{n=-\infty}^{\infty} \exp\left[i\left(k_z - q_z\right) n a_{\alpha}\right] - 1 \right\}, \qquad (6)$$

and

$$\hat{\varepsilon}_{n\alpha}^{(0)} \equiv \hat{\varepsilon}_{\alpha}^{(0)}, \quad \hat{\mu}_{n\alpha}^{(0)} \equiv \hat{\mu}_{\alpha}^{(0)}.$$

Chapter 3

DEPENDENCE OF THE POLARITON SPECTRUM ON THE CONCENTRATION OF IMPURITY LAYERS IN A NONIDEAL SUPERLATTICE

The variation in the composition. A nonideal system whose disorder is related to the variation in the composition (rather than in the thickness) of impurity layers (therefore, $a_{n\alpha} \equiv a_{\alpha}$) is considered. The configuration-dependent tensors $\hat{\varepsilon}_{n\alpha}$, $\hat{\mu}_{n\alpha}$ in our model of a nonideal superlattice are represented in terms of random quantities $\eta_{n\alpha}^{\nu}$ ($\eta_{n\alpha}^{\nu}$ *=1*, if in the site $(n\alpha)$ of the crystal chain the layer of type $\nu(\alpha)$ is situated, and $\eta_{n\alpha}^{\nu}$ *=0*, otherwise),

$$\begin{pmatrix} \hat{\varepsilon}_{n\alpha} \\ \hat{\mu}_{n\alpha} \end{pmatrix} = \sum_{\nu(\alpha)} \begin{pmatrix} \hat{\varepsilon}_{\alpha}^{\nu(\alpha)} \\ \hat{\mu}_{\alpha}^{\nu(\alpha)} \end{pmatrix} \eta_{n\alpha}^{\nu(\alpha)} . \qquad (4)$$

Normalizing condition for this case is $\sum_{\nu(\alpha)=1}^{r(\alpha)} \eta_{n\alpha}^{\nu(\alpha)} = 1$, $r(\alpha)$ is number of layer types. The polariton spectrum of a nonideal superlattice is calculated in the framework of the VCA (in analogy with the

quasiparticle approach) by applying the following replacements: $\hat{\varepsilon} \to \langle \hat{\varepsilon} \rangle$, $\hat{\mu} \to \langle \hat{\mu} \rangle$ (the angular brackets denote the configuration averaging). In this case, (4) and [21] imply

$$\begin{pmatrix} \langle \hat{\varepsilon}_{n\alpha} \rangle \\ \langle \hat{\mu}_{n\alpha} \rangle \end{pmatrix} = \sum_{\alpha, \nu(\alpha)} \begin{pmatrix} \varepsilon_\alpha^{\nu(\alpha)} \\ \mu_\alpha^{\nu(\alpha)} \end{pmatrix} C_\alpha^{\nu(\alpha)}, \tag{7}$$

where $C_\alpha^{\nu(\alpha)}$ is the concentration of the impurity layer of the type $\nu(\alpha)$ in the α th sublattice, $\sum_{\nu(\alpha)} C_\alpha^{\nu(\alpha)} = 1$. Since the configuration averaging "restores" the translational symmetry in the crystal system, as applied to the case of the nonideal superlattice under study, the "acquired" translational invariance of the one-dimensional chain provides the possibility to represent system (2) in the form of the following integral matrix equation:

$$\int d\vec{q} \begin{pmatrix} \frac{\omega}{c} \langle \hat{\varepsilon}(\vec{K} - \vec{q}) \rangle & \delta(\vec{K} - \vec{q}) \hat{q} \\ \delta(\vec{K} - \vec{q}) \hat{q} & -\frac{\omega}{c} \langle \hat{\mu}(\vec{K} - \vec{q}) \rangle \end{pmatrix} \cdot \begin{pmatrix} \vec{E}(\vec{q}, \omega) \\ \vec{H}(\vec{q}, \omega) \end{pmatrix} = 0 \tag{8}$$

Here, $\hat{q} = \begin{pmatrix} 0 & -q_z & q_y \\ q_z & 0 & -q_x \\ -q_y & q_x & 0 \end{pmatrix}$ is the antisymmetric tensor dual to the wave vector $\vec{q}$. In (8), the arbitrary wave number $\vec{k}$ was replaced by the Bloch wave vector $\vec{K}$. This is possible for a nonideal superlattice owing to the configuration averaging that has "restored" the periodicity of the medium. According to the Floquet theorem, a general solution to system (2)

$\begin{pmatrix} \vec{E}(\vec{r}, \omega) \\ \vec{H}(\vec{r}, \omega) \end{pmatrix} = \int d\vec{k} \begin{pmatrix} \vec{E}(\vec{k}, \omega) \\ \vec{H}(\vec{k}, \omega) \end{pmatrix} \exp(i\vec{k} \cdot \vec{r})$ in a periodic medium represents a superposition of the normal modes $\vec{E}_{\vec{K}}(\vec{r}, \omega) = \exp(i\vec{K} \cdot \vec{r}) \varphi(x, y, z, \omega)$, and

$\varphi(x,y,z,\omega)=\varphi(x,y,z+d,\omega)$; $\vec{K}=(0,0,K)$, $K=2\pi\ m/Nd$; $m=\pm1,\pm2,\pm3,...,\pm N$ (among all possible values of m, there are only N values yielding N independent modes).

For nonmagnetic systems, $\hat{\mu}=\hat{I}$, and the dielectric permittivity of the nonideal superlattice under study is the function $\langle\varepsilon_{il}(z)\rangle=\langle\varepsilon(z+d)\rangle\delta_{il}$. In this case, the dispersion relation $\omega=\omega_j(\vec{K})$ of the general form, which follows from (5) and from the condition of solvability of integral equation (8), has the form

$$\omega^2_{j(\pm)}(K)=c^2K^2\times$$
$$\times\left\{\sum_{\alpha=1}^{\sigma}\frac{a_\alpha}{d}\langle\varepsilon_{n\alpha}\rangle\pm\frac{1}{2\pi j}\left|\sum_{\alpha=1}^{\sigma}\langle\varepsilon_{n\alpha}\rangle\left[\begin{array}{l}\exp\left(-i\frac{2\pi j}{d}\sum_{j=1}^{\alpha}a_j\right)-\\-\exp\left(-i\frac{2\pi j}{d}(\sum_{j=1}^{\alpha}a_j-a_\alpha)\right)\end{array}\right]\right|\right\}^{-1}. \quad (9)$$

The integer j enumerates the polariton branches.

The variation in the thickness of impurity layers. For an imperfect superlattice, in which disordering is connected with variation of the thickness (rather then of the composition) of admixture layers we have to use the following procedure of configuration averaging: $a_{n\alpha}\to a_\alpha\left\{C_\alpha^{\nu(\alpha)}\right\}$, $d\to d\left\{C_\alpha^{\nu(\alpha)}\right\}$ (here $C_\alpha^{\nu(\alpha)}$ 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 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 present 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) in the form:

$$\nabla\times\vec{E}(\vec{r},\omega)=\frac{i\omega}{c}\langle\hat{\mu}(z)\rangle\cdot\vec{H}(\vec{r},\omega),\ \nabla\times\vec{H}(\vec{r},\omega)=-\frac{i\omega}{c}\langle\hat{\varepsilon}(z)\rangle\cdot\vec{E}(\vec{r},\omega)\cdot \quad (10)$$

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:

$$\left[\vec{\beta}+\left(K+p\frac{2\pi}{d}\right)\vec{e}_z\right]\times\begin{pmatrix}\vec{f}_{K,p}^{(H)}\\ \vec{f}_{K,p}^{(E)}\end{pmatrix}=\frac{\omega}{c}\begin{bmatrix}-\sum_l \hat{\varepsilon}_l\cdot\vec{f}_{K,p-l}^{(E)}\\ \sum_l \hat{\mu}_l\cdot\vec{f}_{K,p-l}^{(H)}\end{bmatrix} \qquad (11)$$

Here $\vec{\beta}$ is an arbitrary planar (in the XOY plane) wave vector, $\vec{e}_z$ is a unit vector along the *z*-axis, the Bloch vector is $\vec{K}=(0,0,K)$. The system (11) defines normal modes of electromagnetic waves, propagating in the considered "periodic" medium. Furthermore, we (like in [24]) assume, that K is 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 of plane waves between the components $\vec{f}_{K,p}^{(E,H)}$ at $p=0,\,-1$ (these terms dominate in the system (11)). After eliminating the $\vec{f}^{(H)}$ variables, Eqs. (11) with respect to $\vec{f}^{(E)}$ take the form:

$$\begin{bmatrix}K^2-\frac{\omega^2}{c^2}\varepsilon^{(0)} & -\frac{\omega^2\varepsilon^{(1)}}{c^2}\\ -\frac{\omega^2\varepsilon^{(-1)}}{c^2} & \left(K-\frac{2\pi}{d}\right)^2-\frac{\omega^2}{c^2}\varepsilon^{(0)}\end{bmatrix}\begin{pmatrix}f_{K,0}^{(E)}\\ f_{K,-1}^{(E)}\end{pmatrix}=0, \qquad (12)$$

where $\varepsilon_{l=0}\equiv\varepsilon^{(0)}$, $\varepsilon_{l=-1}\equiv\varepsilon^{(-1)}$. Putting the determinant of the system (12) equal to zero we obtain the dispersion relations $\omega_\pm=\omega\left(K\right)$. 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 AND DISCUSSION

For simplicity, we shall restrict our study to the case of light, propagating along the *z*-axis ($\vec{\beta} = 0$) in a nonmagnetic diamond - Si crystal system ($\hat{\mu} = \hat{I}$ is a unit matrix) with admixture layers of a variable composition only. The layers we treat as macroscopically homogeneous and isotropic ($\varepsilon_{ij} = \varepsilon\delta_{ij}$). Let us limit ourselves to the consideration of propagation of electromagnetic radiation in a nonmagnetic superlattice with two isotropic layers, elements, per unit cell. We denote the concentration and the dielectric permittivity of the main substance (matrix) in the first and second sublattices by $C_1^{(1)}$, $\varepsilon_1^{(1)} = 5.7$ and $C_2^{(1)}$, $\varepsilon_2^{(1)} = 11.7$ respectively, while these quantities for the impurity are designated as $C_1^{(2)}, \varepsilon_1^{(2)}$ and $C_2^{(2)}, \varepsilon_2^{(2)}$.

Taking into account the aforesaid, the dispersion of the polariton spectrum of a nonideal binary diamond-silicon system is determined by the following dispersion equation that is derived from (9):

$$\omega_{j(\pm)}^2(K) = c^2 K^2 \left\{ \begin{array}{l} f_1\left(C_1^{(2)}\right)\dfrac{a_1}{d} + f_2\left(C_2^{(2)}\right)\dfrac{a_2}{d} \pm \\ \\ \pm \left| f_1\left(C_1^{(2)}\right)\dfrac{\sin(\pi\ j\ a_1/d)}{\pi\ j} + f_2\left(C_2^{(2)}\right)\dfrac{\sin(\pi\ j\ a_2/d)}{\pi\ j} \right| \end{array} \right\}^{-1}, \quad (13)$$

where $f_1\left(C_1^{(2)}\right) = \varepsilon_1^{(1)} + \left(\varepsilon_1^{(2)} - \varepsilon_1^{(1)}\right)C_1^{(2)}$, and $f_2\left(C_2^{(2)}\right) = \varepsilon_2^{(1)} + \left(\varepsilon_2^{(2)} - \varepsilon_2^{(1)}\right)C_2^{(2)}$. The same approximations as in [15] (where an ideal periodic structure was studied) were used to obtain relation (10); therefore, the shape of the dispersion curves does not differ qualitatively from those given in [16]. Nonetheless, unlike the case studied in [16], the specific feature of the problem under study is that the

parameters of the family of dispersion curves depend on the concentration $C_{\alpha}^{\nu(\alpha)}$ of defective layers. In particular, our model makes it possible to obtain an expression for the width of the forbidden band, which, with $\omega = \omega_j\left(\vec{K}\right)$ in the form of (13), is given by

$$\Delta\omega_j = \\ = \omega \frac{\left|\left(\varepsilon_1^{(1)}C_1^{(1)} + \varepsilon_1^{(2)}C_1^{(2)}\right)\sin\left(\pi\ j\ a_1/d\right)/\pi\ j + \left(\varepsilon_2^{(1)}C_2^{(1)} + \varepsilon_2^{(2)}C_2^{(2)}\right)\sin\left(\pi\ j\ a_2/d\right)/\pi\ j\right|}{\left(\varepsilon_1^{(1)}C_1^{(1)} + \varepsilon_1^{(2)}C_1^{(2)}\right)a_1/d + \left(\varepsilon_2^{(1)}C_2^{(1)} + \varepsilon_2^{(2)}C_2^{(2)}\right)a_2/d} . \quad (14)$$

The concentration dependence of the energy gaps in the diamond-silicon superlattice for different values of j was shown in [25]. Below we are considered the case of admixture layers of a variable both thickness and composition only in Si-sublattice. Concentration, dielectric permeability and thickness as well of the base material in the first and the second sublattice are denoted by $C_1^{(1)}, \varepsilon_1^{(1)}, a_1^{(1)}$ and $C_2^{(1)}, \varepsilon_2^{(1)}, a_2^{(1)}$ respectively. For admixture this quantities are denoted by $C_{1C}^{(2)}$ (it is related to the variable composition) and $C_{1T}^{(2)}$ (it is related to the variable thickness) $\varepsilon_1^{(2)}, a_1^{(2)}$ as well as (there are no admixtures in the Si-sublattice). Simple transformations (with the account that $\left|\varepsilon^{(-1)}\right| = \left|\varepsilon^{(1)}\right|$) lead to the following relations for the refractive index $n_{\pm} \equiv cK/\omega_{\pm}$ of the studied system:

$$n_{\pm}^2\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right) = \varepsilon^{(0)}\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right) \pm \left|\varepsilon^{(1)}\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right)\right| \cong \varepsilon^{(0)}\left[1 \pm \frac{\Delta\omega_1\left(C_{1C}^{(2)}, C_{1T}^{(2)}\right)}{\omega}\right] \quad (15)$$

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

$$\varepsilon^{(0)} = \varepsilon_2\left(1 + f_C f_T\right)/\left(1 + f_T\right), \quad (16)$$

$$\varepsilon^{(1)} = \frac{\varepsilon_2}{\pi}\left|1 - f_C\right| Sin\frac{\pi f_T}{1+f_T}. \qquad (17)$$

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 $\Delta\omega_1 = \left|\omega_+ - \omega_-\right|$, $\Delta\omega_1/\omega \cong (n_+^2 - n_-^2)/2\varepsilon^{(0)}$. It follows from Eq. (15) 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 Refs. [16,25] it was shown that the band gaps of higher orders are as well determined by corresponding Fourier-coefficients of the dielectric permeability.

Figure 1 shows the concentration dependence of the refractive index $n_\pm \equiv cK/\omega_\pm$ of the studied composite superlattice. It is readily seen, that the form of the corresponding surfaces has a complex character, it depend on the dielectric permeability of both admixtures and its thicknesses. In Figure 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 layers for a superlattice with alternating silicon and diamond layers. The energy gap $\Delta\omega_1$ vanishes at $\left|1 - f_C\right| Sin\frac{\pi f_T}{1+f_T} = 0$ for the case a) on Figure 2.

a)

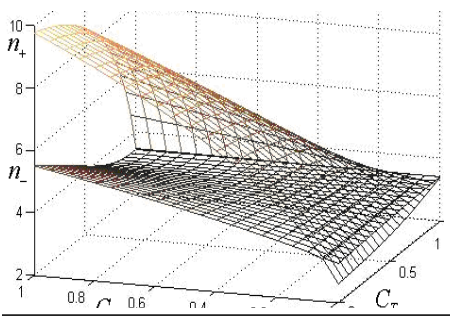

Figure 1. (Continued).

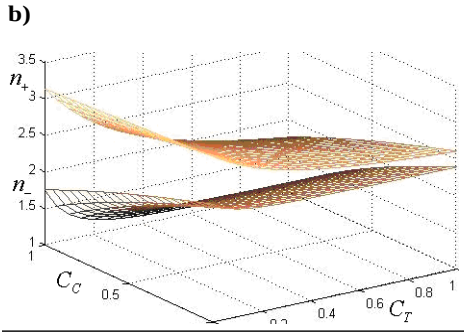

Figure 1. Refractive index $n_+, n_-(C_C, C_T)$ of the composite superlattice (with alternating diamond and silicon layers) vs. the concentrations of admixture layers of a variable thickness and composition for $a_1^{(1)}/a_2 = 1$: a) $a_1^{(2)}/a_1^{(1)} = 0.001$, $\varepsilon_1^{(2)}/\varepsilon_1^{(1)}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

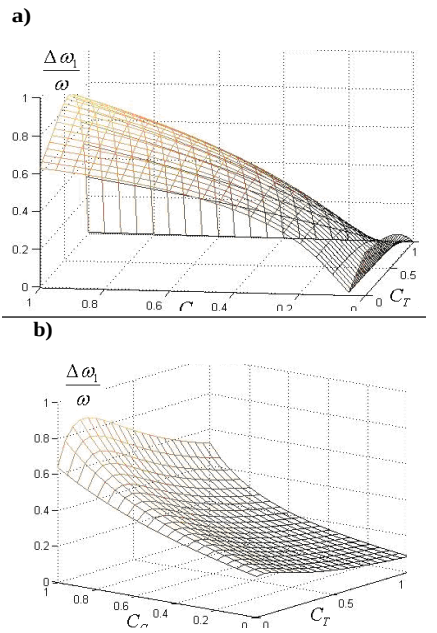

Figure 2. Relative width of the lowest photonic band gap $\Delta\omega_1/\omega$ of the composite superlattice (with alternating diamond and silicon layers) vs. the concentrations of admixture layers of a variable thickness and composition for $a_1^{(1)}/a_2 = 1$: a) $a_1^{(2)}/a_1^{(1)} = 0.001$, $\varepsilon_1^{(2)}/\varepsilon_1^{(1)}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

Chapter 4

PROPAGATION OF ELECTROMAGNETIC EXCITATION IN IMPERFECT QUASI-TWO-DIMENSIONAL PHOTONIC 1D CRYSTAL

Previously (see [26] and refs therein) we studied the propagation of electromagnetic waves localized in an ultrathin homogeneous film and found the dispersion laws that determine the relevant integral optical characteristics. At the same time, the up-to-date progress in nanotechnology and photonics [27-30], as well as the necessity of the creation of ultrathin composite materials, stimulates the investigation of more complex quasi-two-dimensional structures than the structures studied in [26]. This investigation can be most easily performed for ultrathin films that consist of strips that differ from each other both in the composition and in the thickness. In this case, the methods developed previously in [31] for the calculation of the concentration dependence of polariton spectra can be used directly for the calculation of corresponding excitations. In this chapter, we studied the propagation of electromagnetic excitation localized in a nonideal quasi-two-dimensional system, which, in the general case, is a topologically ordered ensemble of strips with a random number of defect strips. 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). In this chapter we studied the concentration dependence of the lowest photonic band gap of a striped quasi-two-

dimensional binary or ternary film (the 1D-superlattice has two or three elements in the unit cell) which contains defect strips of both variable composition and variable thickness.

THEORETICAL FUNDAMENTALS

In the case of an ultrathin film (with the thickness d on the order of the electronic excitation radius), the interaction of the electromagnetic field with the film can only be macroscopically described based on model representations, for example, as, e.g., in [26]. Let us consider the propagation of a plane electromagnetic wave with a frequency ω and a wave vector $\vec{q}$ in the plane of an ultrathin film according to the phenomenological approach. The long-wavelength field ($\lambda >> d$) outside the film does not depend on the characteristics of the crystal structure and on the polarization distribution along the film thickness. It is described by the D'Alembert equation, and the sole nontrivial information about the effect of the film on the electromagnetic field consists of the boundary conditions, which couples the field amplitudes from both sides of the film. The latter circumstance allows us to use the continuous approximation to find the exciting field $\vec{E}_{in}$ and field induced polarization of the plane layer. The material relations take the form

$$\begin{pmatrix} \vec{\Pi} \\ \vec{m} \end{pmatrix} = \hat{\chi}^{E,H} \cdot \begin{pmatrix} \vec{E}_{in} \\ \vec{H}_{in} \end{pmatrix}. \qquad (18)$$

Here, $\vec{\Pi}$ and $\vec{m}$ are the surface densities of the electric and magnetic dipole moments, respectively. The tensor function $\hat{\chi}^{E,H}$ of the film response in our quasi-two-dimensional case has the dimension of length. The joint solution of the system of equations relating to the boundary conditions and the material relations (18) yields the dispersion laws of exciton polaritons of the α, β and n polarizations localized in the layer

[32]. Here $\vec{n} \parallel z$ is the vector normal to the film, $\vec{\beta} = \vec{q}/q$ ($\vec{\beta} \parallel x$) and $\vec{\alpha} = \vec{n} \times \vec{\beta}$.

Let us study 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 replacement $\hat{\chi}^{E,H} \to \hat{\chi}^{E} \equiv \hat{\chi}$. Thus, in the general case of an inhomogeneous film, the material relation takes the form

$$\vec{E}_{in}(\vec{q},\omega) = \int d\vec{k}\,\hat{\chi}^{-1}(\vec{q}-\vec{k})\cdot\vec{\Pi}(\vec{k},\omega) = S_n(\vec{q},\omega)\vec{\Pi}(\vec{q},\omega). \quad (19)$$

As shown in [31,32], $S_n(\vec{q},\omega) = q^2\left(q^2 - \omega^2/c^2\right)^{-1/2}$.

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 superlattice can have an arbitrary number of elements α with a thickness $a_{s\alpha}$ that are oriented perpendicular to the *x* axis (Figure 3).

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

$$\chi(x) = \sum_{s,\alpha} \chi_{s\alpha}\left\{\theta\left[x-(s-1)L-\left(\sum_{j=1}^{\alpha} a_{sj} - a_{s\alpha}\right)\right] - \theta\left[x-(s-1)L-\sum_{j=1}^{\alpha} a_{sj}\right]\right\}. \quad (20)$$

In Eq. (20) $\theta(x)$ is the Heaviside function, $s = \pm 1, \pm 2, \ldots$ is the number of a 1D-crystal cell, index $\alpha = 1,2,\ldots,\sigma$ designates the elements of the cell. Here, *L* is the cell spacing; for the ideal 1D structure, $\chi(x) = \chi(x+L)$. The latter allows us to describe the vector of the surface density of electric dipole moment using the Floquet theorem

$$\Pi(x) = \exp(-iKx)\sum_{p} f_{K,p}\exp\left(ip\frac{2\pi}{L}x\right), \quad (21)$$

the Bloch vector $\vec{K} = (K,0,0)$ being directed along the *x* axis. Thus, since the Fourier representation $\Pi(x)$, owing to (21), has the form $\Pi(q) = \sum_p f_{K,p} \delta\left(q + K - \frac{2\pi}{L} p\right)$, we obtain from (19) the following system of equations with respect to the Fourier amplitude $f_{K,p}$:

$$S_n(K,\omega) f_{K,p} = \sum_l \left(\chi^{-1}\right)_l f_{K,p-l} \,. \tag{22}$$

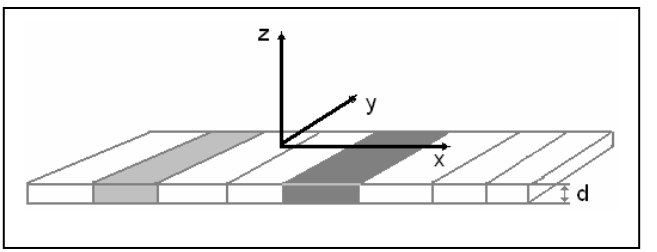

Figure 3. 1D superlattice composed of compositionally homogeneous elements (strips).

The object of this study is a nonideal 1D superlattice. The imperfection in our case can be caused by variations in the both composition and thickness 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 the case of the variations in the composition configuration-dependent value is the film polarizability

$$\chi_{s\alpha} = \sum_{\nu(\alpha)} \chi_{\alpha}^{\nu(\alpha)} \eta_{s\alpha}^{\nu(\alpha)} \,. \tag{23}$$

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 a procedure of configurationally averaging. In addition, from Eq. (23) we have the relation

$$\left\langle \chi_{s\alpha} \right\rangle = \sum_{\alpha,\nu(\alpha)} \chi_{\alpha}^{\nu(\alpha)} C_{\alpha}^{\nu(\alpha)} \,. \tag{24}$$

Where $C_{\alpha}^{\nu(\alpha)}$ is the concentration of the $\nu(\alpha)$-th sort 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. (20) 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 (24) are related as

$$\left(\chi^{-1}\right)_l = -\frac{i}{2\pi l} \sum_{\alpha} \left\langle \left(\chi^{-1}\right)_{s\alpha} \right\rangle \left\{ \exp\left(i \frac{2\pi}{L} l \sum_{j=1}^{\alpha} a_j \right) - \exp\left[i \frac{2\pi}{L} l \left(\sum_{j=1}^{\alpha} a_j - a_\alpha \right) \right] \right\} \tag{25}$$

If the strips are inhomogeneous in their thickness, the configuration-dependent value is $a_{s\alpha}$:

$$a_{s\alpha} = \sum_{\nu(\alpha)} a_{\alpha}^{\nu(\alpha)} \eta_{s\alpha}^{\nu(\alpha)} \,. \tag{26}$$

After averaging the configuration of expression (26) and the corresponding replacements:

$a_{s\alpha} \to \left\langle a_{s\alpha} \right\rangle \equiv a_{\alpha}\left(C_{\alpha}^{\nu(\alpha)}\right)$, $L \to L\left(C_{\alpha}^{\nu(\alpha)}\right)$, we have

$$a_{s\alpha} = \sum_{\nu(\alpha)} a_{\alpha}^{\nu(\alpha)} C_{s\alpha}^{\nu(\alpha)} \,. \tag{27}$$

The configurationally averaging "restores" the translational symmetry of a crystalline system. The normal modes of electromagnetic waves

propagating in this "periodic" structure are determined by the system of Eqs. (22). For simplicity, below we assume that the value of the Bloch vector *K* is close to the values determined by the Bragg's condition. In this case, when the main terms of (22) are $f_{K,p}$ at $p = 0$ and $p = -1$, which corresponds to the resonance between these components of the plane waves, the system of equations (22) takes the form

$$\begin{bmatrix} S_n(\omega, K) - \left(\chi^{-1}\right)_0 & -\left(\chi^{-1}\right)_1 \\ -\left(\chi^{-1}\right)_{-1} & S_n(\omega, K - 2\pi / L) - \left(\chi^{-1}\right)_0 \end{bmatrix} \cdot \begin{pmatrix} f_{K,0} \\ f_{K,-1} \end{pmatrix} = 0 . \quad (28)$$

The dispersion relations $\omega_{\pm} = \omega(K)$ follow from the equality of the determinant of the system (28) to zero.

RESULTS AND DISCUSSION

To specify the results, consider the propagation of electromagnetic excitation in an imperfect quasi-two-dimensional 1D superlattice with two elements (strips) in the cell, namely, with the first strip of silicon and the second strip of SiO_2 ($\varepsilon_2 = 3.7$). Note that the approximation of the film by a thin isotropic plate with the thickness *d* allows one to obtain the relation between $\chi_{nn} \equiv \chi$ component of the polarizability tensor and the plate permittivity ε ,

$$\chi = d(\varepsilon - 1) / 4\pi\varepsilon . \quad (29)$$

Below we are considered the case of admixture layers of a variable thickness and composition only in Si-sublattice. The concentration and thickness of the basic material layer in the first and second sublattices are denoted as $C_1^{(1)}, a_1^{(1)}, \varepsilon_1^{(1)} \equiv \varepsilon_1$ and $C_2^{(1)}, a_2^{(1)}, \varepsilon_2^{(1)} \equiv \varepsilon_2$, and the corresponding parameters of impurity strips (strips with a different composition and thickness), as $C_1^{(2)} \equiv C_C$ or $C_1^{(2)} \equiv C_T$ and $a_1^{(2)}, \varepsilon_1^{(2)}$. Simple calculations taking into account (25)-(29), 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:

$$\Delta\omega = |\,\omega_{+}\left(K_{\min}\right) - \omega_{-}\left(K_{\max}\right)| \cong c\,\frac{|\left(\chi^{-1}\right)_{1} + \left(\chi^{-1}\right)_{0}\,|}{2\pi} \qquad (30)$$

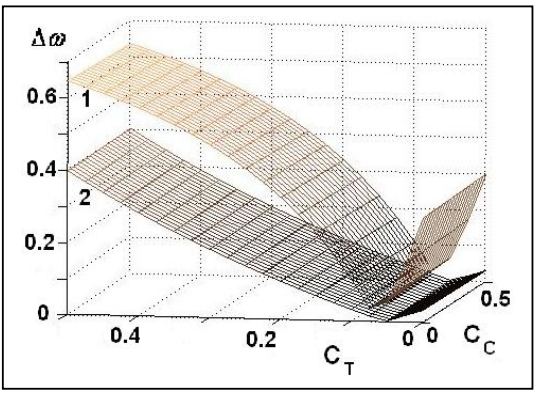

Figure 4. Concentration dependence for a nonideal quasi-two-dimensional Si/SiO_2 1D superlattice which contains defect strips of a variable thickness and composition only in Si-sublattice. $\Delta\omega$ is given in units of $2c/d$ (c is the speed of light and d is the film thickness).

($|K| \le \pi / L$) and allow us to plot the dependences $\Delta\omega\left(C_C\,, C_T\right)$ for different relative both composition and thickness of strips (see Figure 4). Surface 1 refers the case of $\varepsilon_1^{(2)} / \varepsilon_1 = 1.3$ and $a_1^{(1)} / a_2 = 0.9$, $a_1^{(2)} / a_1^{(1)} = 10$, surface 2 corresponds to the case of $\varepsilon_1^{(2)} / \varepsilon_1 = 1.1$ and $a_1^{(1)} / a_2 = 1.5$, $a_1^{(2)} / a_1^{(1)} = 0.01$.

Let us add to Si and SiO_2 strips the third strip of GaAs ($\varepsilon_3 = 11$). 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 $C_3^{(1)}, a_3, \varepsilon_3^{(1)} \equiv \varepsilon_3$ as well as the corresponding parameters of impurity strips (strips with 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 (25,28), yield the following expression for the lowest photonic band gap width $\Delta\omega$ of the system studied (30) and allow us to plot the dependences $\Delta\omega\left(C_2^{(2)}, C_3^{(2)}\right)$ (see Figure 5). Here the values of $\left(\chi^{-1}\right)_0$ and $\left(\chi^{-1}\right)_1$ are found from the relations:

$$\varepsilon_{(0)} = \left(\varepsilon_1 a_1 + \varepsilon_2 a_2 f_2 + \varepsilon_3 a_3 f_3\right)/L ,$$

$$\begin{aligned} |\varepsilon_{(1)}| = \frac{1}{\pi\sqrt{2}}[&(\varepsilon_1)^2\left(1-Cos\frac{2\pi a_1}{L}\right)+(\varepsilon_2 f_2)^2\left(1-Cos\frac{2\pi a_2}{L}\right)+ \\ &+(\varepsilon_3 f_3)^2\left(1-Cos\frac{2\pi a_3}{L}\right)+\varepsilon_1\varepsilon_2 f_2\left(-1+Cos\frac{2\pi a_1}{L}+Cos\frac{2\pi a_2}{L}-Cos\frac{2\pi a_3}{L}\right)+ \\ &+\varepsilon_1\varepsilon_3 f_3\left(-1+Cos\frac{2\pi a_1}{L}+Cos\frac{2\pi a_3}{L}-Cos\frac{2\pi a_2}{L}\right)+ \\ &+\varepsilon_2\varepsilon_3 f_2 f_3\left(-1+Cos\frac{2\pi a_2}{L}+Cos\frac{2\pi a_3}{L}-Cos\frac{2\pi a_1}{L}\right)]^{1/2} \end{aligned} \qquad (31)$$

using eq. (29) and the following expressions:

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

$$f_2 = 1 - C_2^{(2)}\left(1 - \frac{\varepsilon_2^{(2)}}{\varepsilon_2^{(1)}}\right) , \quad f_3 = 1 - C_3^{(2)}\left(1 - \frac{\varepsilon_3^{(2)}}{\varepsilon_3^{(1)}}\right) . \qquad (32)$$

Figure 5 (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 structure, as 1D composite superlattice, for different relative composition of strips. It is clearly seen that the shape of corresponding surfaces considerably depends on both thickness of strips and composition of randomly included admixture strips. For some values of the parameters the energy

gap of a quasi-two-dimensional $Si/SiO_2/GaAs$ photonic crystal may be equal to zero (see case a), but for another ones it is monotonic (see cases b and c).

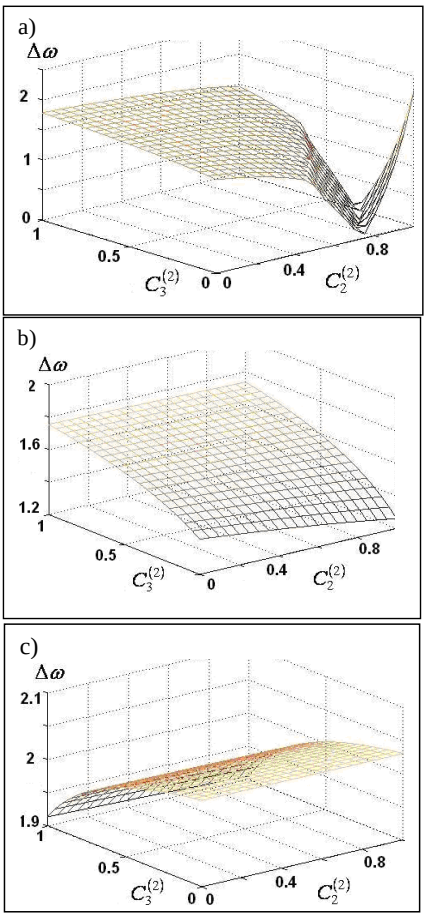

Figure 5. Concentration dependence $\Delta\omega\left(C_2^{(2)}, C_3^{(2)}\right)$ of imperfect quasi-two-dimensional $Si/SiO_2/GaAs$ superlattice for different relative thickness of strips and composition of randomly included admixture strips:

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).

Chapter 5

CONCLUSION

In the current interpretation, the quasi-particle excitation (e.g. polaritons) can be easily described using the Green function. For the disordered macroscopically homogeneous (in particular, topologically ordered) nonideal systems the averaged single-particle Green functions are applied, which are translational invariant within site representation and expressed through resolvent $\left\langle \hat{R}(\omega) \right\rangle = \left\langle \left(\frac{1}{\hbar\omega - \hat{H}} \right) \right\rangle$ of the corresponding quasi-particle Hamiltonian $\hat{H}$ [21,33]. It is well known that $\hat{R}(\omega)$ calculation reduces to the calculation of self-energy part $\hat{\Sigma}(\vec{k}, \omega, C)$ dependent on concentration C of impurities, frequency ω and wave vector $\vec{k}$. The real part of $\hat{\Sigma}(\vec{k}, \omega, C)$ defines renormalization of quasi-particle spectrum, the imaginary one – damping (and, as a consequence, the free path length) of corresponding excitations. This description is just only for those frequency intervals when the inequality

$$\mathrm{Im}\,\hat{\Sigma} << \mathrm{Re}\,\hat{\Sigma} \qquad (33)$$

is satisfied. The frequency intervals (for which (33) is satisfied) depend on specific relationships between parameters of the system, as well as on value of defect concentration. Definition of the criteria for inequality (33) to be satisfied is a rather complicate problem solved, in particular, in papers [34]. As (33) is not always satisfied, the choice and application of

the approximation for finding $\hat{\Sigma}(\vec{k},\omega,C)$ should be based on experimental data.

In this chapter (the same as in [24,25,31,35]) to consider translational invariant model systems (the configuration averaging restores configuration invariance) the virtual crystal approximation [19,20] is used, hence $\mathrm{Im}\,\hat{\Sigma}=0$ [21,23]. We were not concerned with the proving of VCA applicability (or with finding limits for satisfying conditions of (33). It is evident that the VCA is the roughest one among the mentioned [19-21,33,34] approximations, which is suitable for a general (without going in for details of quasi-particle spectrum fine structure) interpretation of experimental data (the values expressed through the averaged Green function). It is not universal.

It should be noted that here as well as in previous papers dealing with the analysis of three-dimensional [24,25,31] or quasi-two-dimensional [35] systems (as 1D superlattices), a one-dimensional chain is not the object of study. That's why, the Fourier transform of the averaged Green function (and of the self-energy part) depends on three-dimensional wave vector $\vec{k}$ (not on one-dimensional). In this chapter the problem relates to a particular case of electromagnetic excitation propagation with $\vec{k}$ directed along the normal to the layers. We can state that under certain conditions for three-dimensional [24,25,31] and quasi-two-dimensional [35] layered systems with arbitrary number of extrinsic layers or stripes, there exist frequency range in which propagation of electromagnetic excitations through these structures is allowed.

Our results show that the optical characteristics of imperfect 1D superlattice may be significantly altered owing to transformation of their polariton spectrum resulted a presence of admixture layers (strips). Graphic representation $\Delta\omega\left(C_1^{(2)},C_2^{(2)}\right)$ proves that the concentration dependence for the binary or ternary systems considered above differs for different relative composition or thickness of layers (strips). The case of nonideal multilayered (multistriped) systems with a larger number of sublattices and components of alien layers (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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