Two-dimensional photonic crystals: method of coherent transmission and reflection coefficients computation

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A method of two-dimensional (2D) photonic crystal (PC) coherent transmission and reflection coefficients calculation is proposed. It is based on the radial distribution function of an actual PC simulation by blurring the coordination circles of an ideal PC. The computations are performed under the quasi-crystalline approximation of the theory of multiple scattering of waves.

INTRODUCTION

We used the quasicrystalline approximation (QCA) of the theory of multiple scattering of waves to calculate coherent transmittance and reflectance [1-3] of the two-dimensional periodically modulated refractive-index structure, namely photonic crystal (PC) [4]. Using this approximation the spatial arrangement of particles is described by the radial distribution function (RDF) [5], characterizing the probability of particles to be located at a distance R from each other. In partially ordered layers short-range ordering is realized, and RDF tends toward unity at short separation distances (less than ten particle diameters) [3]. In the PCs a long-range ordering of particles is realized. RDF converges toward unity at very large distances between particles, making the problem of numerical calculation of transmittance and reflectance under the quasicrystalline approximation extremely cumbersome. We propose a method of 2D PC radial distribution function simulation, which takes into account long-range ordering of particles and allows for a dramatically simpler scattering solution.

METHOD OF PHOTONIC CRYSTAL RADIAL DISTRIBUTION FUNCTION SIMULATION

We consider the 2D PC with triangular, square, and hexagonal arrangements of identical spherical particles (see Fig. 1). To calculate coherent transmission and reflection coefficients of the PC we use the QCA. This approximation takes into account the spatial distribution of particles in a layer, which determines their optical interaction. The spatial distribution of particles is described by a radial distribution function. It characterizes the probability of finding of particle in space relative to any selected particle [5].

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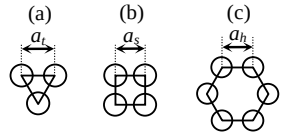

Figure 1. Schematic presentation of unit cells of triangular (a), square (b), and hexagonal (c) lattices. Circles in the lattice sites represent spherical monodisperse particles. a_t, a_s, and a_h are lattice constants for triangular, square and hexagonal lattices, respectively.

To simulate the RDF of an actual PC, we first compute the dependence of the number of particles on distance for the ideal PC. Thereto we select the center of any particle as a coordinate origin and compute relative to it the amount of particle centers as the function of distance *N(R)*. All particle centers located on the same distance *R* from the coordinate origin lie on a coordination sphere [5] (or circle in the case of 2D layer) with radius $R=R_i$. Function $N(R)=N_i$ if $R=R_i$, and $N(R)=0$ if $R \neq R_i$ (N_i is the number of particle centers on the coordination circle with radius R_i). For illustration, we show function *N(R)* for the triangular lattice in Fig. 2.

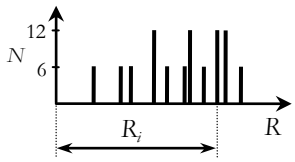

Figure 2. Function showing the number of particles as a function of distance for the triangular lattice. R_i is the radius of the *i*-th coordination circle.

On the basis of the obtained *N(R)* function we simulate the RDF of the actual PC. We use the equation for calculation of the RDF of the simulated photonic crystal:

$$g(u) = \rho_0^{-1} \sum_i \frac{N_i}{2\pi R_i} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(u-R_i)^2}{2\sigma^2} \right). \quad (1)$$

Here $u=R/D$ is dimensionless distance (in particle diameters *D*), ρ_0 is the mean surface numerical concentration (i.e., the ratio of the number of layer particles to the layer area when the area tends to infinity) of particles, N_i is the number of particle centers on the coordination circle with radius R_i (here R_i are determined in particle diameters *D*). We specify parameter σ as a function of distance: $\sigma = \sigma(u)$ that determines the dispersion of the coordination circles radii of the simulated PC and the distance, where the RDF converges to unity. This distance is called the length of correlation (or the correlation length) l_c. The correlation length of a system characterizes the scale of its spatial order. To find the minimal correlation length $l_c^{\min}$ of the PC (i.e. the minimal radius of the coordination circle in which we have to take into account the influence of the particle ordering on light scattering) we estimated the change of its concentration on distance from the coordinate origin. We reveal that $l_c^{\min}$ of the PC is about several tens. We specify $\sigma(u)$ so that the RDF converges to unity with distance

approximately equal to $l_c^{\min}$. We have found that function $\sigma(u) = \sigma_0 u$ can be used to simulate the radial distribution function in a wide range of photonic crystal parameters (σ_0 is the "initial deviation" of radii). It allows us to simulate the RDF with good agreement with the experimental data [6]. The simulated RDF of the PC calculated by the Eq.(1) for the triangular lattice is displayed in Fig. 3. The results are obtained with $\sigma(u) = \sigma_0 u$, $\sigma_0 = 0.01$ and the filling coefficient of a layer (the ratio of particle projections to the area, where they are located) $\eta = 0.5$. The summations in Eq. (1) are implemented over the range of $\pm 10\sigma$ from each u-point.

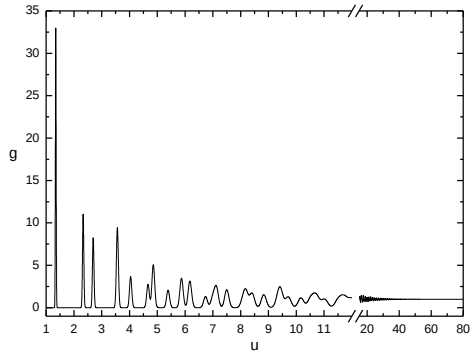

Figure 3. Simulated RDF of PC with the triangular lattice: η=0.5, $\sigma(u) = \sigma_0 u$, σ_0=0.01.

CONCENTRATION DEPENDENCES OF COHERENT TRANSMISSION AND REFLECTION COEFFICIENTS OF PHOTONIC CRYSTAL

We used simulated by Eq. (1) RDFs to calculate coherent transmission T_c and reflection R_c coefficients of PC under the QCA[2,3]. These dependences on size parameter $x=\pi D/\lambda$ (where D is the particle diameter, λ is wavelength of incident light) for PC with the triangular lattice are displayed in Fig. 4 at different filling coefficients η.

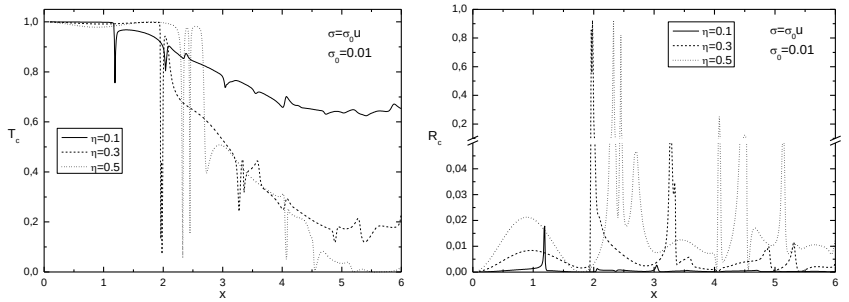

Figure 4. Dependences of coherent transmittance T_c (left) and reflectance R_c (right) of PC with triangular lattice on x at different η. Particles complex refractive index m=1.4+5×10^{-5}i.

The dependences of T_c and R_c for a partially ordered layer with the same filling coefficients and particle refractive indices (as in Fig.4) are displayed in Fig. 5. The data are calcu-

lated under the QCA using the RDF of the partially ordered layer simulated on the base of the Percus-Yevick approximation[3,5]. The data displayed in Figs. 4 and 5 show a dramatic influence of spatial ordering on coherent transmittance and reflectance of the layer. The filling coefficient of the layer has a profound influence (Fig.4) on the location and depth of the photonic band gap (PBG). The displayed data indicate as well, that the PBG occurs even at low concentrations of particles in the PC. The dependencies $T_c(x)$ and $R_c(x)$ of partially ordered layers are smooth.

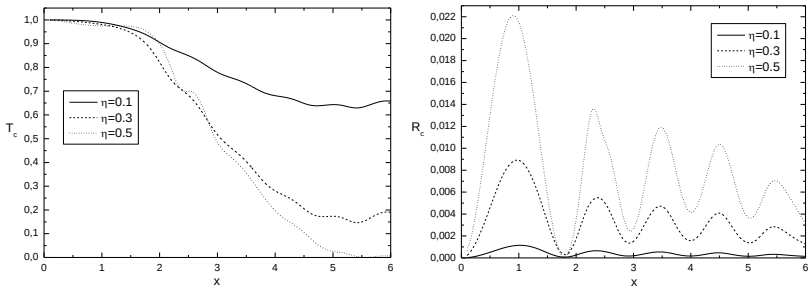

Figure 5. Dependencies of coherent transmittance T_c (left) and reflectance R_c (right) of partially ordered layer on x at different η. Particles complex refractive index $m=1.4+5\times10^{-5}i$.

CONCLUSION

A method for calculation of coherent transmittance and reflectance of a PC is proposed. The obtained radial distribution function is in good agreement with the experimental data. The criterion of correlation length of the PC is derived. Calculation of coherent transmission and reflection coefficients of a PC and partially ordered layer were performed under the QCA. There is a strong difference in the concentration dependencies of transmittance and reflectance of PC and partially ordered layers.

The results can be applied to the design and fabrication of high-efficiency solar cells, highlight-emitting diodes, antireflection layers, extraordinary-transmitting electrodes, etc.

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