Collective resonances in hybrid photonic-plasmonic nanostructures

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Abstract. We present the theoretical model to predict the spectral position of Rayleigh anomalies emerged in hybrid system consisting of periodic array of plasmonic nanodisks embedded into the middle of defect layer of 1D photonic crystal (PhC). The spectral positions of these new emerged Rayleigh anomalies agree well with the results of exact simulations with Finite-Difference Time-Domain (FDTD) method.

1. Introduction

The rapid development of modern technology emerges completely new fields of science aimed at the development of new materials as alternative to semiconductors, such as photonic crystals (PhC). These are materials in which dielectric permittivity changes periodically with a characteristic scale which coincide with the wavelength of light [1]. An important feature of PhC is the possibility of light localization by artificial structural defect in periodic system, so called defect layer.

Of particular interest are PhCs with tunable spectral characteristics in which the defect layer can be made of liquid crystals [2], layer with high Kerr nonlinearity [3] or materials with resonance dispersion [4]. In recent years periodic arrays of plasmonic nanoparticles are of the great interest, because of emergence of collective modes due to the strong coupling between the localized surface plasmon resonance (LSPR) and Wood-Rayleigh anomalies [5]. This hybridization leads to a narrow-band surface lattice resonances (SLRs) which greatly surpass the quality factor of LSPR. SLRs have attracted considerable attention only in the last decade, starting with the pioneering theoretical works of Prof. Schatz [6, 7] and Prof. Markel [8], where they have showed the conditions for the manifestation of extremely narrow collective modes in a one-dimensional periodic chain of silver nanoparticles. While the most of publications study only general properties of regular NPs arrays embedded in the non-homogeneous environment, the physics behind sophisticated coupling regimes between plasmonic and photonic modes is usually hindered. The understanding of modes coupling in such systems, and the development
of analytical models that predict their optical properties represent quite important applied problem. In this paper, we study hybrid nanostructure comprised of a 1D PhC with 2D periodic lattice of plasmonic nanoparticles embedded in its defect layer. We present analytical model to predict spectral position of Rayleigh anomalies in such hybrid plasmon-photonic structures.

2. Description of the structure
We consider PhC with unit cell which consists of two layers with thickness $d_a$ and permittivity $\varepsilon_a$ and $d_b$ and permittivity $\varepsilon_b$ respectively. We assume that PhC is comprised of $N$ unit cells and the optical glasses defect layer (with thickness $L$ and permittivity $\varepsilon_{\text{def}}$) in between, as shown in Fig. 1. Regular 2D array of plasmonic nanodisks with period $h$, height $H$ and radius $R$ is embedded in the middle of the PhC defect layer.

![Figure 1. Schematic representation of PhC and 2D NPs array embedded in its defect layer.](image)

3. Model of the Mode Coupling
In the case of NPs array embedded in PhC defect layer, Wood-Rayleigh anomalies emerge due to the multiple reflections of light scattered by NPs in PhC. In general case, the wavevector $\mathbf{k}$ in the defect layer reads as:

$$k^2 = k_x^2 + k_y^2 + k_z^2 = \varepsilon_{\text{def}} \left( \frac{2\pi}{\lambda_{p,q,s}} \right)^2,$$

where $k_{x,y,z}$ are corresponding components of $\mathbf{k}$. The conditions of constructive interference for PhC with NPs embedded in the middle of its defect layer, can be found from:

$$k_x h = 2\pi p, \quad k_y h = 2\pi q, \quad k_z L = 2\pi s - \varphi .$$

Here $s$ is the integer which denotes the order of the phase difference in $z$ direction. Eq. (2) takes into account the coupling of NPs through the multiple reflections from PhC. Note that for $L \to \infty$, the coupling between NPs and PhC becomes negligible, and $k_z$ vanishes in Eq. (1) and Eq. (2).

Equation (2) takes into account the phase shift $\varphi$ that occurs due to reflection from the PhC:

$$\varphi = \arg \left[ \frac{CU_{N-1}}{AU_{N-1} - U_{N-2}} \right].$$

Here $U_N = \sin [(N + 1) K \Lambda] / \sin [K \Lambda], \quad K = \arccos [(A + D) / 2] / \Lambda$ is the Bloch wavenumber, $\Lambda = d_a + d_b$, and $N$ is the number of PhC periods. $A$, $C$ and $D$ are the elements of the $2 \times 2$
Fig. 2 the transmission spectra of the structure for different values of height $H$ with theoretical predictions. Numerical simulation (i.e., spectral position of avoiding crossings) are in good agreement of NPs in the array with each other via reflections from PhC. As can be seen the results of theoretical model were verified by FDTD simulation of the optical properties of the structure. In this paper, we denote TE polarization as perpendicular to the plane of incidence, while TM is parallel to it.

Thus $ABCD$ matrix is equal:

$$
ABCD = \begin{bmatrix}
e^{ik_{ax}d_a} \left( \cos k_{bz}d_b + \frac{1}{2} i \mathbf{k}_{+} \sin k_{bz}d_b \right) & e^{-ik_{ax}d_a} \left( \frac{1}{2} i \mathbf{k}_{+} \sin k_{bz}d_b \right) \\
e^{ik_{az}d_a} \left( \frac{1}{2} i \mathbf{k}_{-} \sin k_{bz}d_b \right) & e^{-ik_{az}d_a} \left( \cos k_{bz}d_b - \frac{1}{2} i \mathbf{k}_{-} \sin k_{bz}d_b \right)
\end{bmatrix}
$$

Here $\mathbf{k}_{\pm} = k_{bz} \pm k_{az}$ for TE mode, $\mathbf{k}_{\pm} = \frac{\varepsilon_b k_{az}}{\varepsilon_a k_{bz}} \pm \frac{\varepsilon_a k_{bz}}{\varepsilon_b k_{az}}$ for TM mode,

$$
k_{az} = \sqrt{\frac{\varepsilon_a}{\varepsilon_{\text{def}}} k^2_z + \left( \frac{\varepsilon_a}{\varepsilon_{\text{def}}} - 1 \right) k^2_x + \left( \frac{\varepsilon_a}{\varepsilon_{\text{def}}} - 1 \right) k^2_y},
$$

$$
k_{bz} = \sqrt{\frac{\varepsilon_b}{\varepsilon_{\text{def}}} k^2_z + \left( \frac{\varepsilon_b}{\varepsilon_{\text{def}}} - 1 \right) k^2_x + \left( \frac{\varepsilon_b}{\varepsilon_{\text{def}}} - 1 \right) k^2_y},
$$

are the wave vectors for corresponding layers of PhC.

The numerical solution of Eq. (1) for the given configuration of PhC and array of NPs (which are described in Eq. (2) and Eq. (3)) provides the set of $(p, q, s)$-order Wood-Rayleigh anomalies for both TE and TM polarizations. It should be noticed, that solutions of Eq. (1) are symmetrical with respect to the following permutations and transformations: $p \leftrightarrow q$, $p \rightarrow -p$, and $q \rightarrow -q$. Thus, for convenience and without losing the generality, we consider $q \geq p \geq 0$. Due to the symmetry of the system, we limit the discussion with non-negative values of $k_z$ and $s$. Finally, it should be noticed that the modes with wave vector parallel to the 2D array (i.e. with $k_z = 0$) and observed in bare NPs array are also preserved in the presence of PhC. In what follows, we will denote such modes as $(p, q, -)$.

We would like to emphasize that the PhC-mediated interaction between Wood-Rayleigh anomalies of different orders is not taken into account in presented theoretical treatment. Such interaction can be described within the framework of vector-coupled-mode theory [10]. However, as it will be shown below, our formalism predicts positions of Wood-Rayleigh anomalies with satisfying accuracy. In the case of NPs with height $H$ significantly smaller than the thickness of defect layer $L$, one could ignore the interaction between diffractive modes, though, this approximation has to be used with caution for larger NPs.

4. Model verification

The results of theoretical model were verified by FDTD simulation of the optical properties of the structures. In FDTD simulation we used PhC with unit cell made of silica (SiO$_2$) ($d_a = 70$ nm, $\varepsilon_a = 2.1$) and zirconium dioxide (ZrO$_2$) ($d_b = 40$ nm, $\varepsilon_b = 4.16$). The defect layer thickness $L = 725$ nm and $\varepsilon_{\text{def}} = 2.25$. Regular 2D array of Aluminum nanodisks [11] with period $h$, height $H = 30$ nm and radius $R = 25$ nm is embedded in the middle of the PhC defect layer. In Fig. 2 the transmission spectra of the structure for different values of $h$ are shown. This figure shows detailed insets with regular and additional Wood-Rayleigh anomalies created by coupling of NPs in the array with each other via reflections from PhC. As can be seen the results of numerical simulation (i.e., spectral position of avoiding crossings) are in good agreement with theoretical predictions.
Figure 2. (a) Transmittance of 2D array of aluminum nanodisks embedded in PhC defect layer. Symbols denote Wood-Rayleigh anomalies of \((p,q,s)\) order for TE and TM polarization. (b) Detailed illustration of various hybridization scenarios for Wood-Rayleigh anomalies.

5. Conclusion
To conclude, we have developed a simple yet comprehensive analytical model to explain the emergence of additional Wood-Rayleigh anomalies in 2D arrays of NPs embedded in the defect layer of 1D PhC caused by multiple reflections inside PhC. Exact simulations with the FDTD method show excellent agreement between the predicted positions of Wood-Rayleigh anomalies and regions of PhC modes hybridization. Strong coupling between PhC and NPs leads to multiple splittings of the defect modes which can be tailored by varying period \(h\) of NPs array. Thus, deeper understanding of modes coupling in hybrid NPs-PhC system paves a way for more efficient control of its optical response for photonics applications which is not easy to achieve with other alternative strategies.

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