Optical properties of photonic crystal slabs with an asymmetrical unit cell

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(Received 25 February 2005; published 22 July 2005)

Using the unitarity and reciprocity properties of the scattering matrix, we analyze the symmetry and resonant optical properties of the photonic crystal slabs (PCS) with non-trivial unit cell. We show that the reflectivity does not change upon the 180°-rotation of the sample around the normal axis, even in PCS with asymmetric unit cell, whereas the transmissivity of the asymmetric PCS becomes asymmetrical if the diffraction or absorption are present. The PCS reflectivity peaks to unity near the quasiguided mode resonance for normal light incidence in the absence of diffraction, depolarization, and absorptive losses. For the oblique incidence the full reflectivity is reached only in symmetric PCS.

DOI: 10.1103/PhysRevB.72.045138 PACS number(s): 42.70.Qs, 42.25.Bs, 73.20.Mf, 78.66.−w

I. INTRODUCTION

The physics of photonic crystal slabs (PCS)[1–4] receives much attention in recent years because of many interesting possibilities they open to control the light interaction with matter. The tendency is toward the PCS sophistication: nanostructured metals or semiconductors are included, and the unit cell geometry, using modern technology, becomes more nontrivial. As a result, different tools for photonic engineering become available. A well-known example is the extraordinary optical transmission through subwavelength hole arrays in metal films.[5,6] Another promising example is a polaritonic crystal slab with nanostructured semiconductors.[7–9] The physics behind this is the coupling between photonic and different electronic resonances in such structures. They manifest themselves via pronounced resonant Wood's anomalies[10–12] in the optical spectra because of the excitation of quasiguided[3,4,13–18] or surface plasmon[5,19–21] or both[22] modes. On the other hand, making nontrivial unit cells, e.g., characterized by a lack of 180° rotational symmetry in the PCS plane[20,23] adds ways to control the interaction with light.

Thus, the understanding of the symmetry and resonance properties of the optical response in PCS with nontrivial unit cells becomes important, also for their optical characterization. Measuring reflection from asymmetric structure appears not to be a promising method for the PCS optical characterization, and a question arises: which optical properties are more sensitive to the PCS structure? Meanwhile, notwithstanding a long history of investigation (see, e.g., Refs. 12 and 24), actually starting from the optical gratings, which can be understood as one-dimensional (1D) PCS, their properties sometimes look amazing and even contradictory.

One example is the nontrivial symmetry properties of reflection and transmission from asymmetric PCS. Namely, it was demonstrated[20] experimentally and numerically that the reflectivity from 180° rotationally non invariant (in the PCS plane) metal gratings on a dielectric substrate is always symmetric, whereas the transmission is not. However, the transmission appears to be independent on the side of the illumination, whether it is from the air or from the substrate (see also Refs. 5 and 6). The authors of Ref. 20 find this *astonishing* because the calculated fields distributions inside the PCS appear to be very different for the illumination from different sides.

Another example is the so-called anomalous full reflection in the zeroth diffraction order in lossless PCS, when reflectivity peaks to unity resonantly.[12] It is established that excitation of surface or quasiguided modes in PCS is responsible for this resonant behavior. Such resonances, being Fano-type discrete states in the continuum background, are characterized by a finite frequency linewidth because of radiative losses even in lossless materials. The existence of radiative losses seems to contradict to the possibility of full reflectivity. However, all the numerical models[12,14,17,25–28] show this effect in transparent PCS. Moreover, it appears that very different realizations of photonic structures, with only one thing in common—the existence of *any* resonance—predict a qualitatively similar behavior of the PCS optical response (see, e.g., discussions in Refs. 17, 21, 27, 29, and 30).

The most general reasons of such behavior are hidden in the most general properties of the scattering matrix operator of the PCS. These general properties have actually been well known for many years (see, e.g., Ref. 31), but, to the best of our knowledge, their consequences for the photonic crystal slabs with a nontrivial unit cell have not been yet investigated in detail. In this paper, we recall the most general properties of the S matrix of the transparent arbitrary PCS and use them to analyze the symmetry properties of the optical response (Sec. II). We also investigate the resonances of the scattering matrix, especially the conditions of the anomalous full reflectivity in the zeroth diffraction order (Sec. III). For completeness, we also specify in Appendix A the numerical procedure to construct the unitary scattering matrix of a photonic crystal slab based on the scattering matrix method from Ref. 18. The reciprocity properties of the S matrix are proven in Appendix B.

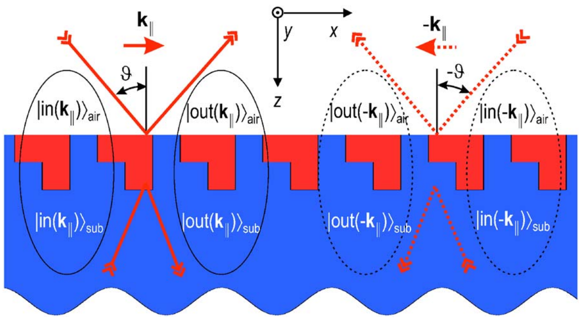

FIG. 1. (Color online) Geometry of light reflection and transmission from PCS. Solid and dashed arrows correspond to a direct and time-reversed process. Only the main harmonics are shown.

II. GENERAL PROPERTIES OF THE SCATTERING MATRIX

Starting from a general scattering matrix operator of a *planar periodic system* made of lossless materials, we note that many scattering channels are closed, e.g., the backscattering for inclined light incidence, as well as all non-Bragg scattering channels. In order to keep all nonzero general S-matrix elements, it is convenient to define the scattering matrix operator as a *unitary* $2N\times 2N$-dimensional matrix S_u, $S_u^\dagger S_u = S_u S_u^\dagger = 1$, coupling the amplitudes of incoming and outgoing harmonics (main and diffracted). Here $N=2+N_{\mathrm{open,air}}+N_{\mathrm{open,sub}}$, the augend 2 stands for the main harmonic (in air and substrate, to be replaced by 1 in the situation of total internal reflection), $N_{\mathrm{open,air}}$ and $N_{\mathrm{open,sub}}$ are the numbers of open diffraction orders (into the air and substrate claddings). Because of there being two polarization states per each harmonic (for example, s and p, or σ^+ and σ^-), there are $2N$ incoming as well as outgoing amplitudes (we assume isotropic air and substrate claddings).

The scattering matrix S_u couples the incoming and outgoing states

$$|\mathrm{out}(\mathbf{k})\rangle = S_u(\omega,\mathbf{k})|\mathrm{in}(\mathbf{k})\rangle, \tag{1}$$

see the scheme in Fig. 1. Here $S_u(\omega,\mathbf{k}_\parallel)$ is a function of the real incoming photon frequency ω and in-plane wave vector

$$\mathbf{k}_\parallel = (k_x,k_y) = \frac{\omega}{c}\sin\vartheta(\cos\varphi,\sin\varphi),$$

where ϑ and φ are the azimuthal and polar angles of light incidence. The wave vectors of the diffracted photons are

$$\mathbf{k}_{\parallel\mathbf{G}} = (k_{x\mathbf{G}},k_{y\mathbf{G}}), k_{x(y)\mathbf{G}} = k_{x(y)} + G_{x(y)}, \tag{2}$$

$$k_{z\mathbf{G}} = \pm\sqrt{\omega^2\varepsilon/c^2 - k_{x\mathbf{G}}^2 - k_{y\mathbf{G}}^2}, \tag{3}$$

where $\mathbf{G}=(G_x,G_y)$ is the reciprocal 2D PCS lattice, and $\varepsilon=1$ or $\varepsilon_{\mathrm{sub}}$, depending on the PCS side; $k_{z\mathbf{G}}$ is real for open diffraction channels.

Such unitary scattering matrix S_u can be constructed from the infinitely dimensional "large" scattering matrix $\mathbb{S}$, accounting for the near-field coupling between all the propagating and evanescent harmonics, and defined, e.g., in Ref. 18. $\mathbb{S}$ has to be reduced[24] to a "small" $2N\times 2N$-dimensional matrix S for propagating harmonics only and transferred into any energy-flow-orthogonal basis (e.g., of sp or $\sigma^\pm$ polarizations), we give the details of this transformation in Appendix A.

The symmetry of the system with respect to the time reversal in the case of PCS made of nongyrotropic transparent materials (compare to Ref. 32), means that for any solution $E(\omega,\mathbf{k}_\parallel)$, $H(\omega,\mathbf{k}_\parallel)$ of Maxwell equations for electric and magnetic fields, $E^*(\omega,-\mathbf{k}_\parallel)$, $-H^*(\omega,-\mathbf{k}_\parallel)$ remains a valid solution. This property, as well known,[27,31,33] leads to the *reciprocity* between the input and output channels. In the definition of the unitary matrix S_u it makes sense to fix the ordering of the channels in such a way that the input channels in $S_u(\omega,\mathbf{k}_\parallel)$ transfer into the output ones in $S_u(\omega,-\mathbf{k}_\parallel)$ and vice versa, upon time reversal, see the scheme in Fig. 1. In the case of s, p-polarizations basis, this can be written as

$$|\mathrm{in}\rangle \equiv |\mathrm{in}(\omega,\mathbf{k}_\parallel)\rangle = |\mathrm{out}(\omega,-\mathbf{k}_\parallel)^*\rangle \equiv |\widetilde{\mathrm{out}}\rangle. \tag{4}$$

Note the important complex conjugates in Eq. (4). We use here the conventional notations $\langle\psi| = |\psi\rangle^\dagger \equiv |\psi^*\rangle^\mathsf{T}$, so that $\langle\psi^*| = |\psi\rangle^\mathsf{T}$, where T stands for the matrix transpose. Then, the reciprocity of the unitary S_u matrix means[27,31] (see Appendix B) that

$$S_u(\omega,\mathbf{k}_\parallel) = S_u^\mathsf{T}(\omega,-\mathbf{k}_\parallel). \tag{5}$$

The most general form of S_u allowing for the time reversal can be then written as

$$S_u = \sum_{j=1}^{2N} e^{i\beta_j}|\mathrm{out}_j\rangle\langle\mathrm{in}_j| = \sum_{j=1}^{2N} e^{i\beta_j}|\mathrm{out}_j\rangle\langle\widetilde{\mathrm{out}_j}|, \tag{6}$$

where the input (output) orthogonal bases $|\mathrm{in}_j\rangle(|\mathrm{out}_j\rangle)$ and the scattering phases β_j, $j=1,\ldots,2N$ are functions of $(\omega,\mathbf{k}_\parallel)$ which are characteristic for the given PCS. The phases are actually even functions of $\mathbf{k}_\parallel$, $\beta_j(\omega,\mathbf{k}_\parallel)=\beta_j(\omega,-\mathbf{k}_\parallel)$, as follows from Eqs. (4) and (5). Equation (6) means the existence of a special "diagonal" input and output basis sets, which do not mix up in the process of scattering.

It follows from Eq. (5) that, with the change of sign of $\mathbf{k}_\parallel$ in *any* asymmetric PCS, the reflection with linear polarization conservation is always symmetric,

$$r_{ss}(\omega,\mathbf{k}_\parallel) = r_{ss}(\omega,-\mathbf{k}_\parallel), \quad r_{pp}(\omega,\mathbf{k}_\parallel) = r_{pp}(\omega,-\mathbf{k}_\parallel) \tag{7}$$

(r is the amplitude reflection coefficient). This is because these reflection coefficients are just the diagonal components of S_u, whereas the reflection with change of polarization from p to s (if it exists) is asymmetrical in asymmetric PCS,

$$r_{sp}(\omega,\mathbf{k}_\parallel) \neq r_{sp}(\omega,-\mathbf{k}_\parallel), \tag{8}$$

but equal to that from s to p,

$$r_{sp}(\omega,\mathbf{k}_\parallel) = r_{ps}(\omega,-\mathbf{k}_\parallel). \tag{9}$$

Simultaneously, the transmission (for $\mathbf{k}_\parallel$) with the conservation of linear polarization from the air to substrate always equals to that in the inverse direction (for $-\mathbf{k}_\parallel$ and from the substrate to air).

To the contrary, in the case of circular polarization, because now the time reversal switches from $\sigma^\pm$ to $\sigma^\mp$, the reflection with change of polarization is symmetrical,

$$r_{+-}(\omega,\mathbf{k}_{\parallel}) = r_{+-}(\omega,-\mathbf{k}_{\parallel}). \tag{10}$$

Simultaneously,

$$r_{++}(\omega,\mathbf{k}_{\parallel}) = r_{--}(\omega,-\mathbf{k}_{\parallel}), \tag{11}$$

but the reflection with conservation of polarization is asymmetrical,

$$r_{++}(\omega,\mathbf{k}_{\parallel}) \neq r_{++}(\omega,-\mathbf{k}_{\parallel}) \tag{12}$$

in asymmetric PCS. Additionally,

$$r_{+-}(\omega,\mathbf{k}_{\parallel}) \neq r_{-+}(\omega,-\mathbf{k}_{\parallel}). \tag{13}$$

These symmetry properties of the *reflection* (and *transmission* in *reverse* direction) are independent of how many diffraction channels are open. They are even more general and hold for PCS with absorptive materials simply because any absorption channel can be included into a more general unitary S matrix of the full system as an additional scattering channel. The symmetry of transmission in reverse direction is just what was found in Refs. 5, 6, and 20. There is no contradiction here with the different field distributions because the reciprocity exists only between the time-reversal channels, whereas the full solution is not reciprocal because of different reflected waves in the cases of incidence from the air and from the substrate.

As to the symmetry of *transmission* for illumination from the *same* side of the PCS, in case of asymmetric PCS it holds only at frequencies when all diffraction channels are closed, and only in lossless PCS, because the $\mathbf{k}_{\parallel}$ and $-\mathbf{k}_{\parallel}$ transmission processes from the same side of the PCS are not reciprocal (see Fig. 1).

An example of such an asymmetric optical response is given in Fig. 2 for a model lossless asymmetric one-dimensional (1D) photonic crystal slab made of Γ-shaped rods (see the insert atop). The transmission, diffraction, and reflection spectra versus incoming photon energy (vertical axes) and angle of incidence (horizontal axes) are shown by color; the color scheme is explained in the insert of Fig. 2(b). The incoming light is s polarized (electric field parallel to the rods), and the plane of incidence is perpendicular to the rods. The calculations are done for the PCS period d=500 nm, and the characteristic sizes (see Fig. 2) are taken $l=d/3$, and h =300 nm. The dielectric constants of the rod material (red) and substrate (blue) are taken $\varepsilon=4$ and $\varepsilon_{\text{sub}}=2$, respectively. The S-matrix method[18] is used, with 21 harmonics in Eq. (2) and accuracy better than 10^{-3}.

It is clearly seen from Fig. 2(c) that the reflection is always invariant against the change of the incidence angle sign (or direction of $\mathbf{k}_{\parallel}$), notwithstanding the asymmetry of the PCS and in agreement with the discussion above, whereas the transmission is symmetrical only if the diffraction is absent (i.e., in the zeroth diffraction order). In this particular case, it happens for photon energies below ≈1.65–1.75 eV, depending on the angle of incidence.

The calculated optical spectra of symmetric and asymmetric PCS (with Γ- and T-shaped rods of the same sizes and materials) for $\vartheta=0,\pm3°,\pm5°$ are compared in Fig. 3. Again, the angular symmetry of the reflection is clearly seen in Fig. 3(c): the circles (for the negative angles) always coincide with the solid lines of the same color (for the positive angles). As to the diffraction, it appears to be very asymmetrical for Γ-shaped rods. And, as a consequence, the transmissivity becomes asymmetrical, too, after the diffraction opens: note the separation of circles and solid lines in Fig. 3(a) when the energy exceeds the diffraction threshold.

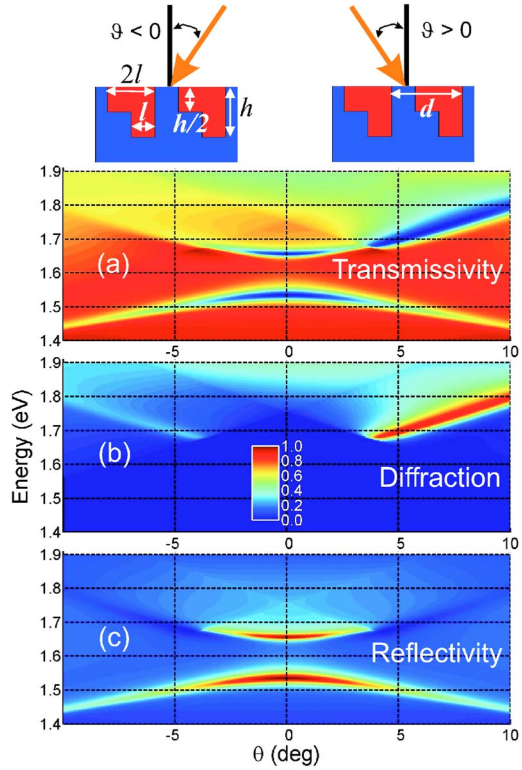

FIG. 2. (Color online) Calculated angular and energy dependencies of the transmissivity $T=|t|^2$ (a), reflectivity $R=|r|^2$ (c), and total diffraction $D=1-T-R$ (b) spectra of the s-polarized light in the asymmetric 1D PCS with Γ-shaped rods, with cross section shown in the inset above. The magnitude of the optical coefficients T, D, R is shown by different colors, and the color scheme is explained in the inset in (b). The inset above (a) explains the geometry of the PCS and light incidence.

III. RESONANCES AND FANO LINE SHAPES

The transmissivity dips in Figs. 2 and 3 are resonant Wood's anomalies[10–12] (see also Ref. 18 and references therein) because of quasiguided modes in PCS. Less pronounced wrinkles (or cusps) are the diffractive Wood's anomalies. The energies of the latter coincide with the diffraction channel openings; they are square-root anomalies, see the analysis in Refs. 34–36.

In the particular case of s polarization and structures shown in Figs. 2 and 3, the resonant Wood's anomalies are the lowest Bragg resonances of the TE-guided modes in the slab. Generally, there are two resonances at any angle, but one of them is odd and cannot be excited at normal incidence in the symmetric structure. The energy gap between the two resonant Wood's anomalies at normal incidence corresponds

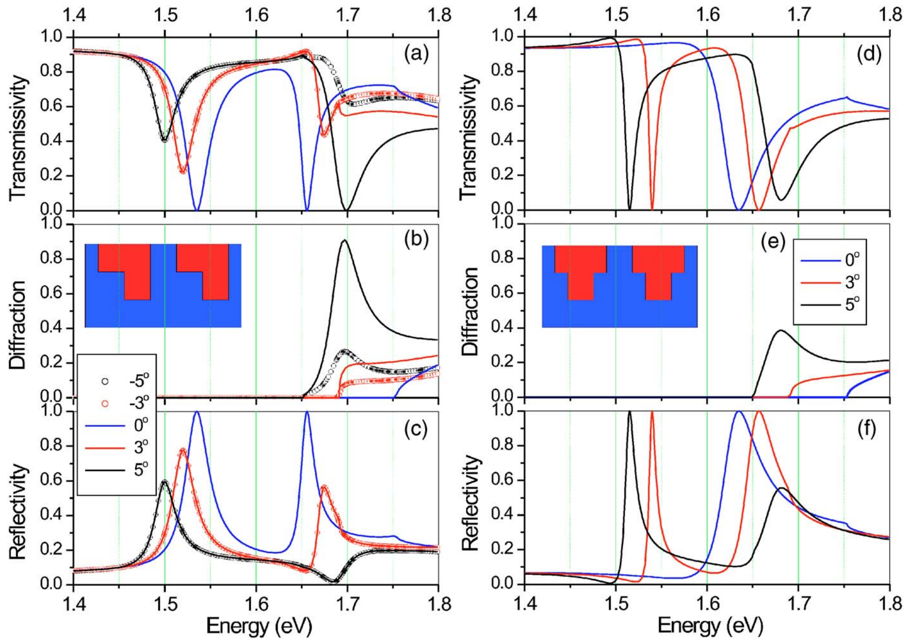

FIG. 3. (Color online) Calculated spectra of the transmissivity $T=|t|^2$ (a), (d), reflectivity $R=|r|^2$ (b), (e), and total diffraction $D=1-T-R$ (c), (f) for different angles of incidence of the s-polarized light in the asymmetric Γ-shaped (left panels) and symmetric T-shaped (right panels) 1D PCS with cross sections shown in the insets. All sizes and dielectric constants are same as in Fig. 2. The angles of incidence ϑ are indicated in the legends of (b) and (e). Solid lines show the optical coefficients for positive angles of incidence. Open circles in (a)–(c) show the optical coefficients of the asymmetric PCS for negative angles of incidence. The plane of s-polarized light incidence is perpendicular to grooves ($\varphi=0$). Note that in the Γ-shaped PCS the reflectivity is always symmetrical (open circles coincide with the solid lines of the same color), the diffraction is asymmetrical, and the transmissivity is symmetrical if only the diffraction is zero.

to the 1D stopband for in-plane photon propagation along the x direction (see Ref. 18 and references therein).

The corresponding peaks in the reflectivity have characteristic asymmetric Fano line shape[37] because they are quasidiscrete states on the background of the photon continua in air and substrate. The reflectivity near the Wood's resonant anomaly can become full in a lossless PCS in the zeroth diffraction order, i.e., when all the diffraction channels are closed. Numerical examples of such a full reflectivity can be seen in bottom panels of Fig. 3. In the case of an asymmetric 1D PCS, the full reflectivity happens for normal incidence only; the maxima of the reflection peaks decrease with the increase of the incidence angle, whereas in a symmetric PCS the full reflectivity can be seen for *any* ϑ. The full reflectivity is possible unless the first diffraction channel opens: compare to the corresponding middle panels. These properties of the resonant reflectivity in transparent PCS can be deduced from the general properties of the unitary scattering matrix S_u.

Let det $\mathbb{S}^{-1}(\omega,\mathbf{k}_\parallel)$ has a zero at $\omega_0(\mathbf{k}_\parallel)=\Omega_0(\mathbf{k}_\parallel)-i\gamma_0(\mathbf{k}_\parallel)$ in the lower half of the complex energy plane, corresponding to the quasiguided photonic mode,[18] or

$$\mathbb{S}^{-1}(\omega_0,\mathbf{k}_\parallel)|\mathbb{O}(\mathbf{k}_\parallel)\rangle=0, \tag{14}$$

where $|\mathbb{O}\rangle$ is the resonant output eigenvector in the large basis, $\Omega_0(\mathbf{k}_\parallel)$ and $\gamma_0(\mathbf{k}_\parallel)$ are the energy and linewidth dispersions of the quasiguided mode. Here we analyze the simplest case of a nondegenerate quasiguided mode. Equation (14) means that all components of $\mathbb{S}$ have the pole at $\omega=\omega_0$. The components of the unitary matrix S_u, which is a rotated submatrix of $\mathbb{S}$, see Eq. (A6), also have the same pole.

S_u has to be unitary for real ω, and it imposes significant restrictions on its possible form. In fact, near the resonance one of the scattering phases (the resonant phase) is a quickly changing function of energy,[33] and Eq. (6) can be rewritten in a form

$$S_u(\omega,\mathbf{k}_\parallel)=\sum_{j\neq 1} e^{i\beta_j}|o_j\rangle\langle\tilde{o}_j| + \eta(\omega,\mathbf{k}_\parallel)|o_1\rangle\langle\tilde{o}_1|, \tag{15}$$

$$\eta(\omega,\mathbf{k}_\parallel)\equiv e^{i\beta_1}=-\frac{\omega-\omega_0^*(\mathbf{k}_\parallel)}{\omega-\omega_0(\mathbf{k}_\parallel)}=\frac{2i\gamma_0(\mathbf{k}_\parallel)}{\omega-\omega_0(\mathbf{k}_\parallel)}-1, \tag{16}$$

where $|o_1\rangle\equiv|o_1(\mathbf{k}_\parallel)\rangle$ (i.e., the resonant "small" outgoing vector in the orthogonal basis corresponding to the large resonant vector $|\mathbb{O}\rangle$, $|\tilde{o}\rangle_1\equiv|o(-\mathbf{k}_\parallel)^*\rangle_1$) and $|o_{j\neq 1}\rangle$ are the output basis vectors in the subspace *orthogonal* to $|o_1\rangle$.

The existence of pole at $\omega=\omega_0$ still leaves an arbitrary constant phase multiplier in the definition of η; in Eq. (16) it is chosen in such a way that $\eta|_{\omega=\Omega_0}=1$ exactly at the resonance. To ensure $\eta(\omega,\mathbf{k}_\parallel)=\eta(\omega,-\mathbf{k}_\parallel)$ (the reciprocity of the reflection near the resonance), we have to set $\omega_0(\mathbf{k}_\parallel)=\omega_0(-\mathbf{k}_\parallel)$. However, the resonant vectors $|o_1(\mathbf{k}_\parallel)\rangle$ and $|o_1(-\mathbf{k}_\parallel)\rangle$ can be different if there is no additional symmetry of the structure transforming $\mathbf{k}_\parallel$ to $-\mathbf{k}_\parallel$.

Equation (15) is the most general form of the Breit-Wigner formula (see, e.g., Ref. 33) for the resonant optical response in a transparent PCS. Except for η, all quantities in

Eq. (15) are slow functions of ω; neglecting this ω dependence gives a very good resonant approximation for S_u in the vicinity of Ω_0.

In the zeroth diffraction order Eq. (15) can be simplified further. In this case S_u is a 4×4 matrix. However, in the case of 1D PCS, and for linearly polarized light with plane of incidence perpendicular to the grating grooves ($\varphi=0$), the s and p polarizations are decoupled. Then, S_u becomes a block-diagonal matrix with uncoupled 2×2 blocks for different polarizations. The resonances in different polarizations differ, generally. Then, S_u becomes effectively a 2×2 matrix (for each polarization). By proper selection of the outgoing harmonics phases, the corresponding 2D vector $|o_1\rangle$ can be made real, and

$$|o_1\rangle = \begin{pmatrix} \sin\xi \\ \cos\xi \end{pmatrix}, \quad |o_2\rangle = \begin{pmatrix} \cos\xi \\ -\sin\xi \end{pmatrix}. \tag{17}$$

The most general form of the (2×2)-dimensional unitary scattering matrix in this polarization becomes

$$S_u(\omega,\mathbf{k}_\parallel) = \begin{pmatrix} \cos\xi \\ -\sin\xi \end{pmatrix}(\cos\tilde{\xi}, -\sin\tilde{\xi})e^{i\beta} + \begin{pmatrix} \sin\xi \\ \cos\xi \end{pmatrix}(\sin\tilde{\xi}, \cos\tilde{\xi})\,\eta(\omega,\mathbf{k}_\parallel), \tag{18}$$

where β, ξ, and $\tilde{\xi}\equiv\xi(-\mathbf{k}_\parallel)$ are slowly changing with ω, $\mathbf{k}_\parallel$ parameters of the system near the resonance. For the coefficients of reflection $r\equiv(S_u)_{11}$ and transmission $t\equiv(S_u)_{21}$ we have, respectively,

$$r(\omega,\mathbf{k}_\parallel) = e^{i\beta}\cos\xi\cos\tilde{\xi} + \eta(\omega,\mathbf{k}_\parallel)\sin\xi\sin\tilde{\xi}, \tag{19}$$

$$t(\omega,\mathbf{k}_\parallel) = -e^{i\beta}\sin\xi\cos\tilde{\xi} + \eta(\omega,\mathbf{k}_\parallel)\cos\xi\sin\tilde{\xi}. \tag{20}$$

In the case of *normal incidence* ($\mathbf{k}_\parallel=0$) for any PCS and in symmetric PCS for *any incidence* we have $\xi=\tilde{\xi}$, and as a result,

$$r(\omega,\mathbf{k}_\parallel) = e^{i\beta}\cos^2\xi + \eta(\omega,\mathbf{k}_\parallel)\sin^2\xi, \tag{21}$$

$$t(\omega,\mathbf{k}_\parallel) = [\eta(\omega,\mathbf{k}_\parallel) - e^{i\beta}]\cos\xi\sin\xi. \tag{22}$$

Obviously, $t=0$ and $|r|=1$ at the energy when $\eta(\omega)=e^{i\beta}$. This condition always matches at some energy near the resonance, provided $e^{i\beta}$ is not too close to -1, because β is a slow function of energy and η makes a circumnutation from $\eta|_{\omega\ll\Omega_0-\gamma_0}\approx -1$ through $\eta(\Omega_0)=1$ back to $\eta|_{\omega\gg\Omega_0+\gamma_0}\approx -1$.

The quantity $\sin\xi\cos\xi=\frac{1}{2}\sin 2\xi$ reaches its maximum $\frac{1}{2}$ at $\xi=\pi/4$. Thus, the only possibility to reach a full transmission $|t|=1$, as seen from Eq. (22), is to have $\xi=\pi/4$ and $\eta(\omega)=-e^{i\beta}$ simultaneously. $\xi=\pi/4$ means the symmetry between the scattering from the top and bottom sides of the structure, compare to Eq. (17). Generally speaking, it happens provided the system has a horizontal mirror plane. For example, the full transmissivity is reached exactly at the resonance, $\omega=\Omega_0$, in the only case if $\beta=\pi$ and $\xi=\pi/4$, simultaneously. This is the case of a well-known Fabry-Perot resonator with symmetrical lossless mirrors.

In asymmetric PCS at *oblique incidence*, as can be understood from the inspection of Eq. (19), the reflectivity still peaks (or antipeaks) near the resonance energy. However, now the maximum value of $|r|$ is obviously <1 because $\xi\neq\tilde{\xi}$ (i.e., the resonant vectors are different $|o_1(\mathbf{k}_\parallel)\rangle \neq |o_1(-\mathbf{k}_\parallel)\rangle$ for the asymmetric PCS).

If the PCS has an additional symmetry transforming the input channels with $\mathbf{k}_\parallel$ to that with $-\mathbf{k}_\parallel$, then we have $\xi=\tilde{\xi}$. Then Eqs. (21) and (22) hold for *any* angle ϑ. As a consequence, the reflection can be full near the resonance for oblique incidence, not only for $\mathbf{k}_\parallel=0$ as in the asymmetric gratings. This additional symmetry can be, e.g., a vertical mirror plane [symmetric PCS made of T-shaped rods on a substrate, see insert in Fig. 3(e)]. The numerical examples shown in Figs. 3(d)–3(f) fully agree with this analysis. We would like to note that the property of full reflectivity is obviously destroyed by any losses, including absorption, defect, and PCS edge scattering for finite sample size.

The resonance approximation neglecting slow ω dependences in Eqs. (19)–(22) gives a very good description of the Fano-shaped optical response near the resonance, see examples in Fig. 4. The parameters Ω_0, γ_0, ξ, $\tilde{\xi}$, and β for any PCS can be calculated from the full scattering matrix $\mathbb{S}$; their particular values are specified in the corresponding panels. This resonance approximation gives, e.g., a rigorous explanation of an intuitive model of the interference between direct and indirect pathways,[17] with a minimal number of directly calculated parameters (five for general PCS and four for normal incidence or symmetric PCS), and it is applicable for arbitrary PCS.

Note that the two polarizations couple in the case of a general 2D-periodic photonic crystal slab with an asymmetric unit cell. As a consequence, there is no full reflectivity at any incidence angle, including the normal incidence. In symmetric 2D PCS the polarizations may, however, decouple if the incidence plane contains the high-symmetry directions in the first Brillouin zone. For example, $\Gamma-X(Y)$ or $\Gamma-M$ directions in PCS with square lattice and C_{4v} symmetry of the unit cell, or $\Gamma-K$ or $\Gamma-M$ directions in PCS with hexagonal lattice and C_{6v} symmetry of the unit cell. Then the full reflectivity happens for the cases of such light incidence (see, e.g., Ref. 17).

To conclude, using the unitarity and reciprocity properties of the scattering matrix, we theoretically analyze the nontrivial symmetry properties and near-resonance behavior of the optical response in photonic crystal slabs (PCS) with asymmetric unit cells. As a direct consequence of the reciprocity, the reflection with conservation of linear polarization is always symmetrical, whereas that with a change of polarization state, if it exists, is asymmetrical. For the circularly polarized light the opposite rule holds: reflection with a change of circular polarization state is always symmetrical, whereas that with conservation of circular polarization is asymmetrical. As a direct consequence of unitarity, the PCS reflectivity peaks to unity near the quasiguided mode resonance for normal light incidence in the absence of diffraction, depolarization, and losses. For the oblique incidence the

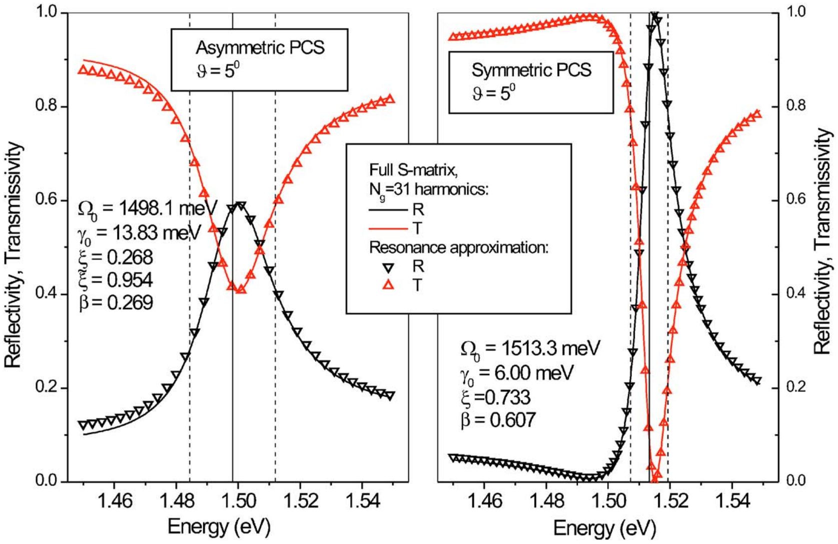

FIG. 4. (Color online) Comparison between the transmissivity $T=|t|^2$ and reflectivity $R=|r|^2$, calculated via full scattering matrix (solid lines) and resonance model Eqs. (19)–(22), open triangles. The resonance parameters are indicated in the panels. The lower-energy resonances in Fig. 3 for $\vartheta=5°$ are shown, for asymmetric (left panel) and symmetric (right panel) PCS. Vertical black solid lines mark the resonance eigenenergies Ω_0, and dashed lines are $\Omega_0 \pm \gamma_0$.

full reflectivity in the zeroth diffraction order is reached only in symmetric 1D PCS; in asymmetric PCS the reflectivity maximum decreases with the angle of incidence increase.

ACKNOWLEDGMENTS

The authors are thankful to I. Avrutsky, L. V. Keldysh, and V. A. Sychugov for discussions. This work was supported, in part, by the Russian Foundation for Basic Research, Russian Ministry of Science, and Russian Academy of Sciences.

APPENDIX A: MATRICES $\mathbb{S}$ AND S_u

The large scattering matrix $\mathbb{S}$ has been defined (e.g., in Ref. 18) as an infinitely dimensional matrix connecting the (x,y) electric field components of the incoming and outgoing waves in vacuum and substrate,

$$\begin{pmatrix} E_{x,\mathbf{G}}^{\text{out,sub}} \\ E_{y,\mathbf{G}}^{\text{out,sub}} \\ E_{x,\mathbf{G}}^{\text{out,vac}} \\ E_{y,\mathbf{G}}^{\text{out,vac}} \end{pmatrix} = \mathbb{S} \begin{pmatrix} E_{x,\mathbf{G}}^{\text{in,vac}} \\ E_{y,\mathbf{G}}^{\text{in,vac}} \\ E_{x,\mathbf{G}}^{\text{in,sub}} \\ E_{y,\mathbf{G}}^{\text{in,sub}} \end{pmatrix}, \tag{A1}$$

where $\mathbf{G}$ is the reciprocal PCS lattice. Both propagating and evanescent waves have been taken into consideration, with wave vector components $k_{x(y),\mathbf{G}} = k_{x(y)} + G_{x(y)}$, and $k_{z,\mathbf{G}} = \pm\sqrt{\omega^2\varepsilon/c^2 - k_{x,\mathbf{G}}^2 - k_{y,\mathbf{G}}^2}$ with, e.g., pluses for incoming waves in vacuum and outgoing ones in the substrate.

Let us note first that $\mathbb{S}$ is not unitary even for PCS made from transparent materials because it is defined on the nonorthogonal basis. The latter is orthogonal for specific geometries only: of xz and yz light incidence planes. In all other cases the total Poynting vector contains interfering terms between different scattering channels in $\mathbb{S}$.

Second, although $\mathbb{S}$ is infinitely dimensional, in the far-field zone, because the evanescent parts vanish, it contains nonzero blocks only in the open channels $i=1,2,\ldots,N$, $N=N_{\text{open}}$.

Thus, it makes sense to deal with finite $(2N_{\text{open}} \times 2N_{\text{open}})$-dimensional scattering matrix over open channels

$$S_n = \mathbb{S}\{\text{open channels}\}. \tag{A2}$$

It is still nonunitary. In order to transfer to a unitary scattering matrix, we have to transform S_n to any flux orthogonal basis. A convenient choice is, e.g., to use s and p polarizations [i.e., the waves with electric field perpendicular (parallel) to the light incidence plane]. The basis of circular $\sigma^{\pm}$ polarizations can be used as well. However, we have to be careful with the circular polarization basis because $\sigma^{\pm}$ polarization transfers into $\sigma^{\mp}$ under the time conjugation. For each *open* channel i the harmonics are propagating waves in vacuum or in substrate. Let $\mathbf{s}_i$, $\mathbf{p}_i$, and $\mathbf{n}_i$ be the ith open-channel unit vectors of s, p polarization, and propagation direction, respectively (where $\mathbf{s}_i \times \mathbf{p}_i = \mathbf{n}_i$). Then, the (x,y) and (s,p) electric field components are connected as

$$\begin{pmatrix} E_{x,i} \\ E_{y,i} \end{pmatrix} = U_i \begin{pmatrix} E_{s,i} \\ E_{p,i} \end{pmatrix}, \tag{A3}$$

$$U_i = (\sqrt{\varepsilon_i} n_{z,i})^{-(1/2)} \begin{pmatrix} s_{x,i} & p_{x,i} \\ s_{y,i} & p_{y,i} \end{pmatrix}. \tag{A4}$$

Here ε_i is the dielectric susceptibility of the media of the ith channel (1 or ε_{sub} for vacuum-substrate geometry). The factor $(\sqrt{\varepsilon_i} n_{z,i})^{-(1/2)}$ in Eq. (A4) normalizes s and p waves on a constant z projection of the Poynting vector.

Now we are ready to transfer from the nonunitary infinite matrix $\mathbb{S}$ to a unitary $(2N_{\text{open}} \times 2N_{\text{open}})$-dimensional matrix S_u. Introducing $(1+N_\alpha) \times (1+N_\alpha)$ matrices

$$U_\alpha = \prod_{i \in \alpha} \otimes U_i, \quad \alpha = \text{vac,sub}, \tag{A5}$$

which are direct products of transformation matrices (A4) over all open channels, we define the unitary scattering matrix as

$$S_u = \begin{pmatrix} 0 & U_{\text{vac}}^{-1} \\ U_{\text{sub}}^{-1} & 0 \end{pmatrix} S_n \begin{pmatrix} U_{\text{vac}} & 0 \\ 0 & U_{\text{sub}} \end{pmatrix}. \tag{A6}$$

By this definition, the unitary scattering matrix transfers the amplitudes of s and p incoming waves, into that of the outgoing waves,

$$\begin{pmatrix} E_{s,i}^{\text{out,vac}} \\ E_{p,i}^{\text{out,vac}} \\ E_{s,i}^{\text{out,sub}} \\ E_{p,i}^{\text{out,sub}} \end{pmatrix} = S_u \begin{pmatrix} E_{s,i}^{\text{in,vac}} \\ E_{p,i}^{\text{in,vac}} \\ E_{s,i}^{\text{in,sub}} \\ E_{p,i}^{\text{in,sub}} \end{pmatrix}, \tag{A7}$$

which is equivalent to Eq. (1).

APPENDIX B: RECIPROCITY OF S_u

Taking the complex conjugate of Eq. (1)

$$|\text{out}(\mathbf{k})^*\rangle = S_u^*(\mathbf{k})|\text{in}(\mathbf{k})^*\rangle$$

and using Eq. (4), we get

$$|\text{in}(-\mathbf{k})\rangle = S_u^*(\mathbf{k})|\text{out}(-\mathbf{k})\rangle.$$

It means that

$$|\text{out}(-\mathbf{k})\rangle = S_u^*(\mathbf{k})^{-1}|\text{in}(-\mathbf{k})\rangle.$$

Comparing to the definition Eq. (1), we see that

$$S_u^*(\mathbf{k})^{-1} = S_u(-\mathbf{k}).$$

Using unitarity $S_u^{-1} = (S_u^*)^\top$, we arrive at Eq. (5).

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