Optical properties of one-dimensional photonic crystals based on multiple-quantum-well structures

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A general approach to the analysis of optical properties of photonic crystals based on multiple-quantum-well structures is developed. The effect of the polarization state and a nonperpendicular incidence of the electromagnetic wave is taken into account by introduction of an effective excitonic susceptibility and an effective optical width of the quantum wells. This approach is applied to consideration of optical properties of structures with a pre-engineered break of the translational symmetry. It is shown, in particular, that a layer with different exciton frequency placed at the middle of an MQW structure leads to appearance of a resonance suppression of the reflection.

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I. INTRODUCTION

Structures with spatially modulated dielectric properties (photonic crystals) attract an ever-growing interest since the early papers where they were considered.[1,2] This interest is caused by unique opportunities that such structures provide, to affect, in a controllable way, fundamental *microscopic* processes of light-matter interaction through a modification of *macroscopic* geometric characteristics of the structures. This makes such structures of obvious interest not only for fundamental physics but also for applications. Most of the works devoted to photonic crystals considered structures made of materials with a frequency-independent dielectric constant.[3,4] Recently, however, a class of structures, which can be described as resonant or optically active photonic crystals, has attracted particular attention.[5–13] In these structures periodic modulation of the dielectric constant is accompanied by the presence of internal excitations of constituent materials resonantly interacting with light within a certain frequency region and resulting in a strong frequency dispersion of constituent dielectric constants. Extreme cases of such structures are so-called optical lattices, in which well-localized resonant elements are periodically distributed through the medium with a uniform dielectric constant. Originally, the concept of optical lattices referred to structures formed by cold atoms,[14] but it was also applied to a special kind of multiple-quantum-well structure (MQW), which was considered as a semiconductor analog of a one-dimensional optical lattice.[15]

MQW is a periodic multilayer structure built of two semiconductor materials, for instance, GaAs and $Al_xGa_{1-x}As$, in which electrons and holes are confined in narrower layers of a material with a smaller band gap (quantum wells) separated by wide layers of a semiconductor with larger band gap (barriers). In this case, the role of dipole active resonant excitations is played by excitons confined to respective quantum wells, and if the width of the barriers is large enough, excitons from different quantum wells do not interact directly. They, however, still can interact through their common radiation field, and in this sense they are similar to atomic optical lattices. This analogy is exact only if one can neglect a difference in refractive indexes of wells and barriers. This approximation was widely used in most papers devoted to long-period MQW structures, in which the period of the structure is comparable to the wavelength of exciton radiation.[16,17] Of special interest are so-called Bragg structures, in which the excitonic wavelength is in Bragg resonance with the periodicity and which are characterized by a significantly enhanced radiative coupling between quantum-well excitons. As a result of this coupling, light propagates through such a structure in the form exciton polaritons, whose dispersion law is characterized by two branches with a band gap between them.[16,17] The width of this stop band is significantly enhanced compared to off-Bragg structures, and this is what makes such structures of particular interest for applications.

In realistic MQW structures, however, dielectric constants of the wells and barriers are not equal to each other, and the presence of resonant optical excitations is accompanied by a periodic modulation of the background dielectric constant. These structures, therefore, represent a special case of one-dimensional resonant photonic crystals, optical properties of which are characterized by an interplay between interface reflections and resonant light-exciton interaction. The effects of the refractive index contrast on the optical properties of MQW structures have not been overlooked, of course, in previous studies. In particular, a modification of the Bragg condition and reflection spectra at normal incidence of Bragg MQWs in the presence of the contrast have been discussed in Refs. 18 and 19. The effects of the dielectric mismatch on optical properties of single quantum wells[20,21] or a MQW structure embedded in a dielectric environment[22,23] was also taken into account. In principle, optical spectra of any given MQW-based structure can be easily obtained numerically. Numerical calculations, however, do not provide a real physical insight into relations between structure and optical properties of the systems under consideration. At the same time, such an insight is crucial for understanding fundamental physics of these materials, as well as for efficient design of structures with predetermined optical properties, which is a key element in utilizing these structures for optoelectronic applications. In order to achieve such a qualitative understanding of optical properties of these materials, one needs a unified *analytical* framework, which has not yet been developed. The main difficulty of this task is the presence of a large number of experimental parameters, such as an angle of incidence, a polarization state, indices of refraction, widths of the barriers, the quantum wells, etc., which are in a complicated way related to spectral characteristics of a structure. The problem becomes even more difficult if one needs to consider complex systems, such as periodic MQW structures with several wells in an elementary cell[19] or with intentionally introduced "defects."[24–26] In order to resolve these difficulties, one needs a general effective analytical approach that would facilitate establishing relationships between material parameters and spectral properties of MQW-based structures for an arbitrary angle of incidence and polarization state of incoming light.

Developing such a method is the main objective of the present paper. The method is based on the transfer matrix approach and consists of two steps. In the first step, we show that a quantum well embedded in a dielectric environment can be described in exactly the same way as a quantum well in vacuum by introducing an effective excitonic susceptibility and an effective optical width of the quantum-well layer. In the second step, we establish relations between these effective quantum-well characteristics and parameters of the total transfer matrix describing propagation of light throughout the entire structure. The method is rather general and can be applied to a great variety of different MQW structures with light of an arbitrary polarization, incident at an arbitrary angle. In order to demonstrate the power of our approach, we consider reflection spectra of a MQW structure in which a central well is replaced with a well having a different resonant frequency. Such structures have been considered previously in a number of papers[24–26] in the optical lattice approximation. Here we show how such a structure can be effectively described even in the presence of the refractive index contrast and that its presence does not destroy the remarkable reflection properties of such structures, confirming, therefore, their potential for optoelectronic applications.

II. A SINGLE QUANTUM WELL IN A DIELECTRIC ENVIRONMENT

Propagation of the electromagnetic wave in structures under discussion is governed by the Maxwell equation

$$\nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2}[\epsilon_\infty(z)\mathbf{E} + 4\pi \mathbf{P}_{\rm exc}], \tag{1}$$

with modulated background dielectric permeability $\epsilon_\infty(z)$, which is assumed to take values n_b^2 and n_w^2 in the barriers and the quantum wells materials, respectively. For the sake of concreteness we assume hereafter that $n_w > n_b$, unless otherwise explicitly specified. $P_{\rm exc}$ is the excitonic contribution to the polarization and is defined by

$$\mathbf{P}_{\rm exc} = \chi(\omega) \int \Phi(z)\Phi(z')\mathbf{E}(z')dz', \tag{2}$$

where $\Phi(z)$ is the exciton envelope function. Here we have restricted ourselves by taking into account 1s heavy-hole excitons only and have neglected the in-plane dispersion of the excitons. The frequency dependence of the excitonic susceptibility is described by

$$\chi(\omega) = \frac{\alpha}{\omega_0 - \omega - i\gamma}, \tag{3}$$

where ω_0 is the exciton resonance frequency, γ is the nonradiative decay rate of the exciton, $\alpha = \epsilon_b \omega_{\rm LT} a_B^3 \omega_0^2/4c^2$, $\omega_{\rm LT}$ is the exciton longitudinal-transverse (LT) splitting, and a_B is the bulk exciton Bohr's radius.

Because of the absence of an overlap of the exciton wave functions localized in different quantum wells and the linearity of the Maxwell equations, the propagation of the electromagnetic wave along the structure can be effectively described by a transfer matrix. Using the usual Maxwell boundary conditions, the transfer matrix through one period of the structure in the basis of incoming and outgoing plane waves can be written in the form

$$T = T_b^{1/2} T_{bw} T_w T_{wb} T_b^{1/2}, \tag{4}$$

where

$$T_b^{1/2} = \begin{pmatrix} e^{i\phi_b/2} & 0 \\ 0 & e^{-i\phi_b/2} \end{pmatrix} \tag{5}$$

is the transfer matrix through the halves of the barriers surrounding the quantum well. Here $\phi_b = \omega n_b d_b \cos\theta_b / c$ with d_b being the width of the barrier and θ_b being an angle between the wave vector $\mathbf{k}$ inside the barrier and the direction of the z axis, $\hat{\mathbf{e}}_z$.

The scattering of the electromagnetic wave at the interface between the quantum well and the barrier caused by the mismatch of the indices of refraction of their materials is described by

$$T_{bw} = T_{wb}^{-1} = T_\rho(\rho) \equiv \frac{1}{1+\rho}\begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}, \tag{6}$$

where ρ is the Fresnel reflection coefficient. The interface scattering depends upon both the angle of incidence of the wave and its polarization state. These effects are effectively described by Fresnel coefficients (see, e.g., Ref. 27) ρ_s and ρ_p

$$\rho_s = \frac{n_w \cos\theta_w - n_b \cos\theta_b}{n_w \cos\theta_w + n_b \cos\theta_b},$$

$$\rho_p = \frac{n_w \cos\theta_b - n_b \cos\theta_w}{n_w \cos\theta_b + n_b \cos\theta_w} \tag{7}$$

for $s[\mathbf{E} \perp (\mathbf{k}, \hat{\mathbf{e}}_z)]$ and $p[\mathbf{E} \parallel (\mathbf{k}, \hat{\mathbf{e}}_z)]$ polarizations, respectively. The angular dependence of these coefficients on the angle of incidence measured inside the barrier is schematically shown in Fig. 1.

Finally,

$$T_w = \begin{pmatrix} e^{i\phi_w}(1 - iS) & -iS \\ iS & e^{-i\phi_w}(1 + iS) \end{pmatrix} \tag{8}$$

is the transfer matrix through the quantum well. Here $\phi_w = \omega n_w d_w \cos\theta_w / c$, where d_w is the width of the quantum well

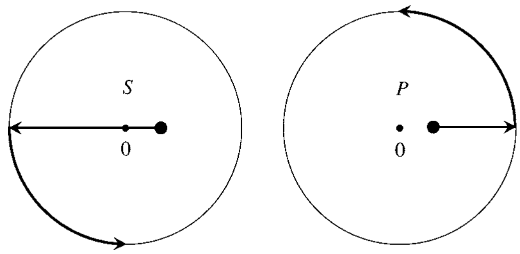

FIG. 1. A scheme of the angular dependence of the Fresnel coefficients ρ_s and ρ_p on the angle θ_w is shown on the complex plane. At normal incidence the coefficients have values shown by small filled circles (the same for both polarizations). When the angle of incidence increases, the coefficients follow the arrows on the lines. ρ_p passes through zero at the Brewster's angle, both coefficients reach the unit circle at the angle of total internal reflection. When the angle increases further, the Fresnel coefficients become complex with the unit modulus and increasing argument.

and θ_w is the angle between $\mathbf{k}$ inside the quantum well and $\hat{\mathbf{e}}_z$. The excitonic contribution to the scattering of the light is described by the function

$$S = \frac{\Gamma_0}{\omega - \omega_0 + i\gamma}, \tag{9}$$

which we will call the excitonic susceptibility in what follows. The radiative decay rate Γ_0 at normal incidence is determined by

$$\Gamma_0 = \frac{1}{2}\pi k \omega_{\mathrm{LT}} a_B^3 \left(\int \Phi(z) \cos kz \, dz \right)^2. \tag{10}$$

For oblique incidence the radiative decay rates are renormalized in different ways for different polarizations. For p polarization in addition to this renormalization it is also necessary to take into account a possible splitting of Z- and L-exciton modes,[30–32] which gives rise to a two-pole form of S. However, in materials with the zinc-blende structure, the Z mode of the heavy-hole excitons is optically inactive and one can describe angle dependencies of the radiative decay rate for s and p polarizations, respectively, by simple expressions

$$\Gamma_0^{(s)} = \Gamma_0/\cos \theta_w, \quad \Gamma_0^{(p)} = \Gamma_0 \cos \theta_w. \tag{11}$$

Thus, propagation of light in the structures under consideration depends on a number of natural parameters (such as Fresnel coefficients, exciton frequencies, and radiative decay rate) and optical widths, which (with the exception of ω_0) depend on the angle of incidence of the wave and its polarization state.

Our next step will be to simplify the presentation of the total transfer matrix through the period of the structure in such a way that makes the relations between the elements of the transfer matrix and the natural parameters of the structure more apparent. The most complicated part of the transfer matrix is the product $T_{bw}T_wT_{wb}$, which describes the reflection of the wave from the interface and its interaction with quantum-well excitons. We simplify it by noting that this product can be presented as $T_{bw}T_wT_{wb} = \widetilde{T}_w$, where $\widetilde{T}_w$ has the same form as T_w, Eq. (8), but with renormalized parameters

$$\widetilde{T}_w = T_{bw}T_wT_{wb} = \begin{pmatrix} e^{i\widetilde{\phi}_w}(1 - i\widetilde{S}) & -i\widetilde{S} \\ i\widetilde{S} & e^{-i\widetilde{\phi}_w}(1 + i\widetilde{S}) \end{pmatrix}, \tag{12}$$

where the effective excitonic susceptibility $\widetilde{S}$ and the phase shift $\widetilde{\phi}_w$ are defined as

$$\widetilde{S} = S\frac{1 + \rho^2 - 2\rho \cos \phi_w}{1 - \rho^2} + 2\rho \frac{\sin \phi_w}{1 - \rho^2},$$

$$e^{i(\widetilde{\phi}_w - \phi_w)} = \frac{1 - \rho e^{-i\phi_w}}{1 - \rho e^{i\phi_w}}. \tag{13}$$

Here ρ denotes the Fresnel coefficient for the wave of a respective polarization. Taking into account the diagonal form of the transfer matrix through the barrier T_b, one can see that the total transfer matrix through the period of the structure again has the form of a single-quantum-well transfer matrix and is determined by Eq. (8), where the phase $\widetilde{\phi}_w$ is replaced by a total phase $\phi = \phi_b + \widetilde{\phi}_w$.

Thus, we have shown that the propagation of the wave in MQW-based photonic crystals can be described in terms of properties of a respective optical lattice with renormalized parameters. The renormalization of the phase is the simplest one: the expression for $\widetilde{\phi}_w$ can be rewritten as

$$\widetilde{\phi}_w = \phi_w \frac{1 + \rho}{1 - \rho}, \tag{14}$$

provided that the change of phase ϕ_w across the well is much smaller than 2π, which is usually true for long-period MQW structures. Hence, one of the effects of the index-of-refraction contrast is reduced to a simple renormalization of the optical width of the quantum well.

The effective susceptibility $\widetilde{S}$ consists of two terms. One of them has a singularity at the exciton frequency, whereas the second varies slowly in a wide frequency region. The relation between these terms essentially depends on the frequency, and near the exciton resonance the second term is negligibly small. The frequency region where the nonsingular addition is negligible can be found from Eq. (13) and is determined by

$$|\omega - \omega_0| < \omega_{\min} = \frac{\Delta_\Gamma^2}{2\Delta_{PC}} \frac{1 + \rho^2 - 2\rho \cos \phi_w}{1 - \rho^2}. \tag{15}$$

Here $\Delta_\Gamma = \sqrt{2\Gamma_0\omega_0/\pi}$ is the half-width of the forbidden gap in a Bragg MQW without a mismatch of the indices of refraction, and $\Delta_{PC} = 2\omega_r \rho \sin[\phi_w(\omega_0)]/\pi(1 - \rho^2)$ is the half-width of the forbidden gap in a nonresonant (passive) photonic crystal with the same mismatch calculated in the limit $\Delta_{PC} \ll \omega_r$, where ω_r is the central frequency of the gap. In the presence of broadening (both homogeneous and inhomogeneous), there is an additional restriction on this frequency interval: $|\omega_0 - \omega| > \gamma$, and for sufficiently large γ it may cease to exist. This will mean that the exciton resonances play a very small role in the system, which, in this case, can be considered as a regular photonic crystal. In real GaAs/GaAlAs systems, this happens when γ exceeds the value of about 10 meV, which is significantly larger than

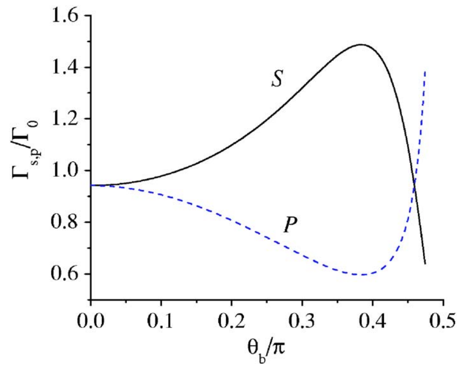

FIG. 2. Change of the effective radiative decay rates Γ_s (solid line) and Γ_p (dotted line) with the angle of incidence for a single quantum well.

inhomogeneous broadening in most QW structures, and corresponds to room temperatures for homogeneous broadening. Thus, in good quality samples and at sufficiently low temperatures there always exists a frequency region determined by Eq. (15), where the nonsingular addition to the effective susceptibility [Eq. (13)] is negligible regardless of how strong the mismatch between refractive indexes is. Depending on the strength of the mismatch, this region, however, can cover all or only part of the spectral interval affected by excitons. In the case of a single QW or of a MQW with a small number of periods, the frequency region of interest is of the order of Γ_0, which is typically much smaller than $\omega_{\min}$ in Eq. (15). In this case the refractive-index mismatch can be described in the resonant approximation with only the first term in Eq. (13) for the effective susceptibility retained. In this approximation, the effects of the mismatch of the indices of refraction, nonperpendicular incidence, and polarization are reduced to a renormalization of the radiative decay rate. This means that these effects can be taken into account by using standard expressions obtained for normal incidence in the absence of the mismatch with the radiative decay rate replaced with its effective value

$$\Gamma_{s,p} = \Gamma_0^{(s,p)} \frac{1 + \rho^2 - 2\rho \cos \phi_w}{1 - \rho^2}. \quad (16)$$

Depending on the value of the Fresnel coefficient one can observe either an enhancement (when $\rho<0$) or a reduction (when $\rho>0$) of the exciton radiative recombination. Since usually $n_w>n_b$, the Fresnel coefficient for the normal incidence is positive and therefore the oscillator strength is diminished compared to the case of the absence of the contrast. When the angle of incidence increases, in addition to different dependencies of the Fresnel coefficients corresponding to different polarization states following from Eqs. (7), it is necessary to take into account direct modification of the oscillator strength given by Eqs. (11). Figure 2 shows the dependence of the factor modifying the radiative decay rate on the angle of incidence.

III. OPTICAL PROPERTIES OF MQW STRUCTURES

In the previous section of the paper we showed that incorporating the mismatch in the refractive indexes of the wells and barriers into the description of the optical properties of MQW structures can be reduced to replacing exciton susceptibility and photon optical width with the respective effective parameters given by Eq. (13). It was also shown that for the single-QW case the effective susceptibility can be described in the resonant approximation, in which the role of the refractive-index mismatch is reduced to the renormalization of exciton radiative rate [Eq. (16)]. We start this section with ascertaining conditions when the same resonant approximation can be applied to Bragg MQW structures. The main difference between this case and the one considered in Sec. II is the width of the spectral interval of interest. In the case of Bragg MQW with a large number of periods we are interested in the region of the polariton stop band with width equal to Δ_Γ. The resonant approximation is valid for this entire part of the spectrum if $|\omega_{\min}-\omega_0| \gg \Delta_\Gamma$. It follows from Eq. (15) that this inequality is satisfied when

$$\Delta_\Gamma > 2\Delta_{PC}. \quad (17)$$

In real MQW structures based on III-V compounds the Fresnel coefficient at normal incidence,[33] ρ_0, are <0.03 and $\phi_w(\omega_0) \sim 0.1\pi$ can be considered as typical, so both quantities Δ_Γ and Δ_{PC} are of the same order of magnitude $\sim 10^{-2}$ eV. Therefore, both signs of the inequality (17) are possible, depending on details of the composition of the structures. The condition of Eq. (17) is, for instance, fulfilled for InGaAs/GaAs samples used in experiments of Ref. 35. In GaAs/$Al_xGa_{1-x}As$ structures with values of x of the order of 0.3 the opposite situation can take place. Therefore, in the remainder of the paper we will use an exact form of the effective susceptibility taking into account both resonant and nonresonant contributions.

Keeping in mind subsequent application to more complicated structures, it is convenient to introduce a special formal representation for a transfer matrix

$$T(\theta,\beta) = \begin{pmatrix} \cos\theta - i\sin\theta\cosh\beta & -i\sin\theta\sinh\beta \\ i\sin\theta\sinh\beta & \cos\theta + i\sin\theta\cosh\beta \end{pmatrix}, \quad (18)$$

where the parameters of the representation, θ and β, are related to the "material" parameters S and ϕ_w entering the transfer matrix by

$$\cos\theta = \mathrm{Tr}\, T/2 = \cos\phi + S\sin\phi,$$

$$\coth\beta = \cos\phi - S^{-1}\sin\phi. \quad (19)$$

This representation is valid for an arbitrary system that possesses a mirror symmetry with respect to a plane passing through the middle of the structure. It can be easily derived taking into account the equality of the determinant of the matrix to one and the circumstance that the mirror symmetry requires off-diagonal elements to be imaginary. Because of the general character of the representations (18), the material parameters entering Eq. (19) can be either the parameters of a single quantum well [Eq. (8)] or the effective parameters $\tilde{S}$ and $\tilde{\phi}$ [Eqs. (12) and (13)] of a barrier-well sandwich or even parameters characterizing the entire MQW structure as long as the latter possess the mirror symmetry.

Using this representation we can introduce the following transformation rule for transfer matrices

$$T_H(\psi)T(\theta,\beta)T_H^{-1}(\psi) = T(\theta,\beta+2\psi), \tag{20}$$

where matrix T_H describes a hyperbolic rotation with a dilation and has the form of

$$T_H(\psi) = e^{\psi}\begin{pmatrix} \cosh\psi & -\sinh\psi \\ -\sinh\psi & \cosh\psi \end{pmatrix}. \tag{21}$$

This transformation rule can be used, for instance, for diagonalization of transfer matrices, which can be achieved by choosing parameter $\psi=-\beta/2$. Matrix T_H can be turned into matrix T_{bw} [Eq. (6)], which describes propagation of waves through interface between two media with different refraction coefficients by using the following relation between ψ and the Fresnel parameter ρ: $\rho=-\tanh(\psi)$ (a detailed discussion of a relation between interface scattering and the hyperbolic rotation can be found in Ref. 34). This means that the transformation [Eq. (20)] can be either used to describe the interface between two different structures or in order to present any type of nondiagonality of the transfer matrix as resulting from some effective interface. With the help of Eq. (20), any symmetric multilayer structure can be replaced by a uniform slab with the width given by θ and the index of refraction determined by ψ. Therefore, it can be used to describe structures that are more complicated than a simple three-layer barrier-well sandwich considered in Sec. II. For instance, using Eq. (20) we can immediately derive an expression for the transfer matrix T_N of a sequence of identical blocks described by $T(\theta,\beta)$

$$T_N = T(\theta,\beta)^N = T(N\theta,\beta). \tag{22}$$

Because the reflection from the structure described by the transfer matrix T given in the basis of incoming and outgoing waves is

$$r = -T_{21}/T_{22}, \tag{23}$$

for a structure containing N blocks we have

$$r_N = -\frac{i\sinh\beta}{\cot N\theta + i\cosh\beta}. \tag{24}$$

The reflection coefficient written in terms of the parameters θ and β does not depend on the specific form of the transfer matrix and therefore Eq. (24) can be applied to a variety of different structures. In the case of $\Gamma_0=0$, Eq. (24) can be easily shown to reproduce the result well known for a passive multilayer structure.[4,28,29]

To find a relation between the quantities entering this expression and the elements of the transfer matrix through the period of the structure it is convenient to multiply both the numerator and denominator by $\sin\theta$ and to use Eq. (19). If each block is characterized by an effective susceptibility $\tilde{S}$ and the phase $\phi=\phi_b+\tilde{\phi}_w$, then we obtain for the reflection coefficient an exact expression

$$r_N = \frac{i\tilde{S}}{\cot(N\theta)\sin\theta + i(\tilde{S}\cos\phi - \sin\phi)}. \tag{25}$$

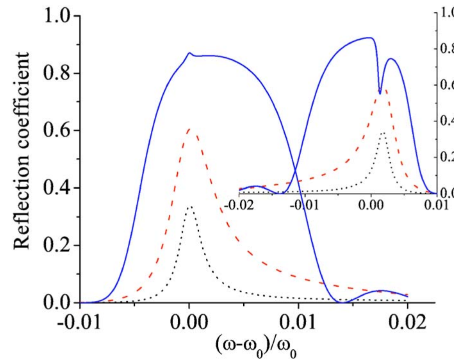

FIG. 3. Dependence of the amplitude reflection coefficient $|r_N|^2$ on the frequency. The main plot shows the reflection of structure satisfying the modified Bragg condition with $\rho=0.005$, the radiative decay rate $\Gamma_0=67$ μeV, the exciton frequency $\omega_0=1.491$ eV, the homogeneous broadening $\gamma=500$ μeV and the length $N=10$, 25, 100 (dotted, dashed, solid lines, respectively). On the inset reflection spectra of structures that satisfy the standard Bragg condition are shown. To make the correspondence with the results of Ref. 35 clearer we chose $\rho=-0.005$.

Below we analyze the reflection coefficient for Bragg and slightly off-Bragg structures. For frequencies close to ω_0 we can use $\theta=\pi+i\lambda$, where λ is a complex number with a small modulus. Moreover, in most applications of MQW structures it is naturally to assume that structures are not too long, that is $N\ll N_c=(\mathrm{Re}\,\lambda)^{-1}$. In this approximation, $\coth(N\lambda)\sinh\lambda \approx N$ and the reflection can be written directly in terms of the material parameters

$$r_N = \frac{iN\tilde{S}}{1 + iN(\tilde{S}\cos\phi - \sin\phi)}. \tag{26}$$

The amplitude of reflection $|r|^2$ has the typical form shown in Fig. 3. It is characterized by a strong reflection band around the exciton frequency, which is a manifestation of the strong resonant exciton-light interaction. The reflection has an asymmetric form since it is a sum of two terms: one of them is even with respect to the frequency ω_0 and the second is odd. The latter is due to nonzero mismatch and in the approximation used above does not vanish at infinity. Both these terms have a typical width

$$\delta = \frac{N\Gamma_0(1-\rho)^2\cos\phi_+}{(1-\rho^2)^2 + N^2(\sin\phi_+ - \rho^2\sin\phi_-)^2}, \tag{27}$$

where $\phi_\pm=\phi_b\pm\phi_w$. It should be noted that the actual optical width of the quantum well determined by ϕ_w enters the definition of $\phi_\pm$, rather than the modified $\tilde{\phi}_w$. We are interested in maximizing exciton-related effects in the reflection spectra of our structures, which means designing structures with as large a width δ as possible. One can see from Eq. (27) that the width demonstrates essentially nonmonotonous dependence on the number of quantum wells in the structure: it grows linearly for small N, but starts decreasing as N^2 for larger N. If the coefficient in front of N^2 in the denominator of Eq. (27) vanishes, then the linear growth of δ would go unchecked as long as N does not exceed N_c. Thus, the condition for maximizing the excitonic effects in the reflection spectrum can be formulated as

$$\rho^2 = \sin \phi_+(\omega_0)/\sin \phi_-(\omega_0). \tag{28}$$

If one neglects the mismatch of the indices of refraction, this equation takes a well-known form of a condition for the Bragg resonance between the period of the structure and the exciton radiation.[16] One can consider Eq. (28) as an equation for the period of the structure, d, for a given ρ. Then for the case of small ρ it gives approximately the same results as that obtained from

$$\rho = \cos(\phi_+/2)/\cos(\phi_-/2), \tag{29}$$

which coincides with a modified Bragg condition introduced in Ref. 19. This condition actually requires that the exciton frequency is equal to the low-frequency boundary of the passive (without excitons) photonic crystals' stop band. This consideration shows that the most prominent effect of the light-exciton interaction on the optical properties of long MQW structures with a mismatch of the indices of refraction occurs when the modified Bragg condition is met.

To establish the relation between the modified Bragg condition and the reflection spectrum of the structure, it is convenient to obtain the dispersion equation from the transfer matrix written in terms of $\tilde{S}$ and $\tilde{\phi}_w$ [Eq. (12)]. Using the relation $\cos Kd = \mathrm{Tr}\, T/2$, where K is the Bloch wave number, d is the period of the structure, one obtains the dispersion equation in the standard form

$$\cos Kd = \cos \phi + \tilde{S} \sin \phi, \tag{30}$$

where the change of the phase on the period of the structure ϕ is determined by the modified optical width of the quantum well, i.e., $\phi = \phi_b + \tilde{\phi}_w$. The Bragg resonance condition is written in a usual form $\phi(\omega_0) = \pi$ that can be shown to coincide with the modified Bragg condition from Ref. 19.

Thus, for Bragg MQWs the expression for the reflection coefficient [Eq. (25)] is essentially simplified and can be approximated as

$$r_N = \frac{iN\tilde{S}}{1 + iN\tilde{S}}. \tag{31}$$

This expression gives a generalization of a well-known result about the linear dependence of the width of the exciton-polariton reflection band on the number of quantum wells in Bragg MQW structures.[17]

When the system is detuned from the Bragg resonance, the transparency window appears in the band gap. It shows up in the form of a dip near the exciton frequency in the reflection spectrum (see inset in Fig. 3). For example, in Ref. 35 the reflection was measured for MQW structures that satisfied the Bragg condition for structures without the mismatch. In other words, the period of those structures was made to coincide with the half-wavelength at the exciton frequency calculated without taking into account photonic crystal modification of light dispersion. These effects, however, significantly modify the wavelength of light resulting in a detuning of the structures studied in Ref. 35 from actual

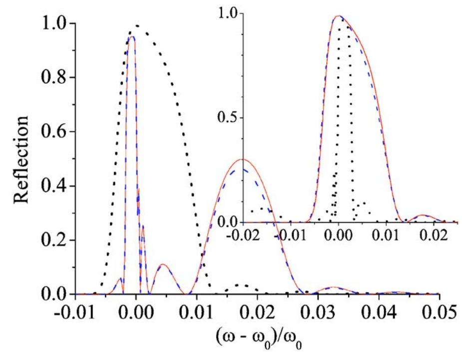

FIG. 4. The change of the reflection spectrum with the angle of incidence. The parameters of the structure are the same as those used in Fig. 3 except $\gamma = 25$ μeV, $\rho = 0.01$. The dotted line shows the reflection at normal incidence. The solid and dashed lines show the reflection at $\theta_b = \pi/18$ of s- and p-polarized waves, respectively. The main plot corresponds to the structure that is tuned to the Bragg resonance at normal incidence. The inset shows the reflection of a structure that is tuned to the Bragg resonance at $\theta_b = \pi/18$.

Bragg resonance. As a result, spectra observed in that paper demonstrate features specific for slightly off-resonance structures (see Fig. 3).

The general results presented in this section allows one to qualitatively analyze modifications in spectra of MQW structures caused by changes of the angle of incidence or polarization state of the wave. Indeed, using Eq. (14) we can write an expression for the renormalized phase ϕ in the form

$$\phi = \frac{\omega}{c}\left(n_b d_b \cos \theta_b + n_w d_w \frac{1+\rho}{1-\rho} \cos \theta_w \right). \tag{32}$$

This expression shows that the dependence of the Bragg condition on the angle of incidence differs significantly from the intuitive assumption that it can be accounted for by a simple replacement of the wave number k with $k \cos \theta$, which was suggested in some earlier works.[35] Although the latter assumption is true in the optical lattice approximation, the presence of the refractive-index contrast makes this dependence more complicated. Equation (32) also describes dependence of the Bragg condition on polarization.

Figure 4 demonstrates changes in the reflection spectrum for the structure tuned to the Bragg resonance for the normal incidence with the change of the angle. First, the spectrum for the oblique incidence looks as a typical spectrum for slightly off-Bragg structures. On the other hand, if a structure has a period that is bigger than what is required by the Bragg condition for normal incidence [i.e., $\phi(\omega_0, \theta=0) > \pi$], then it can be tuned to the resonance by increasing the angle of incidence (see inset in Fig. 4). An interesting result apparent from these figures is that tuning the structure to the Bragg resonance by changing the angle preserves, to a great extent, the shape of the spectrum. This fact opens a possibility for shifting the position of the reflection band of these structures by changing the exciton frequency with the help of, for instance, the quantum confined Stark effect[36] with consecutive tuning of the structure back to the Bragg resonance by adjusting the angle of incidence. Estimates show that for the

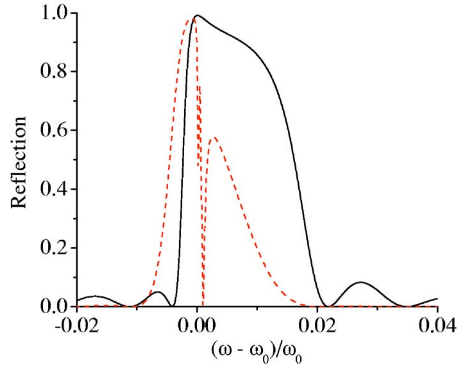

FIG. 5. The reflection spectrum of s- and p-polarized waves (solid and dashed lines, respectively) of a structure that is tuned to the Bragg resonance at $\theta_b = \pi/4$. The Bragg condition is met for s-polarized waves.

available Stark shifts of the exciton frequencies required changes in the angle do not exceed 10–15°, which is similar to the angles used in Fig. 4.

The difference between reflection spectra of waves with s and p polarizations remains rather insignificant for angles used in Fig. 4. In order to observe it one has to consider much larger angles. Figure 5 shows the reflection spectra of a structure that is tuned to the Bragg resonance at the angle $\theta_b = \pi/4$. The difference between the two polarizations occurs because of two circumstances. First is the different renormalization of the optical width of the quantum wells for different polarizations [Eq. (14)]. As a result, the angle at which the structure is tuned to the Bragg resonance depends on polarization. In Fig. 5 the Bragg condition is met for s polarization. Therefore, one has a typical Bragg profile for the reflection spectrum of the s-polarized wave and off-Bragg profile for the p-polarized wave. The second circumstance is the difference between the effective radiative decay rates [see Eq. (16)] for different polarizations. Therefore, the exciton related feature on the reflection spectrum of the p-polarized wave is weaker compared to the s polarization.

It should be noted, however, that such big angles of propagation inside the barriers are not accessible for a usual experimental setup when the wave is emitted and detected outside the structure. The reason is a high contrast of the indices of refraction of the vacuum and the barriers. However, such angles become relevant when the problem of luminescence is considered.

Another prominent effect caused by the refractive index mismatch consists of vanishing of the reflection coefficient $|r_N|^2$ at $\omega = \omega_0 - \omega_{\min}$ [see Eq. (15)] where $\tilde{S} = 0$. This is the consequence of an interference of two channels of scattering of light—by the excitons and by the barrier-well interfaces. For Bragg MQW structures, r_N can be written in a form that explicitly expresses the Fano-like profile of the reflection

$$r_N = r_N^{(0)} \frac{\omega - \omega_0 + \omega_{\min}}{\omega - \omega_0 + \omega_{\min} r_N^{(0)}}, \qquad (33)$$

where

$$r_N^{(0)} = \frac{i\pi N \Delta_{PC}}{\omega_r + iN\pi\Delta_{PC}} \qquad (34)$$

is the reflection in a vicinity of the photonic band gap of a passive, $\Gamma_0 = 0$, N-layer structure, which is not too long compared to the penetration length. When the mismatch of the indices of refraction vanishes, $\omega_{\min}$ turns to infinity and the reflection restores the Wigner-like form with the width $\propto N\Gamma$. This is similar to what one has in the standard Fano resonance case when the Fano parameter tends to infinity.[37] In the other limiting case, $\Gamma_0 = 0$, the reflection turns to what one has for a purely passive multilayer structure.

As discussed above, because of the relation between different contributions to the scattering of light in regular MQW structures, this resonant drop of reflection occurs at the tail of the excitonic susceptibility where the general smallness of the reflectivity masks this effect. In Sec. IV we consider a situation where vanishing of the reflectivity has a much more profound effect on the spectrum.

IV. MQW STRUCTURES WITH DEFECTS

The results obtained in the previous sections are quite general and can be applied directly to more complicated situations. As an example, in this section we consider a reflection spectrum of a system in which one of the barrier-well-barrier elements has properties different from those of all other elements of the structure. These structures can be described as MQW structures with a “defect.” In infinite systems such a defect results in the appearance of a local state, which arises in a band gap of the host structure. Then the transmission of light through finite but sufficiently long structures can be conveniently described in terms of resonant tunneling via such a state. This effect was studied in regular passive one-dimensional photonic crystals[38–42] and in Bragg MQWs in the optical lattice approximation.[24,43] In shorter systems, however, which are the main object of study in this paper, the concept of the resonant tunneling via a local state becomes ill defined, and therefore, we will interpret results of our calculations without resorting to this concept.

We will consider a structure in which the defect is placed in its center; such an arrangement is known to result in strongest modifications of the optical spectra.[24] In this case, the system demonstrates the mirror symmetry, and the results of the previous sections can be used. Indeed, for a structure ABA built of blocks A and B described by the transfer matrices (18) with parameters $\theta_{A,B}$ and $\beta_{A,B}$, one has

$$T(\theta_A,\beta_A)T(\theta_B,\beta_B)T(\theta_A,\beta_A) = T(\theta,\beta). \qquad (35)$$

That is, the whole structure can also be described by the matrix (18) with

$$\cos\theta = \cos\varphi_+ \cosh^2\delta\beta - \cos\varphi_- \sinh^2\delta\beta,$$

$$\coth(\beta - \beta_A) = \cos(2\theta_A)\coth\delta\beta + \frac{\sin\varphi_-}{\sin\theta_N \sinh(2\delta\beta)}, \qquad (36)$$

where $\varphi_\pm = 2\theta_A \pm \theta_B$ and $\delta\beta = (\beta_B - \beta_A)/2$. Applying now relations (19) one can express the result in terms of parameters S

and ϕ and use the results for reflection described above.

In some particular cases, however, the problem of scattering of light can be solved without resorting to the transformation rule (36). Let us consider a situation when the block B is a single-quantum well surrounded by barriers so it can be described by the matrix similar to that given by Eq. (12) with parameters S_d and ϕ_d. Let the block A be a MQW structure described by θ and β. Thus, the transfer matrix through the whole structure is

$$T = T(\theta,\beta)T_\rho(\rho)T(S_d,\phi)T_\rho^{-1}(\rho)T(\theta,\beta), \tag{37}$$

where $T_\rho(\rho)$ takes into account a possible mismatch of the indices of refraction of the defect layer and the host and ρ is the corresponding Fresnel coefficient.

The transfer matrix (37) can be simplified in several steps. First, as has been described before, we can treat β as an addition to the mismatch noting that

$$T_H^{-1}(\beta/2)T_\rho(\rho) = T_\rho(\tilde{\rho}), \tag{38}$$

where $\tilde{\rho}=(\rho+\rho')/(1+\rho\rho')$ and $\rho'=\tanh(\beta/2)$. Then, similar to Eq. (12) we can introduce effective quantities $\tilde{S}$ and $\tilde{\phi}$

$$\tilde{S} = S_d\frac{1+\tilde{\rho}^2-2\tilde{\rho}\cos\phi}{1-\tilde{\rho}^2} + 2\tilde{\rho}\frac{\sin\phi}{1-\tilde{\rho}^2},$$

$$e^{i(\tilde{\phi}-\phi)} = \frac{1-\tilde{\rho}e^{-i\phi}}{1-\tilde{\rho}e^{i\phi}}. \tag{39}$$

The next step is a multiplication of $T(\tilde{S},\tilde{\phi})$ by the diagonal matrices $T(\theta,0)$, which leads to a simple shift of the phase, $T(\tilde{S},\tilde{\phi}+2\theta)$. Finally, the terminating matrices $T_H(\beta/2)$ and $T_H^{-1}(\beta/2)$ are taken into account by modifying $\tilde{S}$ and $\tilde{\phi}$. Thus the resultant transfer matrix T takes the form (12), i.e., $T = T(\tilde{\tilde{S}},\tilde{\tilde{\phi}})$, with

$$\tilde{\tilde{S}} = \tilde{S}\frac{1+\rho'^2+2\rho'\cos(\tilde{\phi}+2\theta)}{1-\rho'^2} - 2\rho'\frac{\sin(\tilde{\phi}+2\theta)}{1-\rho'^2},$$

$$e^{i(\tilde{\tilde{\phi}}-\tilde{\phi}-2\theta)} = \frac{1+\rho' e^{-i\tilde{\phi}-2i\theta}}{1+\rho' e^{i\tilde{\phi}+2i\theta}}. \tag{40}$$

These expressions together with Eq. (24) give a complete solution of the problem of propagation of light through the MQW structure with an arbitrary defect in the middle.

One can consider several particular types of defects. An example is a well with the exciton frequency different from the frequencies of all other wells, an Ω defect. Another possible example could be a defect element with the width of the barriers different from the rest of the structure. It is interesting to note that a standard optical microcavity with a quantum well at its center can also be considered within the same formalism. For example, after substitution of $\tilde{S}$ from (39) into Eq. (40) one obtains an expression that contains a singular term (proportional to S_d) and regular terms. Choosing such widths of the barriers surrounding the quantum well so that the regular terms vanish in the vicinity of the exciton frequency one has the reflection determined by the exciton susceptibility with renormalized oscillator strength. The excitonic contribution to the scattering in such a structure will not be obscured by the interface scattering.

We demonstrate the application of the results obtained above by a detailed consideration of an Ω defect. This type of defect was analyzed in Refs. 24–26 in the scalar model for the electromagnetic wave in MQW structures without a mismatch of the indices of refraction. It has been shown there that in the presence of homogeneous and inhomogeneous broadening of excitons, the effect of the defect is prominent when the frequency of the exciton resonance in the defect layer ω_d is close to the boundary of the forbidden gap in the host system and the length of the system is not too big. The reflection spectrum in this case has the characteristic Fano-like dependence with a minimum followed by a closely located maximum. Such a spectrum makes this structure a potential candidate for such devices as optical switches or modulators.[25,26] It is interesting, therefore, to find out how the refractive-index mismatch affects spectral properties of such a structure.

For the frequencies within the polariton stop band of the host structure one has $\theta=M(\pi+i\lambda)$, where M is the number of quantum wells in the parts of the structures surrounding the defect and $M\lambda \ll 1$. The description becomes much simpler if we assume that the width of the defect layer is tuned to the Bragg resonance at the frequency ω_d; that is, if $\phi(\omega_d)=\pi$. That makes the second term in the expression for $\tilde{S}$ [Eq. (39)] negligible in a wide region of frequencies and the expression for $\tilde{\tilde{S}}$ takes a very simple form

$$\tilde{\tilde{S}} = S_d\frac{1+\rho}{1-\rho} + 2M\tilde{S}_h, \tag{41}$$

where $\tilde{S}_h$ is the effective excitonic susceptibility of the host, given by an expression similar to Eq. (13) with the exciton frequency $\omega_0=\omega_h$. In derivation of Eq. (41) we have neglected the small term $\propto S_d\tilde{S}_h$. The reflection coefficient can be obtained by substituting this expression into Eq. (24) with $N=1$. The reflection has peculiarities near the exciton frequencies of the host and the defect, and in the absence of broadening becomes zero at the frequency where $\tilde{\tilde{S}}=0$. Generally, this equation is suitable for finding the resonance frequency for any value of the photonic band gap Δ_{PC}, which is not much bigger than the excitonic forbidden gap Δ_Γ. Here, however, we only consider the perturbation of the spectrum analyzed in Ref. 25 because of small contrast in the refractive indexes. Therefore we assume here that $\Delta_{PC} \ll \Delta_\Gamma$. In this approximation the resonant frequency ω_R is

$$\omega_R = \omega_d - \frac{\Delta_\omega}{2M+1} - 16\frac{M^2\Delta_\omega^2\Delta_{PC}}{\Delta_\Gamma^2(2M+1)^3}, \tag{42}$$

where $\Delta_\omega=\omega_d-\omega_h$ is the difference between the defect and the host exciton frequencies, and we assume for concreteness that $\omega_d > \omega_h$.

Setting the mismatch of the indices of refraction in this expression to zero we reproduce the expression for ω_R obtained in Ref. 25. The fact that the contrast does not preclude the reflection coefficient from going to zero at a certain point is not at all obvious because it might have been expected that the interface reflection would set a limit on the decrease of the reflection. However, as seen from Eq. (42), the mismatch leads only to an additional shift of the zero point away from the defect exciton frequency. We would also like to comment on the dependence of the resonance frequency on the angle of incidence and the polarization of the electromagnetic wave. These characteristics enter Eq. (42) through the Fresnel coefficients [Eq. (7)], which determine the photonic band gap, $\Delta_{PC} \propto \rho/(1-\rho^2)$. Therefore angular and polarization dependencies of the zero point of reflection follow the behavior of Δ_{PC}. The obtained expression for the reflection coefficient also allows for analyzing the position of the maximum of reflection, and its maximum magnitude, but the resulting expressions turn out to be too cumbersome and we do not present them here.

The formalism presented in this paper allows one to take into account effects of homogeneous and inhomogeneous broadenings because the main results obtained do not use a particular form of the excitonic susceptibility. For example, the reflection coefficient of a structure with an inhomogeneous broadening can be obtained in the effective medium approximation by using Eq. (24) with $\tilde{\tilde{S}}$ instead of S and with inhomogeneously broadened $S_{h,d}$ in Eq. (42)

$$S_{h,d} = \int d\omega_0 f_{h,d}(\omega_0) \frac{\Gamma_0}{\omega - \omega_0 + i\gamma}, \tag{43}$$

where $f_{h,d}$ are the distribution functions of the exciton frequencies in the host and defect layers, respectively.[25,44,45] However, as it has been discussed in Ref. 25, if ω_R is far enough from ω_d (i.e., $|\omega_R - \omega_d| \gg \Delta$), where Δ is the inhomogeneous broadening, the effect of the latter is negligible and the magnitude of the reflection is determined by

$$|\tilde{\tilde{S}}|_{\min} \approx \frac{\pi\gamma(2M+1)}{4M\omega_d\Delta_\omega^2}[\Delta_\Gamma^2(2M+1)^2 + 16M(2M-1)\Delta_{PC}\Delta_\omega]. \tag{44}$$

The reflection is small provided the smallness of the homogeneous broadening, $\gamma \ll \omega_d$, and $\Delta_\omega \gtrsim \Delta_\Gamma \gtrsim \Delta_{PC}$.

There is a certain analogy between this effect of the resonant drop of reflection and turning the reflection to zero considered in Sec. III. In the case of a defect MQW structure, the Fano-like profile of the reflection, in a narrow vicinity of ω_d, can be understood as an interference of the scattering of light by the host structure and by the defect. Comparing Eq. (41) to Eq. (13) one can see that the second term in Eq. (41) plays the role of a background on which the exciton susceptibility of the defect quantum well appears. This is exactly the role played by the second term in Eq. (13). Expanding $\tilde{\tilde{S}}$ near ω_R the reflection can be represented in a form similar to Eq. (33). There is an essential quantitative difference between these two cases, however. In a defect MQW structure the drop of the reflection occurs not far away from the exciton frequency; therefore, this effect becomes more noticeable. A typical form of the reflection, transmission and absorption near ω_R is shown in Fig. 6.

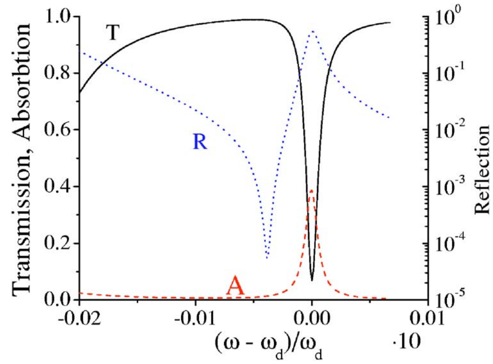

FIG. 6. The reflection (dotted line, right scale), transmission and absorption (solid and dashed lines, respectively, left scale) are shown in a vicinity of ω_R for a Bragg 5-1-5 structure. The parameters of the quantum wells are the same as those used in Fig. 3 except $\gamma = 25$ μeV, $\omega_h = 1.491$ eV, and $\omega_d = 1.495$ eV. To emphasize the resonant character of the change of the reflection it is plotted in the log scale. It should be noted that because of the large (in comparison with γ) separation between ω_R and ω_d the drop of the reflection is *not* accompanied with a resonant absorption.

It should be noted that if a regular term in the effective susceptibility of the defect layer is taken into account, then Eq. (41) for $\tilde{\tilde{S}}$ becomes valid not only in an immediate vicinity of ω_R but in a much wider region, including for example ω_h. In this region, the reflection can be seen to resemble the Fano profile in the case of two metastable states interacting with continuum.[46] As a result, the reflection has two resonances: near ω_h and ω_d. The first resonance is $2N$ times wider than the second one. The reflection reaches zero between these resonances at ω_R.

To conclude this consideration we would like to note that for multiple defect structures composed of several blocks, *ABA* considered above the reflection can be qualitatively described by Eq. (31) where N is understood as the number of such blocks. This expression shows that increasing N can be interpreted as increasing an effective radiative decay rate. This qualitatively explains the results of numerical calculations in Ref. 26 where it was found that the maximal value of the reflection increases with N, while the value of the ratio of the maximal and minimal values remains about the same.

V. CONCLUSION

In the present paper, the general problem of light propagation in a MQW-based photonic crystal characterized by both spatial modulation of the dielectric constant and dipole active exciton states in quantum wells is considered. It is shown that the mismatch of indices of refraction between barriers and wells can be taken into account by introduction of an effective excitonic susceptibility and an effective optical width of the quantum wells. The effective susceptibility has two terms, one of which is almost independent of frequency, whereas the second is resonant in nature. For sufficiently short MQW structures (or in the vicinity of the exciton frequency), the regular term can be neglected and the effect of the mismatch of the indices of refraction reduces to a modification of the excitonic oscillator strength. In a general case, the reflection spectrum becomes essentially asymmetric and nontrivially dependent on the number of quantum wells in the structure. It is shown that in order to obtain the strongest exciton-induced reflection band the structure must satisfy a certain resonance condition. This is a Bragg resonance condition between the period of the MQW structures and the wavelength of the electromagnetic wave. The latter has to be calculated from a dispersion law for a structure with the spatially modulated refraction index.

The developed approach is applied to analysis of the reflection spectrum of a structure with an intentionally introduced defect element, which breaks the translational symmetry of a system. A more detailed analysis is carried out for a special kind of defect, characterized by the presence of a layer in the middle of the structure with a different frequency of the exciton resonance. It is shown that the main characteristics of the reflection spectrum of such structures obtained in the absence of the refraction-index contrast survive in the presence of the additional interface reflections. In particular, a significant decrease of the reflection takes place even in the presence of the contrast, which is important for possible applications of such structures.

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