Journal of Quantitative Spectroscopy & Radiative Transfer 151 (2015) 260–268

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

Three-dimensional ordered particulate structures: Method to retrieve characteristics from photonic band gap data

Alexander A. Miskevich, Valery A. Loiko *

B.I. Stepanov Institute of Physics of NAS of Belarus, 68 Nezalezhnastsi Avenue, Minsk 220072, Belarus

ARTICLE INFO

Article history:
Received 19 June 2014
Received in revised form
6 October 2014
Accepted 10 October 2014
Available online 27 October 2014

Keywords:
Inverse problem
Photonic crystal
Photonic band gap
Quasicrystalline approximation
Transfer matrix method
Refractive index

ABSTRACT

A method to retrieve characteristics of ordered particulate structures, such as photonic crystals, is proposed. It is based on the solution of the inverse problem using data on the photonic band gap (PBG). The quasicrystalline approximation (QCA) of the theory of multiple scattering of waves and the transfer matrix method (TMM) are used. Retrieval of the refractive index of particles is demonstrated. Refractive indices of the artificial opal particles are estimated using the published experimental data.

1. Introduction

Ordered photonic structures, such as photonic crystals (PC), are the subject of intensive investigations in the last decades [1–12]. The interest is caused by the unique feature of such structures to suppress light propagation in some spectral ranges known as photonic band gaps (PBGs) [1–3]. This phenomenon is caused by interference of waves interacted with the ordered structures.

The depth, width and spectral position of the PBG depend on characteristics of the structure. That can be used to find (retrieve) the structure parameters. The retrieval problem is known as an inverse problem [13–22]. Its solution can be based, for example, on the known solution to the respective direct problem, i.e. on the known characteristics of outgoing light. The retrieval can be performed by multiple solution of the direct problem at different values of parameter to be found and comparison of the calculated and experimental PBG data.

In this work we consider the inverse problem for a three-dimensional (3D) ordered particulate structure (photonic crystal). We develop a method to retrieve characteristics of a structure by the known PBG data. The refractive index retrieval is considered as an example.

2. Basic approaches

We consider three-dimensional ordered particulate structure consisting of monodisperse spherical particles as a stack of the ordered plane-parallel monolayers of particles. To solve the direct problem we use the quasi-crystalline approximation (QCA) [23,24] of the theory of multiple scattering of waves [23–25] and the transfer matrix method (TMM) [26–28]. First, we calculate the amplitude coherent transmission and reflection coefficients of individual monolayers in the QCA. Using these coefficients, we next calculate coherent transmittance and reflectance of the multilayer under the TMM.

* Corresponding author. Tel.: +375 17 284 2894; fax: +375 17 284 0879.
E-mail addresses: miskevic@dragon.bas-net.by (A.A. Miskevich), loiko@dragon.bas-net.by (V.A. Loiko).

http://dx.doi.org/10.1016/j.jqsrt.2014.10.007
0022-4073/

2.1. Spatially ordered monolayer of particles

Let us consider a spatially ordered monolayer of monodisperse spherical particles with known parameters, such as refractive index, size, and concentration of particles, type and degree of their spatial ordering. Let it be normally illuminated by a plane wave and situated in a medium with a known spectral refractive index. We use the quasicrystalline approximation of the statistical theory of multiple scattering of waves to find the coherent transmission and coherent reflection coefficients of the monolayer. This approximation is based on the assumption that the mean (coherent) field at one fixed particle equals the field at two fixed particles [24]. The spatial correlation of particles is taken into account by the radial distribution function (RDF) [29,30], which characterizes the probability of finding a particle in a certain position relative to another one.

There is a number of methods to calculate the RDFs of short-range ordered monolayers (partially ordered monolayers) [31–35]. Nevertheless it is a challenge to find the RDFs for long-range ordered monolayers (for example, planar photonic crystals). Besides, these functions should be adapted for the QCA.

We showed that the expression for calculating the RDF $g(u)$ of an actual planar photonic crystal (monolayer with long-range order) can be written as [10,11]

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

Here $\sigma(u)$ is a function that characterizes the coordination circles "blurring" (broadening) with the distance u. It is reasonable to use the linear blurring function:

$$\sigma(u)=\sigma_0(au+b). \quad (2)$$

In Eqs. (1) and (2) $u=R/D$ stands for the dimensionless distance expressed in diameters D of the particles ($u\geq 1$); R is the distance in a monolayer plane (plane, where the particle centers are located) relative to the origin; ρ_0 is the averaged numerical particle concentration in the monolayer; N_i is the number of particle centers on the coordination circle with radius R_i in an ideal lattice; σ_0 is the dimensionless initial dispersion of coordination circles radii (expressed in particle diameters); and a and b are the coefficients. The ordering degree and the scale of the spatial order of the simulated crystal are specified by σ_0, and by a and b coefficients, respectively. Eq. (2) takes into account asymmetry of the individual peaks of the RDFs observed experimentally. It enables one to calculate RDFs of crystals in a wide range of ordering. The RDFs [Eq. (1)] obtained with Eq. (2) are well adapted for the QCA. Calculation of such RDFs and, consequently, coherent transmission and reflection coefficients of the monolayer with long-range order in the QCA is fast and requires low amount of computational resources.

At small distances from the coordinate origin, the RDF of highly ordered PC is a sequence of sharp peaks. For example, in Fig. 1c is shown such RDF describing the PC with triangular lattice (Fig. 1a,b). With distance increasing, the peaks become wider, the function oscillates and converges to unity. Note that for $\sigma(u)=$const, expression (1) is transformed into the known one, which describes the Gaussian blurring of the coordination circles [30]. Function (1) describes imperfect lattices with different degree of imperfection, which is specified by function (2) and consists in the deviations of particle centers from the points of perfect lattice (other defects are not considered in this model).

Using the described RDF allows one to calculate in the QCA coherent transmission T_c and coherent reflection R_c coefficients [23–25,34], which describe direct transmission and specular reflection, of monolayers with imperfect lattices. The detail consideration of the lattice geometry and ordering degree effects on the coherent transmittance and reflectance spectra is made in our previous works [10,11].

Compare the results for coherent reflection coefficient R_c obtained by our approach described in [10,11] with the results for total reflection coefficient $\Re$ (reflectivity) calculated by the method based on the low energy electron diffraction (LEED) theory developed for perfect lattices [36–38]. Fig. 1d shows the QCA-calculations of spectral coherent reflection coefficient R_c and of sum T_c+R_c (T_c is the spectral coherent transmission coefficient) for a monolayer with a triangular lattice (see Fig. 1a,b), which is close to the perfect one. Concentration of particles is characterized by filling coefficient η, i.e. by the surface fraction of particles in the monolayer. The calculations were fulfilled at $\eta=0.9$. The results published in [38] for monolayer with perfect triangular lattice with maximum filling coefficient $\eta=\eta_{max}=\pi/(2\sqrt{3})\approx 0.9069$ (see Fig. 2 of [38]) are displayed as well.

Fig. 1d illustrates that our calculations coincide with data of [38] at $\omega<1$ ($\omega=\sqrt{3}a_t/(2\lambda)$, where a_t is the triangular lattice constant, λ is the wavelength of incident light), except for narrow resonance peaks. The agreement is caused by existence of only coherent components of light: direct transmission and specular reflection. The value of T_c+R_c is unity (see Fig. 1d). In this ω-range only zero diffraction order exists.

At $\omega\geq 1$ the incoherent components (nondirect light) [23–25,34] are appeared. The $1-(T_c+R_c)$ values characterize the fraction of such light. The difference in the R_c and $\Re$ characterizes the fraction of higher diffraction orders. Although as a whole for $\omega\geq 1$ coherent reflection is less than reflectivity, in the ranges of peaks R_c can be larger than $\Re$ (see, for example, calculation results in the vicinity of $\omega=1.35$). The possible reason can be that the QCA does not consider the near field effects [23,24]. They can make contribution to the resulting coherent component of the transmitted and reflected waves at a high concentration of particles. Fig. 1d shows the maximum intensity of the near field $|E|^2_{max}(\omega)$ at distance of $D/2$ (particle radius) from the monolayer plane obtained in [38] (see dotted line linked with right axis).

The calculations by the both methods show sharp resonance peaks in the spectra of regularly packed monolayers (see Fig. 1). As shown in [38], they coincide with the peaks of the near field that are predominantly caused by the evanescent waves. Note that the QCA results and results of [38] agree well with respect to peak positions at $1<\omega<1.5$, although the QCA itself does not consider