Optical bio and chemical sensor in a one-dimensional photonic structure with bound states in the continuum

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***Abstract* — In this paper, we present the main results of the numerical calculation of the bound states in the continuum (BICs) application in the refractive index (RI) sensing. We consider a one-dimensional rectangular photonic structure at subwavelength regime and study the Fano resonance shift for off-Г BIC. The results obtained will make it possible to create photonic structures for biosensing, for which a high-Q resonance is observed at nonzero incidence angles.**

Keywords — bound states in the continuum, photonic structure, Fano resonance, sensitivity

I. INTRODUCTION

Bound states in a continuum (BIC) can be considered as a resonant mode with an infinite quality factor Q in an open system. It was shown that in Г point BIC is observed for odd modes, while outside the Г point the modes are not divided into even and odd ones with due to the presence of a nonzero Bloch phase, and the appearance of BIC outside the Г point (off-Г BIC) is achieved by selecting the optimal geometric parameters of the structure[1]. When the symmetry of the structure is broken or the diffraction channel is opened, BICs transform into quasi-BICs. The RI contrast between substrate and superstrate breaks the flip symmetry and transforms the off- Г BIC into a resonant state with a finite, but high, Q factor [1]. Therefore, the spectral position of high-Q quasi-BIC is sensitive to changes in the refractive index of the medium, which makes it possible to design sensors with high sensitivity [2].

One of the important characteristics of sensors is the figure of merit (FOM), which is proportional to the sensitivity and Q factor. It should be noted that the presence of a high Q factor is confirmed in the form of a narrow Fano resonance in the transmittance (or reflectance) spectrum [3]. For sensors based on surface plasmon resonance (SPR sensors), which are commercially available, it is impossible to achieve the narrow Fano resonance in the experiment, because the absorption in metal leads to low Q factor [2]. In contrast, photonic crystal (PhC) devices support high Q factor [4], and despite the fact that their sensitivity is several times less than SPR sensors have [2], the high Q factor compensates low sensitivity that leads to extremely high values of FOM in comparison with SPR sensors [5]. The spectral position of these extremely narrow Fano resonances is sensitive to the change on refractive index of surrounding medium, which makes it possible to create sensors with high FOM [3]. Nowadays research is actively conducted on creation of PhC sensors with high performance [4], and for such structures there are several theoretical approaches to increasing their sensitivity [2,3]. Although the problem of optimisation in presence of the substrate has not been completely solved; moreover, most of the works are devoted to structures that support only In-Г BIC, which appear at normal incidence of beam [3].

In this paper, we investigate the resonance shift of off- Г BIC depending on the refractive index (RI) contrast between substrate and superstrate in a dielectric grating. We calculate the sensitivity of the system and show how it changes with the RI of superstrate (analyte).

II. RESULTS AND DISCUSSION

We have considered a one-dimensional periodic gallium phosphide (GaP) grating with n_g =3.17, period d =0.4μm, width w =0.28μm and height h =0.33μm, which is located on a substrate of sapphire (Al_2O_3) with n_s =1.75 (Fig. 1 (a)). Since the next step of our research is an experimental study, the structure parameters were matched to the technological possibilities. As Al_2O_3 and GaP has small absorption [6] in the operating wavelength range that is available in the experiment, they were chosen as the components for the sensor. Since we are working in subdiffractive regime, the period must less than the wavelength. Since off-Г BIC is observed only at certain values of the structure's geometry, the height and width of the grating were obtained by fitting.

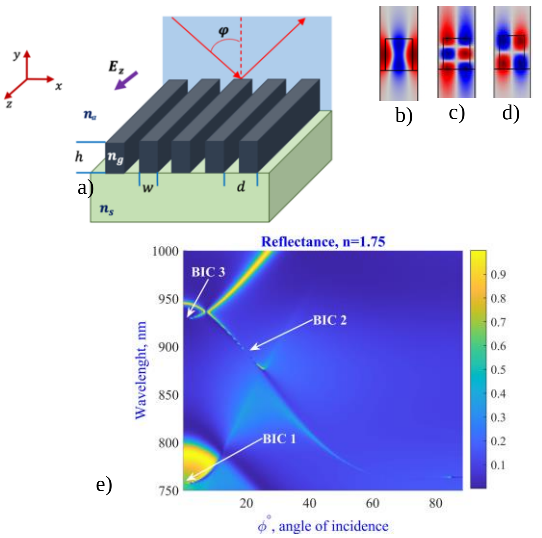


Fig. 1. Schematic representation of the structure (a); field profile E_z for BIC 1 (b), BIC 3 (c), which are observed in Г point and for BIC 2, which appears outside the Г point; e) reflectance map for the case $n_s = n_a$ =1.75

The numerical calculation was realized by Fourier Modal Method (FMM) [7], while the field profiles were obtained on the COMSOL Multiphysics software. In COMSOL we used «Wave Optics» module – «Eigenfrequency» study, in which eigenmodes and eigenfrequencies of a linear or linearized model are obtaining by the solving of following equation [8]:

$$\nabla \times \mu_r^{-1}(\nabla \times \mathbf{E}) - k_0^2\left(\varepsilon_r - i\frac{\sigma}{\omega\varepsilon_0}\right)\mathbf{E} = 0 \tag{1}$$

where **E** is electric field strength, k_0 is vacuum wavenumber, ε_r, μ_r and σ are permittivity, magnetic permeability, and conductivity. For our case $\mu_r = 1$ and σ is equal to zero. When solving the equation (1) as an eigenfrequency problem the eigenvalue is the complex eigenfrequency $\lambda = -i\omega + \delta$, where δ is the damping of the solution [8]. The grating schematically shown in the Fig. 2. As we considered 1D periodic structure, the Floquet conditions were applied along the periodicity direction.

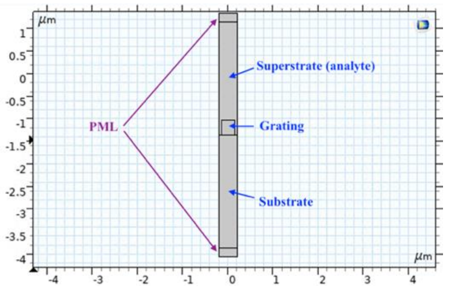
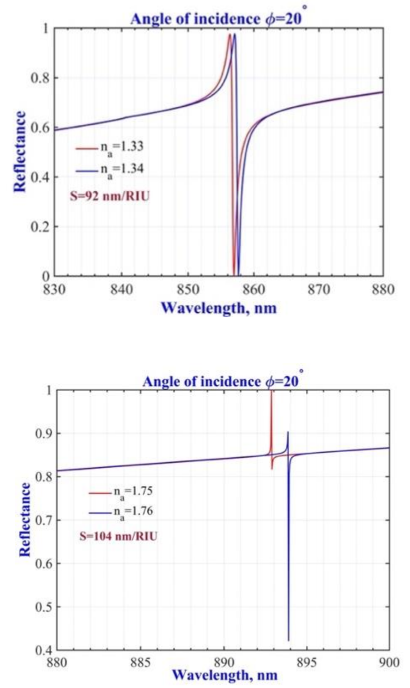


Fig. 2. Schematic representation of the considered model in COMSOL Multiphysics software (PML means perfectly matched layer)



a)

b)

Fig. 3. Reflectance spectrum as a function of wavelength at ϕ =20° for n_a =1.33, n_a =1.36 (a), n_a =1.75, n_a =1.76 (b). The results of the sensitivity calculation are shown in the insets

It should be noted that the calculation in COMSOL was realized without considering the material dispersion, while it was taken into account during the FMM calculation of the reflection spectra.

For this structure, BIC 1 and BIC 3 are observed in Γ point and BIC 2 outside the Γ point (Fig. 1 (b-d)). For the case when $n_s \neq n_a$ off-Γ BIC turns into a quasi- BIC with a finite quality factor. We calculate the sensitivity S from the shift of resonances for quasi-BIC at different values of the analyte refractive index Fig.3(a, b). One can see from Fig.3 that with on n_a, the sensitivity increases, moreover, when the refractive indices of the substrate and analyte are close to each other, the Fano resonance width decreases, which leads to a high FOM value. In our case, the FOM value is above 10^3, which is an order of magnitude higher than FOM of the structure from the article [2] for the case of quasi-normal incident wave.

For the considered structure the average S equals to 92 nm/RIU. In work [2] authors shows that the S is limited by $S_{max} = {}^{\lambda_{BIC}}/_{n_a}$. In our case, the upper limit of the sensitivity is 510 nm/RIU.

III. CONCLUSION

In this paper, we considered a one-dimensional photonic structure that supports the BICs in Γ point and outside it. It was found that the sensitivity for off-Γ BIC, which is obtained at $\phi = 20°$, reaches 100 nm/RIU. Although the sensitivity we obtained is about 5 times less than S_{max} =510 nm/RIU, it is possible to achieve the upper limit value. One way to achieve maximum sensitivity is to increase the refractive index of the analyte relative to the refractive index of the substrate [2]. Moreover, the narrow Fano resonances that occur in the vicinity of BIC make it possible to detect a small change in the refractive index in biological or chemical environment.

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