RESEARCH ARTICLE / ARAȘTIRMA MAKALESİ

Strongly Confined Electromagnetic Waves in a Hybrid Photonic– Plasmonic Resonator for Enhancing Light–Matter Interaction

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Abstract

In this paper, a 1D photonic crystal waveguide and a plasmonic compound nano-system are utilized to design a hybrid photonic-plasmonic device for enhancement of light-matter interaction. Strongly localized light waves in a very small volume intensify the optical field, via a plasmonic particle, which interacts with the resonator's cavity mode while the photonic crystal nanobeam ensures a high temporal confinement. The enhancement of light-matter interaction in the hybrid resonator is investigated through the single-atom cooperativity parameters based on numerically obtained results, which is calculated to be a factor of 14 as a consequence of the considerably reduced optical mode volume in the presence of the plasmonic nanoparticle. Additionally, the theoretical models and calculation procedures, presented in this paper, are demonstrated to be pioneering for the fabrication of efficient quantum devices based on hybrid photonic-plasmonic resonators.

Keywords: Photonic crystal, Hybrid resonator, Optical mode, Plasmonic nanoparticle, Light-matter interaction

I. INTRODUCTION

Controlling of light-matter interaction has become more of an issue for the scientific and technological developments in the area of photonics [1-3]. In this regard, numerous optoelectronic and photonic devices in various research fields like quantum information, laser and sensor technologies [4-6] have been introduced and efforts have been made to couple quantum sources such as dye molecules, quantum dots (QDs) into these photonic devices to manipulate their spontaneous emission [7]. Photonic resonators are basically designed based on two parameters; the quality factor (Q-factor), which corresponds to the temporal confinement of the electromagnetic waves and the mode volume (V), which accounts for the spatial localization of the photons [8]. The enhancement of the spontaneous emission rate is achieved provided that a resonator has either a high Q-factor or a small mode volume, yielding a high Purcell factor to improve the performance of the photonic devices [9].

Photonic crystal cavities have been demonstrated to offer a remarkable platform to control and manipulate the light emission with their ability to successively trap the photons at desired frequencies [10]. Even a slight change in the design parameters, like the dimensions or the shape of the mirror holes, results in the resonance frequency of the device to change, leading to a different design with a particular *Q*-factor and mode volume [11, 12]. Therefore, a wide variety of 1D or 2D photonic crystal designs, using diversified materials with varied Purcell factors at specific resonant frequencies, have been achieved [13-17] and they have been utilized in various applications; such as, optical trapping of nanoparticles [18], biological detection [19], light modulation [20] by means of vertical component of the light, which strongly emerges in the photonic crystals [21]. Although these dielectric photonic crystals are usually designed to have a high Q-factor based on their design parameters and materials, it is challenging to reduce the mode volume of these devices due to the number of the reflective mirrors used to achieve a high temporal confinement of the optical power [22]. On the other hand, it is a wellknown fact that plasmonic nanoparticles act like nanoantennas with their capability of trapping light waves in a very small volume [23, 24]. It is also known that the plasmonic structures are not generally efficient to fabricate a resonator with a high O-factor because of the radiation loss caused by their high absorption coefficients [25]. However, if metallic nanoparticles are integrated into a photonic cavity, provided that the quality factor of the resonator is essentially preserved, depending on the number and size of the plasmonic nanoparticles; the radiation properties of the device can be improved through the strong light localization [26, 27]. For example, a hybrid device, which comprised of a partially encapsulated photonic crystal waveguide and a single gold nanosphere, was reported to achieve a considerably enhanced Purcell factor, compared to the previously reported values for its counterparts due to the strong light concentration within a very small volume around the plasmonic nanoparticle[28].

Corresponding Author: BELKIS GÖKBULUT, Tel: 0212 359 5400, e-posta: belkis.gokbulut@boun.edu.tr Submitted: 25.11.2022, Revised: 20.01.2023, Accepted: 28.02.2023 Hybrid photonic-plasmonic devices have also been demonstrated to offer unique opportunities for various applications as they provide ideal platforms for enhancing light-matter interaction [29, 30]. For instance, an optical refractive index sensor based on a photonic crystal structure integrated with metallic nanorods was shown to outperform the pure plasmonic or photonic crystal sensors as the localized surface plasmons increase the interaction of the optical field and the matter inside the cavity. This situation enhances the sensitivity and figure of merit of the device [31]. In another study, the synergetic coupling between the plasmonic field and the photonic crystal waveguide mode in a refractive index sensor was also revealed to offer an excellent potential to be used in sensing applications; the device was based on hybrid topology of photonic crystal and nested circular metallic split-ring resonator [32].

In this paper, a hybrid photonic-plasmonic device, which originates from a 1D photonic crystal waveguide and a plasmonic nanostructure is proposed to benefit from the advantages of both photonic and plasmonic systems. First of all, the photonic resonator, with gradually decreasing nanoholes towards the center of the resonator, is designed. Then, a core/shell nanoparticle, which consists of a gold nanoparticle, coated by polystyrene (PMMA) layer and a dipole, placed on the surface of the PMMA layer surrounding the plasmonic nanoparticle is introduced to be integrated on the surface of the photonic crystal cavity. The polymer layer between the dipole and the plasmonic nanoparticle provides a required distance to prevent any radiation loss induced by the excessive electron or energy transfers between the dipole and the metal nanoparticle. In this regard, while the light waves are demonstrated to be localized in a very small volume due to the strong interaction between the surface plasmons and the cavity mode, the *Q*-factor of the system is mainly preserved. The enhancement factor of the light-matter interaction in the hybrid resonator is investigated by the single-atom cooperativity parameters of the designed photonic crystal nanobeam and photonic compound system, which results in a value of about 14. The appropriate theoretical models and calculation procedures presented in this paper ensure fabrication of a highly efficient quantum device based on a hybrid resonator. Therefore, in our photonic design, strongly confined electromagnetic field at nanoscale in a hybrid photonic-plasmonic device, which consists of an efficient photonic resonator and a well-defined core/shell nanoparticle, is demonstrated to be promising for remarkable progresses in nanophotonics, nanoplasmonics, and quantum information technologies.

II. THE DESIGN OF THE PHOTONIC DEVICE

In this work, photonic crystal nanobeam is designed to be a 1D sequential layout of air holes with a lattice constant (p) of 250 nm and a hole radius (r) of 70 nm aiming to have high Q-factor and a small mode volume at the visible wavelength regime via Finite Difference Time Domain (FDTD) Technique. The reasons behind using 1D geometry and an air-bridged design are that 1D photonic crystal beams usually have larger band gaps than their 2D counterparts [33]; and air-bridged designs offer a high refractive index contrast between the waveguide and the air cladding to facilitate obtaining a high Q-factor [34].

The schematic representation of the photonic crystal nanobeam that includes eleven mirror holes as Bragg reflectors and four taper holes on each side, is given in Figure 1.



Figure 1. A display of the designed photonic crystal nanobeam.

A defect mode is introduced at the desired wavelength of 628 nm to obtain a radiation with the optimized simulation parameters. The substrate material is chosen to be SiN with a refractive index of 2.05 because it has a low absorption coefficient at the visible range. The layer thickness and width (ω) of the substrate material are determined to be 200 nm and 300 nm, respectively. There are four taper holes on each side that have linearly decreasing radius from 66 nm to 55 nm towards the center of the beam. Cavity length (*Lc*) is also determined to be the distance between the innermost holes, which is equal to 205 nm.

The design parameters of the photonic crystal nanobeam are optimized to have a high *Q*-factor and small mode volume through the optimization toolbox of the FDTD solver module of the Lumerical Ltd. In the simulations, after the design of the photonic crystal cavity, a gold nanoparticle with a radius of 10 nm is coated by a PMMA shell with a thickness of 15 nm first; and then, an electric dipole is attached to the surface of the layer to introduce a hybrid core/shell-Au/PMMA-dipole nanoparticle. This nanoparticle is integrated at the central region of the photonic crystal nanobeam to produce a hybrid photonic-plasmonic resonator, as shown in Figure 2.



Figure 2. The schematic representation of the hybrid device that includes 1D photonic crystal nanobeam and a core/shell-Au/PMMA-dipole nanoparticle, which is illustrated in detail in the zoomed image.

The coupling of the localized surface plasmons to the mode significantly confines optical the electromagnetic field in the photonic device. However, plasmonic particles near the fluorescent quantum light sources like quantum dots or molecules induce a considerable optical loss because of the quenching of the light intensity [35]. Nonetheless, with a specified thickness of the polymer layer surrounding the gold nanoparticle, a controllable distance between the plasmonic nanoparticle and the dipole is provided to prevent the excessive electron or energy transfer mechanisms between the particles; hence, an efficient dipole-hybrid mode interaction is achieved simultaneously. The numerical calculations have also been performed to optimize the radius of the gold nanoparticle whose diameter is much smaller than the interacting light wavelength after the resonance wavelength of the photonic structure is simulated. According to our results, the local electric field near the plasmonic nanoparticle is observed to be considerably boosted when the gold nanoparticle with a radius of 10 nm is used.

III. RESULTS AND DISCUSSION

In the simulations, the electric field distribution is calculated for each unit cell to obtain the field distribution profiles of the resonators. The mesh grid size in the hybrid structure is determined to be 0.1 nm. The optical mode volume and the Q-factor of the hybrid cavity are also determined by time-domain perfectly-matched calculations using layers surrounding the resonator to calculate the Purcell factor. The optical mode volume calculations are performed over the entire space, including the perfectly matched-layers. The main reason to use perfectly-matched layers at the boundaries of the hybrid resonator is to ensure taking account of the field leakage from the system, induced by the plasmonic nanoparticle. Thus, using perfectlymatched layers facilitates to determine the exact field distribution and the optical mode volume of the hybrid photonic-plasmonic cavity. The top view and electric field distribution profile of the photonic crystal nanobeam are obtained by FDTD technique, which are given in Figure 3a and 3b, respectively. In our numerical calculations, a dipole is also attached to the surface of the shell (PMMA) particle, and then the shell (PMMA)-dipole particle is placed at the central region of the photonic crystal nanobeam. The top view of the photonic crystal beam, after the shell (PMMA)dipole particle is placed, is shown in Figure 3c along with its electric field distribution profile, shown by Figure 3d. Although the electric field distribution profile is observed to change as a result of the effect of the cavity mode on the polymer layer, a strong light localization, which induces a substantially reduced mode volume, is not observed. The top view and electric field distribution profile of the photonic crystal nanobeam after the core/shell-Au/PMMAdipole nanoparticle is integrated on the surface of the structure, are also given in Figure 3e and 3f, respectively. In Figure 3f, the inset figure shows the zoomed electric field distribution around the plasmonic nanoparticle. For visual purposes, the central regions of the resonators are illustrated. After the core/shell-Au/PMMA-dipole nanoparticle is integrated on the surface of the resonator, the local electric field near the plasmonic nanoparticle is shown to be noticeably enhanced when the gold particle with a radius of 10 nm is used, as shown in Figure 3f.



Figure 3. (a) Top view and (b) field distribution of the resonator. (c) Top view and (d) field distribution of the resonator in which a shell-dipole nanoparticle is placed. (e) Top view and (f) field distribution of hybrid resonator.

The Purcell factor is basically determined by Equation 1 when the dipole is oriented with respect to the mode field direction at the resonant frequency [36].

$$F_p = \frac{3Q(\lambda/n)^3}{4\pi^2 V}$$
(1)

in which *n* is the refractive index of the cavity, *V* is the optical mode volume and λ is the resonance wavelength of the device, and *Q* is the quality factor. When the plasmonic particle exists, the mode volume of the hybrid mode is determined by Equation 2,

which accounts for both the confined cavity mode and photonic loss from the cavity due to the absorbtive plasmonic nanoparticle [37]. The Drude model is utilized for the complex dielectric function with the total field ($\tilde{\mathbf{E}}$, $\tilde{\mathbf{H}}$) generated by a dipole, $\mathbf{p}=p\mathbf{u}$ in which \mathbf{u} is a unit vector.

$$V = \frac{\int \left[\tilde{\mathbf{E}} \cdot \frac{\partial \left(\omega\varepsilon\right)}{\partial \omega} \tilde{\mathbf{E}} - \tilde{\mathbf{H}} \cdot \frac{\partial \left(\omega\mu\right)}{\partial \omega} \tilde{\mathbf{H}}\right] d^{3}\mathbf{r}}{2\varepsilon_{0} n^{2} \left[\tilde{\mathbf{E}}\left(\mathbf{r}_{0}\right) \cdot \mathbf{u}\right]^{2}}, \qquad (2)$$

In the numerical calculations, the mode volume of the photonic crystal nanobeam is determined to be around $0.12(\lambda/n)^3$. The mode volume is also determined after the shell (PMMA)-dipole particle is placed on the surface of the photonic crystal beam, which is found to be $0.09(\lambda/n)^3$. The insignificantly decreased mode volume of the structure is induced by the slight confinement of the light waves in a very small volume of the polymer region.



Figure 4. Numerically obtained photoluminescence spectra of (a) the photonic crystal nanobeam and (b) the hybrid device, consisting of a 1D photonic crystal nanobeam and core/shell-Au/PMMA-dipole nanoparticle.

Finally, the core/shell-Au/PMMA-dipole nanoparticle is integrated on the surface of the resonator and the nanostructure with an optimized Au core radius of 10 nm is observed to ideally confine the optical mode field of the photonic crystal cavity in a very small volume through the localized surface plasmons. As a result, the mode volume of the hybrid structure is observed to considerably decrease to a value of $0.007(\lambda/n)^3$ with a negligible imaginary part.

The photoluminescence spectra of the photonic crystal waveguide and hybrid device are also acquired by FDTD technique, which are given in Figure 4a and 4b, respectively. The lasing spectrum is observed not to be changed noticably in the existence of the gold particle because of the minimized dimensions of the plasmonic nanoparticle used in the hybrid system.

The quality factors of the photonic systems presented in Figure 3a, 3c and 3e are also obtained numerically. The *Q*-factor of the photonic crystal nanobeam and the shell (PMMA)-dipole particle integrated photonic crystal nanobeam are calculated to be about 10448 and 10254, respectively. The *Q*-factor of the hybrid resonator is also determined to be about 8434 in the presence of the plasmonic nanostructure.

Table 1. The resonant wavelength λ_c , Mode volume, *Q*-Factor, and the Purcell factor (F_p) values of the designed photonic crystal (PC) nanobeam; photonic crystal nanobeam in which a shell (PMMA)-dipole nanoparticle is placed; and the hybrid resonator in which core/shell-Au/PMMA-dipole nanoparticle is placed.

Structure	Mode volume	<i>Q</i> - factor	$\lambda_c(nm)$	F_P
PC nanobeam	$0.12(\lambda/n)^3$	10448	628.68	6622
PC with the shell-dipole	$0.09(\lambda/n)^3$	10254	628.68	8666
PC with the Au/PMMA- dipole	$0.007(\lambda/n)^3$	8434	628.68	91651

The Purcell factors of the designed photonic crystal nanobeam shown in Figure 3a, the photonic crystal nanobeam after the shell (PMMA)-dipole nanoparticle is placed, which is demonstrated in Figure 3c, and the hybrid resonator after the core/shell-Au/PMMA-dipole nanoparticle is placed, which is presented in Figure 3e, are also calculated and given in Table1 along with their mode volume, *Q*-factor values and resonance wavelengths. The Purcell factor is observed to be considerably enhanced to a value of F_p =91651 in the presence of the plasmonic nanoparticle.

The absorptive nature of the gold nanoparticle, interacting with optical mode is expected to cause a decrease of the Q-factor of the device. However, in our photonic design, interrogating a plasmonic nanoparticle with a radius of 10 nm, reduces the effects of the optical losses and the Q-factor of the structure remains still high. Therefore, it is obviously

seen that the hybrid device proposed here is demonstrated to be highly efficient for developments of the low-threshold lasers since the designed photonic structure with a high *Q*-factor and small mode volume enables to considerably enhance the Purcell factor and reduce the amount of active material in the resonator if a quantum source like a dye molecule or a QD is used to be a dipole to be chemically attached to the surface of the synthesized core/shell-Au/PMMA nanoparticle.

The light-matter interaction enhancement factor is determined in terms of the single-atom cooperativity parameters of the designed photonic resonators based on Equation 3 [38]:

$$C = \frac{2G^2}{\kappa \gamma_s} , \qquad (3)$$

in which γ_s is the decay rate of dipole, κ is the decay rate of the optical mode, and *G* represents the coupling strength, calculated by [38]

$$G = \mu f_c(\mathbf{R}) \left(\frac{\omega_c}{\left(2\hbar\varepsilon_0 \varepsilon_c V_c\right)} \right)^{1/2}, \qquad (4)$$

in which \hbar is the reduced Planck's constant, ε_0 is the vacuum permittivity, μ and ε_c represents the photonic medium permeability and permittivity, respectively, and $f_c(\mathbf{R})$ corresponds to the normalized electric field distribution in the cavity where the distance is represented by R.

The light-matter interaction enhancement factor ($C_{c+m/}$ C_c), is determined by the ratio of the single-atom cooperativity parameters of the dipole coupled into the photonic-plasmonic mode of the hybrid device, consisting of a 1D photonic crystal waveguide and core/shell-Au/PMMA-dipole nanoparticle (C_{c+m}) and the cavity mode of the photonic crystal resonator (C_c) based on the numerically obtained results for both systems. The light-matter interaction enhancement factor is determined to be about 14 in the hybrid resonator. Although our study has no direct analogy to previously published works in the literature, the enhancement factor we have obtained might be compared to the system based on a hybrid structure, which consists of a plasmonic nanoparticle and a WGM cavity [39]. When the radius of the plasmonic nanoparticle in this system is 10 nm and the distance between the dipole and the plasmonic nanoparticle is about 15 nm, the enhancement factor of the lightmatter interaction is determined to be about 5 [39], which seems to be much lower than ours.

In the literature, plasmonic particles integrated to 2D photonic crystal waveguides with low or moderate Q-factors have been demonstrated to improve radiation efficiency [40, 41]. For example, the enhanced mode field has been revealed in a recent study in which

plasmonic rods and nanospheres are excited to enable surface plasmons to be coupled into the cavity field of the resonator as the Q-factor of the device is significantly reduced from Q=2500 to Q=720 because of the absorptive nature of the plasmonic particle [41]. In another study, a plasmonic nanoparticle is located at the center of an integrated photonic device with two different photonic cavities; a Fabry Perot cavity and a 2D photonic crystal waveguide to interact with the mode fields. In the hybrid device, as the electric field is observed to be significantly enhanced around the plasmonic nanoparticle, the Q-factor of the device is also shown to decrease from Q=435 to Q=184 due to plasmonic particle [42]. In addition to all these, the boosted cavity mode field through plasmonic interaction has also been achieved in a recently published study in which a hybrid structure, consisting of a partially encapsulated photonic crystal waveguide and a gold nanoparticle is used [28]. The photonic design is based on a partial encapsulation of a 1D photonic crystal waveguide with a polymer layer of a thickness of 40 nm. The mode volume of the device is demonstrated to considerably decrease to a value of about 0.8 $(\lambda/n)^3$ in the presence of the gold nanoparticle [28]. In the photonic design proposed here, together with appropriate theoretical models and calculation procedures, the light-matter interaction enhancement is accomplished by a hybrid photonicplasmonic design consisting of a 1D photonic crystal core/shell-Au/SiO2-dipole waveguide and а nanoparticle, which offers both high Q-factor and small mode volume. As the polymer layer between the electric dipole and the surface of the gold particle provides an efficient distance for enhancement of light-matter interaction, light waves are demonstrated to be extremely confined through synergetic effect of the cavity mode and the plasmonic fields. Thus, the mode volume of the device is dramatically decreased to a value of $0.007(\lambda/n)^3$. It proves that the stronger light concentration, and hence, the stronger lightmatter interaction is achieved compared to the similar hybrid architecture published earlier as the high Qfactors of the photonic resonators are almost maintained in the presence of the plasmonic nanoparticles in both devices [28]. Therefore, the photonic platform introduced here offers а significantly improved device characteristics through plasmonic effect, which enables fabrication of a nanostructure with a great potential to be used in various applications such as optical trapping or biosensing.

In a future work, the photonic crystal waveguide proposed here will be produced by electron beam lithography and the core/shell-Au/PMMA particle will be synthesized chemically and decorated with a few quantum dots to reduce the amount of active material in the resonator and then, integrated on the surface of the photonic cavity by Atomic Force Microscopy technique. Time-resolved experiments based on single photon counting technique will also be performed to obtain the experimental results to compare with the theoretical model, calculations and the numerically obtained results presented in this paper. The fabrication of such a hybrid photonic-plasmonic resonator would facilitate to produce a nanodevice operating in the quantum regime, which may have a potential to be used in quantum information technologies.

IV. CONCLUSIONS

In this paper, a 1D photonic crystal resonator with gradually decreasing nanoholes towards the center of the structure, is designed. Then, a well-defined which comprises nanoparticle, a plasmonic nanoparticle, coated by a silica layer and a dipole, is integrated on the surface of the cavity to generate a hybrid photonic-plasmonic resonator. The strongly enhanced electromagnetic field at nanoscale is generated as a result of the interaction between the optical mode field and gold particle to enhance the light-matter interaction by a factor of about 14. The theoretical models and calculation procedures introduced in this paper are demonstrated to be leading for the fabrication of a highly efficient quantum device based on a hybrid resonator. Therefore, the photonic design presented in this paper is considered to be promising for the advances in fabrication of hybrid and efficient devices for photonic and optoelectronic platforms, laser and sensor technologies, and quantum information processing.

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