Wood anomalies in the vicinity of 3D Bragg diffraction from hybrid opaline photonic crystals

V S Nikolaev$^{1,2}$, M M Voronov$^1$, S A Yakovlev$^1$, A B Pevtsov$^1$

$^1$Ioffe Physical-Technical Institute, Politekhnicheskaya 26, St Petersburg, 194021 Russia
$^2$St. Petersburg State Electrotechnical University LETI, St. Petersburg, 197376 Russia

E-mail: vudi.vova@gmail.com

Abstract. For hybrid chalcogenide/opal photonic crystals the optical reflection spectra demonstrating the interplay of diffraction resonances such as 3D Bragg diffraction and resonant Wood anomaly have been studied. The coupling coefficient of the Wood and Bragg waves has been estimated on the basis of the coupled-waves approach and the concept of the effective refractive index of the wave-guiding surface layer of the hybrid structure. A phenomenological expression for the coefficient of reflection from a hybrid photonic crystal allowing one to investigate the interference of the Wood anomalies has been proposed.

Introduction

In recent years in the field of photonics a great deal of attention has been paid to the study of the interface radiative states to which the resonant Wood anomalies (WA) [1] can be attributed. The latter represent the reflection or transmission peaks caused by the formation of quasi-guided modes in a spatially periodic surface layer (2D photonic crystals). Since the characteristics of these spectra (e.g., the position and half width of the resonance) depending on the parameters of the system can vary over a sufficiently wide range and the quasi-guided mode formation usually occurs in a thin surface layer, the photonic crystals can serve as basic elements of integrated photonic devices (see for example [2]).

In this work we consider the high contrast hybrid photonic crystals (HPCs) [3], which in our case are opaline photonic crystals covered with chalcogenide $Ge_2Sb_2Te_5$ (GST) films of different thickness, and study the reflection spectra in which the resonant WA and 3D Bragg diffraction can manifest themselves. We show that for certain parameters of the hybrid structure (e.g., the thickness of GST film and period of HPC) the WA maxima arise in the spectral region of 3D Bragg diffraction (the photonic band gap range) on a many-layer opal structure, which leads to the anticrossing of these spectral lines. Depending on the parameters of the system, the anticrossing may be quite strong (in case of a strong interaction between the Wood and Bragg resonances) or rather weak (in the opposite case) resembling an energy level crossing. The difference in intensity of the interaction is associated with different conditions of the propagation and scattering of light in the wave-guiding layer. In the hybrid structures being studied the above difference is determined by the thickness of the GST film because the effective parameters (the effective refractive index $\tilde{n}$ and transverse wave vector component $a$) of the quasi-guided mode invoked to describe the angular-dependent Wood anomalies, are strongly dependent on this thickness [4]. Besides, we study the behaviour of two close modes of the...
WAs and analyze the shape of the reflection coefficient spectra. In some cases (under different conditions) the WA reflection spectrum peaks corresponding to separate quasi-guided modes are symmetric Lorentzians, with their maximum positions being well described by an equation involving two effective parameters (\(\bar{n}\) and \(a\)), which enables us to investigate the interplay of the Wood anomalies from the viewpoint of the interference of the light waves.

On the whole, the proposed approach using a set of the effective parameters for hybrid photonic crystals can be applied to describe some peculiarities of the light reflection spectra demonstrating the interplay of several diffraction resonances such as Wood anomalies, Bragg diffraction and Fabry-Perot oscillations.

1. The coupled-waves approach

The samples of the structures under study are formed from opal films (30 monolayers of a-SiO\(_2\) spheres of diameter about 637 nm) grown from water suspension of a-SiO\(_2\) particles by the vertical deposition technique on fused silica substrates [5]. The GST layers of thickness 40, 80 and 150 nm were deposited on the surface of opal films by the thermal deposition technique [6]. The schematic picture of a hybrid photonic crystal and the geometry of the experiment are shown in figure 1. Experimental reflection spectra of the opal/GST hybrid structures with GST films with the thicknesses of 40, 80 and 150 nm for different light incidence angles (11° < \(\theta_0\) < 66°) are shown in figure 2. For the structures with film thicknesses of 40 and 80 nm these spectra show two kinds of features, one of which is a 3D Bragg diffraction peak moving to shorter wavelengths as the incidence angle increases, while the second is a Wood anomaly peak moving to longer wavelengths with an increase in the incidence angle. It is clearly seen that in the interaction region of the Bragg and Wood resonances the behaviour of the corresponding angular reflection spectra is different, showing a crossing of the lines (figures 2a,b) with the exception of a very narrow frequency region in one case and a strong repulsion typical for an anticrossing (figures 2e,f) in the second.

Since the experimental reflection spectra corresponding to the Wood anomaly and 3D Bragg diffraction are fitted well by Lorentzian shape functions, one can expect that their spectral-angular dependence will be described by the coupled-mode theory [7]. For this purpose we apply the two-coupled wave equation to the quasi-guided modes by analogy with the guided modes in dielectric waveguides [7]. A coupled-wave equation usually contains the wave vectors of the interacting waves, but since the wave vectors of the light propagating in the waveguide layer attributed to the Wood anomaly and Bragg diffraction correspond to the certain outgoing

Figure 1. Schematic image of the surface of a hybrid opal/GST photonic crystal and geometry of the experiment. Here are shown the incident, outgoing and scattering wave vectors \(k_0\), \(k\) and \(k_\parallel\), and also the incident and outgoing angles, \(\theta_0\) and \(\theta\).
Figure 2. Experimental reflection spectra of hybrid opal/\(\text{Ge}_2\text{Sb}_2\text{Te}_5\) photonic crystals for different incident angles (\(\theta_0\)) and \(\text{Ge}_2\text{Sb}_2\text{Te}_5\) thicknesses (\(h\)). The spectra (a,c,e panels) are shifted vertically for clarity; the color maps (b,d,f) are shown to improve visualization of the spectra. The thick full curves (b,d,f panels) passing through the spectral maxima correspond to the coupled-waves modes of 3D Bragg diffraction (BP) and the Wood anomalies (WP) and are calculated by using equation (1). The thin full curves (b,d,f panels) are calculated by expressions for \(\omega_W(\theta)\) and \(\omega_B(\theta)\) (without interaction between the Wood and Bragg resonances). The effective fitting parameters \(n\) and \(a\) for the quasi-guided modes calculated by equation (2) are the following: \(\bar{n} = 1.85, a = 0.38\) (\(h=40\) nm); \(\bar{n} = 3.11, a = 1.04\) for the long-wave Wood anomaly (\(h=80\) nm); \(\bar{n} = 3.25, a = 1.01\) (\(h=150\) nm). The Bragg reflection spectrum (panel c) for an uncoated opal film (30 monolayers of a-SiO\(_2\) spheres of diameter about 637 nm) is marked by arrow "Bragg peak".

Angles of the light, \(\theta\), (in our case \(\theta = \theta_0\)) the equation for the coupled waves can be written in the form:

\[
(\omega - \omega_B(\theta))(\omega - \omega_W(\theta)) = \delta,
\]

where \(\omega_B(\theta) = \frac{2\pi c}{\lambda_B(\theta)}\) and \(\omega_W(\theta) = \frac{2\pi c}{\lambda_W(\theta)}\) are the frequencies corresponding to the reflection spectrum maxima for the Bragg diffraction and Wood anomaly, and \(\delta\) is the effective coupling coefficient of the modes. The spectral position of the WA maximum is determined by the expression [4]:

\[
\lambda_W = \frac{2\pi \sqrt{(\sin \theta \cos \varphi)^2 + (\bar{n}^2 - \sin^2 \theta)(1 + a) - \sin \theta \cos \varphi}}{1 + a}.
\]

Here \(\varphi\) is an angle between the projection \(k_\parallel\) of the incident wave vector \(k_0\), lying in the plane of the surface of a hybrid structure, and \(G\) is 2D vector of the reciprocal lattice formed by the top hexagonally-ordered monolayer of opal spheres of the structure. The parameter \(a = \left(\frac{k_z}{G}\right)^2\), where \(k_z\) is the wave-vector \(k\) projection in the perpendicular direction to the surface waveguide layer.

The spectral position of the reflection coefficient maximum caused by 3D diffraction of electromagnetic waves on the planes (111) of the opal film is determined by a modified Bragg formula

\[
\lambda_B(\theta) = 2d_{111}\sqrt{\varepsilon - \sin^2 \theta} + \Delta\lambda,
\]
where $d_{111}$ is the period of the opal structure in the [111] direction, $\varepsilon$ is the average value of dielectric constant of the opal film, and $\Delta \lambda$ is the value resulting from an additional phase shift due to the thickness of the GST film and to reflection of the light in the interface area of opal-GST. Taking into account the high value ($n > 4$ in frequency wave considered) of the refractive index of GST film one can suppose that the additional phase shift, leading to the spectral shift of the Bragg diffraction peaks, will be about the same for different (not very large, in our case $\theta < 70^\circ$) incident angles of the light beam. This indeed takes place for hybrid structures opal/GST with the film thickness in the range of 40-150 nm. If to consider the coupling coefficient $\delta$ to be a constant (equal to its value in the crossing point of the unperturbed lines), equation (1) will be quadratic relative to the frequency $\omega$, whose roots $\omega_1(\theta) = 2\pi c/\lambda_1(\theta)$ and $\omega_2(\theta) = 2\pi c/\lambda_2(\theta)$ describe the behaviour of the coupled Bragg and Wood modes. Generally speaking, the coupling coefficient decreases when moving off the centre of the interaction region on the frequency scale. Here we set the value of $\delta$ to a constant in the interaction region and equal to zero outside it; in fact, to simplify the final expressions we keep $\delta$ constant in the whole spectral range. This is justified by a rapid divergence of the Wood and Bragg resonances outside the interaction region toward their ultimate values (in the absence of one of the resonances), see the thick and thin full curves for large angles $\theta$ in figures 2b,f. The value of the splitting (the minimum distance between the Bragg and Wood lines, $\lambda_B(\theta)$ and $\lambda_W(\theta)$), is equal $\Delta \omega = 2\sqrt{\delta}$ which is about 80 meV. The estimation of the coupling coefficient $\delta$ in the cases of the weak (figures 2a,b) and strong (figures 2e,f) interaction made with the help of equation (1) gives values $\sim 10^{24}c^{-2}$ and $\sim 10^{27}c^{-2}$, respectively. Such a large difference in the interaction intensity of the resonances is due to a difference in the interference conditions for 3D Bragg diffraction wave and the Wood anomaly wave in the surface waveguide layer. We note that in work [8], where 3D opal-based photonic crystals were studied under similar experimental conditions, the interference of the light waves resulted from 3D Bragg diffraction from the opal planes (111) and from disorder-induced continuous Mie spectrum was found in the transmission spectra. A similar Mie spectrum in our experimental situation (at relatively large angles $\theta_0$) converts to the WA spectrum, which can show the interference of the light waves (and also with those resulted from 3D Bragg diffraction).

It should be noted that in the interaction region of the two resonances there are also the reflection peaks corresponding to the Fabry-Perot interference over the whole thickness of the structure (figures 2a,b and 2e,f), which are characterized by a noticeably smaller value of the reflectance and therefore we do not consider this mode (as the third wave) in the coupled-waves approach. Besides, equation (1) for the coupled modes can include the spectral-angular dependence for some other diffraction resonances, e.g. 2D Bragg diffraction (which in the frequency range studied does not appear) or Wood anomaly corresponding to another quasi-guided mode.

2. Description of the reflection spectra

Let us now explain the main features of the optical spectra of reflection from the hybrid structures with the GST film thickness $h = 50$ nm, see figures 2c,d. A peculiarity of these spectra is the absence of peaks due to 3D Bragg diffraction on the (111) planes of the opal film. Since the value of the reflection coefficient is quite small ($R < 0, 1$) in the considered ranges of both wavelength $\lambda$ and reflection angle $\theta$, this situation is possible under such parameters of the structure when the total phase shift caused by the film thickness and phase change at the interfaces air - GST film and GST film - opal film leads to a condition close to that for a minimum. Therefore in a nearby wavelength range the Fabry-Perot interference can be strongly suppressed, which is indeed almost not seen (see figures 2c,d).

As is seen in figure 2c, there are two ridges of peaks, which are Wood anomalies corresponding to two different quasi-guided modes. The analysis of these spectra shows that at sufficiently
large reflection angles ($\theta = \theta_0 > 30^\circ$) the spectra are quite well described by the Lorentzian functions whose widths increase monotonically with decreasing the angle $\theta$. At small enough angles $\theta$ the reflection spectra are strongly deformed and take an asymmetrical form, so that it becomes impossible to differ between separate quasi-guided modes in the interaction region. The reflection coefficient peaks (for the light reflected in a small spatial angle) also monotonically increase with decreasing the angle $\theta = \theta_0$, reaching their maxima at the normal incidence ($\theta_0 = 0$). At very small angles $\theta$ the Wood anomalies join up to form a broad irregular contour. Thus, the reflectance contour of similar shape that arises at the normal incidence of light on a hybrid structure can suggest the appearance of the Wood anomalies in the reflection spectra at the inclined incidence.

We will now describe the Wood anomaly reflection spectra $R(\omega)$ for not too small angles $\theta$ when the corresponding quasi-guided modes are far enough from each other, see figures 2c,d and figure 3, shown as an example for angle $\theta_0 = 61^\circ$. Since the maximum of the peaks much exceeds the value of the reflection coefficient at some distance from the resonances $(\max(|r_j(\omega)|^2) \gg |r_{0j}|^2, \ j = 1, 2)$, this situation resembles the one seen in the case of the light reflection from a two-dimensional periodic array of objects demonstrating a resonant response in the absence of dielectric contrast, e.g., associated with excitons in isolated or tunnel-coupled quantum dots [9],[10]. Relying on this analogy one can write the transmission coefficient for a hybrid structure as $t(\omega) = 1 + r(\omega)$, and taking into account the relation $|r|^2 + |t|^2 = 1$, one gets that $|r|^2 + R^2(r) = 0$. Further, the reflection coefficient can be presented as a sum of the pole terms $r = \sum_{j=1}^{N} r_j, \ r_j = f_j/(\omega_{0j} - \omega - i\Gamma_j)$, where $\omega_{0j}$ and $\Gamma_j = \Gamma_{0j}$ are the resonant frequency and radiative damping rate of the j-th resonance. As a result, one can obtain the following expression for the reflection coefficient:

$$R = |r|^2 = \sum_{j=1}^{N} \frac{Im(f_j)\Gamma_{0j} + Re(f_j)(\omega - \omega_{0j})}{(\omega - \omega_{0j})^2 + \Gamma_{0j}^2}.$$

If to take into consideration the absorption in the system, the last expression can be recast into the form

$$R(\omega) = \sum_{j=1}^{N} \frac{A_j + \ B_j(\omega - \omega_{0j})}{(\omega - \omega_{0j})^2 + \Gamma_j^2}, \ (4)$$

where $A_j$, $B_j$ and $\Gamma_j$ are some real constants. Alternatively, equation (4) can be derived by considering many wave interference from $N$ resonances.

![Figure 3](image.png)

**Figure 3.** The optical reflection spectrum (black line) for the hybrid photonic crystal (with GST film of thickness 80 nm) for the incidence angle $\theta_0 = 61^\circ$, which demonstrates the Wood anomalies ($WP_1$ and $WP_2$) corresponding to two close quasi-guided modes. The extrapolation of the spectrum is made by equation (4) (red line).

The extrapolation of the reflection spectra shown in figure 3 by equation (4), where the frequency $\omega$ is expressed in terms of energy ($\omega \rightarrow E(eV)$), gives the following fitting parameters: $A_1 = 0.064, B_1 = -0.223, \Gamma_1 = 0.043$ and $A_2 = 0.072, B_2 = -0.024, \Gamma_2 = 0.066$. The resulting
discrepancy between the coefficients $B_1$ and $B_2$ and the condition $B_2 = -B_1$ can be attributed to a significant difference of the spectral shape for the second Wood anomaly from the Lorentzian shape (due to a large broadening of the peak), and to the frequency dependence of the phase shift (due to a difference in the spatial locations of the quasi-guided modes in the waveguide layer).

3. Conclusion

It can be expected that the approach developed in the present work can also be used to estimate the locations of Wood anomalies in the reflection and transmission spectra of weakly disordered structures; in this case the vector’s magnitude $G$ in equation (2) is the same as in the periodic case. Despite the absence of periodicity, these structures have long-range order and therefore would provide effective quasi-guided modes for propagation and scattering of light, leading to Wood anomalies in the optical spectra, albeit of less intensity but more broadened. The simplest system here is a 1D resonant grating waveguide structure with a rectangular profile composed of alternating segments with slightly different lengths to form a weakly disordered periodic structure. The study of the light reflection from such a structure can be made by a method applicable to the case of the analogous periodic structure [11] that leads to a conclusion about the possibility of appearance of resonant Wood anomalies in the reflection spectra for a weakly disordered periodic hybrid structure (and also for some other non-periodic structures having an average period, e.g., for quasicrystals).

To summarize, in the frame of the coupled-waves approach we have studied the anticrossing phenomenon of the Wood and Bragg resonances in the reflection spectra of the synthesized hybrid structures based on the opal photonic crystal. From a comparison of the experimental data with the theoretical model calculations we have determined the effective parameters of the quasi-guided mode responsible for the appearance of the resonant Wood anomalies and the interaction coefficient between the modes of the Wood anomalies and 3D Bragg diffraction. An empirical description of the Wood anomaly reflection spectra is made for the case where all other resonances in the considered frequency range are absent. It is established that in hybrid photonic crystals the interference of the light waves originating from different quasi-guided modes in the Wood anomaly reflection spectra can arise.

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