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Sensitive analysis of 2D photonic bandgaps using boundary integral equations

L. I. Goray[1,2]

[1] Saint Petersburg Academic University, Khlopina 8/3, St. Petersburg 194021, Russia
[2] Institute for Analytical Instrumentation, RAS, Rizhsky Prospect 26, St. Petersburg 190103, Russia

Abstract. A boundary-integral-equation-based method is proposed to calculate sensitive diffraction properties of various photonic crystal slabs (PCS). The numerical results presented demonstrate the significant impact of rod shapes and sizes on diffraction in metallic 2D PCS supporting the polariton-plasmon excitation, particularly close to resonances and at high filling ratios.

Introduction

In the recent decades, we have been witnessing unwaning interest, both of theoreticians and experimenters, in the properties of photonic crystal slabs (PCS) and metamaterials. Progress in the technology of nanostructures with a characteristic surface relief of the order of 10–100 nm has stimulated production of 2D and 3D periodic structures with periods shorter than the wavelength of visible light, i.e. subwavelength diffraction gratings. Nowadays considerable effort is devoted to the investigation of polariton-plasmon PCS with metallic or semiconducting nanostructures supporting strong light-matter interaction. Large photonic band gaps, extraordinary light transmission properties, negative refraction, and strong coupling between the electronic and photonic resonances can be supported in such structures.

Though surface plasmon excitation plays a predominant part in metallic subwavelength PCS, other types of electromagnetic resonances can also exist in complex structures: Rayleigh anomalies, Fabry-Perot resonances, waveguiding anomalies, cavity modes, etc. In some cases it is difficult to distinguish among these phenomena, owing to their gradual mutation from one into another, and determine which is which even using electromagnetic field map distributions inside the grating structure. There is therefore a growing need for methods based on a rigorous theory which would be both accurate and fast enough [1]. Most of the theoretical investigations applied to PCS have been performed using the plane wave method (scattering-matrix formalism), but this method suffers from poor convergence and needs large computation times, especially for the TM-polarized incident light, because of its main accuracy parameter scaling cubically with time [2, 3]. Recently a modeling tool without such limitations has been developed on the basis of the rigorous single-boundary integral equations for conical diffraction [4] and the scattering matrix approach applied to off-plane multilayer gratings [5].

The motivation for the present communication is to introduce the new method as an exact and universal approach to be applied in areas where rapid design and analysis of the most sensitive PCS cases would be at a premium. The aim of this work is to investigate the influence of rod (nanowire) shapes and rod filling ratio on diffraction in metallic 2D PCS supporting the polariton-plasmon excitation, particularly close to resonances.

1. Theory

We employed the boundary integral equation method for a theoretical description of the optical properties of PCS. The theory is covered here necessarily very briefly because its main parts have been described at considerable length in Refs. 4, 5. The electromagnetic formulation of diffraction by gratings, which are modeled as infinite periodic structures, can be reduced to a system of Helmholtz equations for the z-components of the electric and magnetic fields in $\mathbf{R}^2$, where the solutions have to be quasiperiodic in the x-direction, subject to radiation conditions in the y-direction, and satisfy certain jump conditions at the interfaces between different materials of the diffraction grating. In the case of classical diffraction, when the incident wave vector is orthogonal to the z-direction, the system splits into independent problems for the two basic polarizations of the incident wave, whereas in the case of conical diffraction the boundary values of the z-components, as well as their normal and tangential derivatives at the interfaces, are coupled. Thus the unknowns are scalar functions in the case of classical diffraction, and two-component vector functions in the conical case.

A grating diffracts the incoming plane wave into a finite number of outgoing plane waves, the so-called reflected and transmitted modes. The program computes the energies and polarizations of these modes for an arbitrary number of layers with different profile types including closed boundaries (i.e. inclusions). The boundary profiles of the layers must be strictly separated, i.e. the maximal y-value of a given profile is strictly less than the minimal y-value of the next profile above. In this case, it is possible to determine the diffracted field of the grating by computing the scattering matrix separately for any profile. The computation of the scattering amplitude matrices is based on the solution of a 2×2 system of singular integral equations at each interface between two different materials. The integral equations are discretized with a collocation method, the unknowns are sought as trigonometric polynomials which in the case of profiles with edges are partially replaced by splines to improve the approximation of the solution near the edges.

2. Numerical Experiment and Discussion

In this Section, we are going to analyze numerically the optical response of PCS with different cross sections of nanowires invariant with respect to the z axis and different number of gratings stacked one upon the other. The geometric model under study approaches the description proposed for rectan-

gular PCS (Ref. [6], Fig. 1). The model contains M identical gratings of arbitrary cross section displaced vertically (by H_m) and horizontally (by L_m) relative to one another and embedded in a homogeneous medium with dielectric permittivity ϵ_1 and magnetic susceptibility μ_1. We are going to deal here only with materials with $\mu_m = 1$, although the model is applicable to other cases as well, including metamaterials [4]. The dependence of the dielectric permittivity ϵ_2 of the material of nanorods on the incident photon frequency is assumed to be known. The lower medium (substrate) and the upper one are likewise assigned pairs of material constants, but one may conceive of more complicated cases of multilayer structures as well. The model allows also arbitrary incidence of, in the general case, elliptically polarized radiation on PCS, which is prescribed by two angles of incidence and two angles of polarization.

In Fig. 1a, calculated spectra of reflected energy for PCS with Au nanowires of rectangular cross section, measuring 100×15 nm^2 and $M = 1$ ($H = L = 0$) or $M = 2$ ($H = 30$ nm, $L = 0$ and $H = 30$ nm, $L = 100$ nm) are compared with similar spectra derived in Ref. [6] (Fig. 3a) by the plane-wave approach. We consider here TM-polarized radiation (the plane of polarization is perpendicular to the lines) incident normally with respect to the x-z plane) on a grating with a period $d = 200$ nm and refractive indices of Au taken from [7]. To eliminate interference effects, the Au nanorods are embedded in an infinite homogeneous Si matrix with dielectric permittivity $\epsilon_1 = 2.13$. Examining the two figures, we see a very good agreement, which evidences applicability of both rigorous numerical methods to analysis of such PCS.

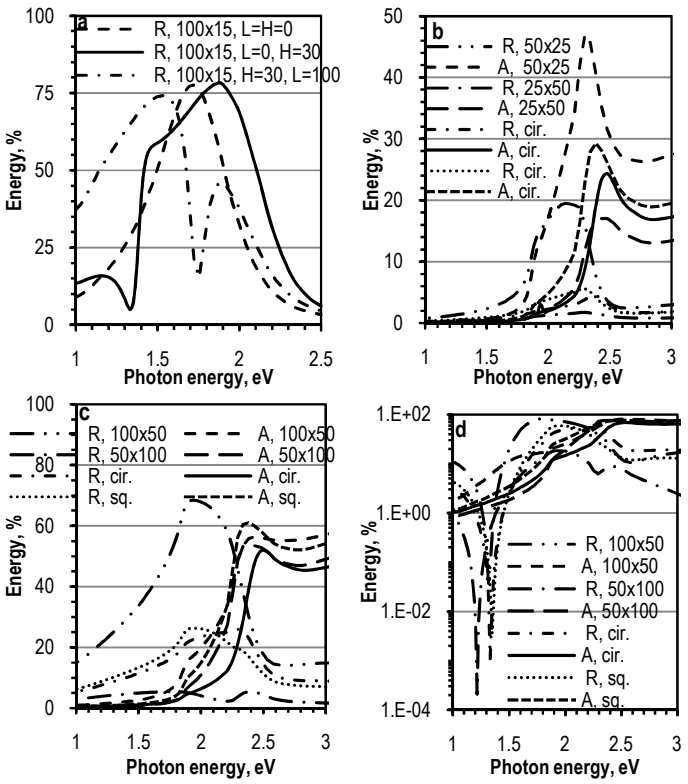

Fig. 1. Calculated reflection (R) and absorption (A) spectra of Si-embedded $d = 200$-nm gratings with Au nanowires of rectangular ($a \times b$ in nm^2), circular (cir.), and square (sq.) shapes and vertical, H, and horizontal, L, displacements in nm are plotted vs. photon energy for normal incidence and TM polarization.

Figure 1b displays for comparison theoretical spectra of energy reflected from, and absorbed by, a PCS with Au nanowires of circular, square, and rectangular cross sections of the same area and with $M = 1$ studied in the 1–3-eV range. In this and subsequent examples we consider light normally falling on Au nanowires with $d = 200$ nm embedded in a Si matrix with refractive indices of Au taken from [8]. The $a \times b$ dimensions of the rectangular rods selected for this example are 50×25 nm^2 or 25×50 nm^2 and the width of the squares and diameter of the circles were chosen so as to obtain equal areas. As seen from Fig. 1b, reflection and, particularly, absorption spectra exhibit a strong difference near the plasmon-polariton anomaly among the four shapes of nanowire cross section chosen. These differences amount to several hundred percent for the rectangles because of their different width-to-height ratio (2 and 0.5) compared with the square and the circle (1). One observes also a noticeable difference in the positions of the absorption and reflection maxima among different grating profiles.

Figure 1c presents energy spectra similar to those displayed in Fig. 2 but for a cross sectional area 4 times that of the preceding example. In this case, $a \times b = 100 \times 50$ nm^2 or 50×100 nm^2. We readily see that the differences in the reflection and absorption spectra among gratings of different profiles increase with increasing filling ratio and are observed now not only close to the plasmon resonances. Near the resonances, they amount to a few tens of absolute percent.

Figure 1d shows spectra similar to those depicted in Fig. 1c but for $M = 2$, $H = 50$ nm, and $L = 0$. In the case of two gratings, the plasmon-polariton resonance frequencies are subtracted or summed [6], and one may expect still larger differences in the spectra of reflected and absorbed energy among crystals with lattice cells of different shape. Indeed, Fig. 1d drawn on a log scale reveals enormous differences, up to an order of magnitude, throughout the spectrum studied. Thus, the simple effective medium theory cannot be applied to design and analysis of such PCS. The minimum reflectance of $1.E-6$ is observed for a photonic bandgap with a rectangular cross section which is the most sensitive shape due to its lower symmetry and different absorption. The relative error calculated from the energy balance for absorption gratings is 0.01% and the computation time is shown to scale quadratically with the main accuracy parameter. The code developed and tested is found to be very accurate and fast for solving complex PCS diffraction problems with any rods including nanowires with real profiles, the cases that should be studied experimentally.

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