FEM Design and Modeling of $\chi^{(2)}$ Second-Harmonic Enhancement in Circular Photonic Crystal

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Abstract—In this paper, we analyze the enhancement of $\chi^{(2)}$ nonlinear process in membrane-type circular photonic crystal (PhC) based on GaAs. This unconventional kind of PhC is well suited for the generation of whispering gallery modes (WGMs) due to the circular symmetric periodic pattern. By using a laser Gaussian beam at $1.55\ \mu\text{m}$ as pump signal, a WGM at $1.55\ \mu\text{m}$ and a second-harmonic (SH) mode at $0.775\ \mu\text{m}$ are obtained. The SH will be generated in the center of the missing-hole microcavity. The periodic pattern and the microcavity are tailored and optimized providing an SH efficiency conversion as high as 50%. We predict the resonances by an accurate 2-D time-domain model including $\chi^{(2)}$ nonlinearity and by a 3-D finite-element method. Finally, by using a 3-D membrane configuration, we found a total quality factor of the SH mode of the order of 35 000.

Index Terms—Nonlinear process, numerical modeling, photonic crystal (PhC), second-harmonic generation (SHG).

I. INTRODUCTION

STUDIES of $\chi^{(2)}$ processes [1]–[5] promote research works on nonlinear optic (NLO) devices for ultrafast signal processing based on second-order nonlinearity. After the development of high-efficiency second-harmonic generation (SHG) devices using ferroelectric crystal waveguides [4], the research was directed to implementation of a compact and efficient coherent light source by combining the SHG device with a semiconductor laser. Moreover, a strong motivation of research on NLO devices has been the need for the development of all-optical wavelength converters for dense wavelength-division multiplexing (DWDM) [5] optical communication systems. In particular, in telecommunications, the SHG in $\chi^{(2)}$ nonlinear process represents a good solution for DWDM systems in which more wavelengths are requested. However, this process requires high intensity input power and large interaction lengths for an efficient second-harmonic

(SH) conversion. To this purpose, the employment of photonic crystals (PhCs) structures enhancing SH field can be very fruitful. PhCs microcavities are actually used in many optical applications such as biosensors [6], optical resonators [7], and wavelength filters [8]. Several architectures of microcavities have been studied in the past by using triangular and square lattices [9], [10], and high performances in microcavities have been achieved by both reducing the size of the holes adjacent to the cavity and by shifting their position. In particular, the properties of PhCs are becoming a new and exciting area of research in NLOs [11]. The enhancement of an SH field localized in the microcavity can be obtained by a circular PhC with central microcavity, as shown in Fig. 1. This kind of circular periodic pattern is well suited for performing active photonic devices such as microcavity lasers based on whispering gallery mode (WGM) [12] or circular resonators [13] that usually exhibit low loss, good confinement, high Q -factor, etc. The WGM generated by the circular pattern allows the enhancement of the SH microcavity coupling efficiency. Microcavities with central defect have been already proposed and analyzed in previous works [14], [15], even though the optimization of the SH coupling efficiency and the SH conversion efficiency has not been yet reported. In this paper, we study the $\chi^{(2)}$ nonlinear process in GaAs circular PhC slab (CPhCS) consisting of air holes (see Fig. 1) disposed along periodic concentric lines. We optimize the radius value and position of all inner holes disposed around the central defect (missing hole) in order to couple a cavity mode corresponding to the SH signal ($\lambda_{\text{sh}} = 0.775\ \mu\text{m}$) generated by a laser beam ($\lambda_0 = 1.55\ \mu\text{m}$) focused on CPhCS. The PhC pattern consists of air holes (Fig. 1) in a GaAs material ($n = 3.374$ at $\lambda_0 = 1.55\ \mu\text{m}$) along circular concentric lines; all the circular lines have the same distance that we defined as the period a of the CPhCS, and all the holes have the same radius, with exception for those around the central cavity. These holes have a reduced radius and are shifted starting from the microcavity center and along the radial direction, in order to improve the resonance properties. The shift of the inner holes and the different radius as compared to the outer holes improve the field confinement in the central region by enhancing the cavity modes. Furthermore, the high dielectric contrast of a membrane-type configuration will localize and enhance these cavities modes by providing a high-quality Q -factor. The particular periodic pattern cannot be analyzed with the traditional numerical modeling, such as the wave expansion method in the frequency domain, which is used often in the modeling of PhCs structures: the Brillouin zone is not defined as in triangular or square lattice, and alternative methods, such as finite-difference

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In this paper: 1) we model the laser pump signal at $\lambda_0 = 1.55 \text{ } \mu\text{m}$; 2) we model and optimize the CPhCS by a time-domain FEM tool in order to select the SH cavity mode at $\lambda_{\text{sh}} = 0.775 \text{ } \mu\text{m}$ with a coupling efficiency of 50%; and 3) finally, we enhance the SH mode, generated by the nonlinear effect, through an air cavity depth below the CPhCS, obtaining a high-quality Q -factor value (total quality factor of $Q = 35\,000$). The pump depletion due to the loss and generation of new frequency components is not taken into account in the presented FEM model.

II. TIME-DOMAIN AND FREQUENCY-DOMAIN FEM MODELING

In this section, we first characterize the laser beam modeling. When a laser beam propagates, it travels as an approximate plane wave with a cross section intensity of Gaussian shape. The waist of the beam is defined as the Gaussian function's characteristic length. A focused laser beam has a minimum waist (see w_0 in Fig. 2) at a certain point along the direction of propagation. The solution of the time-dependent Maxwell's equations gives the following electric field related to a TE-polarized field (y -components) [16]:

$$\mathbf{E}_y(x, y, z; t) = E_0 \frac{w_0}{w(z)} e^{-(r/w(z))^2} \cos\left(\omega t - kz + \eta(z) - r^2 \frac{k}{2R(z)}\right) \mathbf{e}_y \quad (1)$$

where [16]

$$\begin{aligned} w(z) &= w_0 \sqrt{1 + \left(\frac{z}{z_0}\right)^2} \\ \eta(z) &= a \tan\left(\frac{z}{z_0}\right) \\ R(z) &= z \left(1 + \left(\frac{z_0}{z}\right)^2\right). \end{aligned} \quad (2)$$

In these formulas, w_0 is the minimum waist, ω is the angular frequency, r is the radial cylindrical coordinate, k is the

Fig. 2. (a) FEM modeling: transmittivity response as S_{21} evaluation. (b) Microcavity optimization obtained by reducing the inner holes radius r and by shifting the inner holes from the microcavity center.

wavenumber, and z_0 is the peak electric field position. The wavefront of the beam is not exactly planar; it propagates like a spherical wave with radius $R(z)$. Close to the point of the minimum waist, the wave is almost plane. In this manner, (1) and (2) are used to describe a plane wave at one end of a cylinder representing the focusing of the laser beam (see right inset of Fig. 2). In our 2-D time-domain FEMs (TD-FEMs) [17], the simulated laser signal excites the CPhCS from a side, and the equation that represents the wave propagation in the GaAs nonlinear slab is as follows:

$$\mu_0\sigma\frac{\partial\mathbf{A}}{\partial t}+\mu_0\frac{\partial\left(\frac{\varepsilon_0\varepsilon_r\partial\mathbf{A}}{\partial t}-\mathbf{D}\right)}{\partial t}+\nabla\times(\mu_r^{-1}(\nabla\times\mathbf{A}))=0 \quad (3)$$

where $\mathbf{A}$ represents the magnetic potential vector and $\mathbf{D}$ is the electric displacement vector given by the constitutive relationship $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$, where $\mathbf{P}$ is the polarization vector. The nonlinear properties for the SHG in the nonlinear CPhCS are defined with the following matrix:

$$\mathbf{P} = \begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{bmatrix} \begin{bmatrix} E_x^2 \\ E_y^2 \\ E_z^2 \\ 2E_z E_y \\ 2E_z E_x \\ 2E_x E_y \end{bmatrix}. \quad (4)$$

The presented time-domain model uses, for simplicity, only the d_{11} parameter, according to the TE pump source assumption (in the GaAs case, $d_{11} = 200$ pm/V [18]). The thickness T (indicated in Fig. 1) of the CPhCS is optimized by introducing the effective dielectric constant (EDC) approach that provides the effective refractive indexes of the slab TE modes. The micro-cavity transmittivity response is defined by the scattering parameter [19] S_{21} calculated by placing the input and the output ports, as reported in Fig. 2(a): the scattering parameter is found by driving the input port 1 with the pump source and evaluating the wave amplitude coming out from the output port 2 placed above the central region and represented by the circular dashed line of Fig. 2(a).

The Q -factor is evaluated by 3-D frequency-domain FEM tool [19] that provides the total Q -factor evaluated by considering an air cavity below the PhCs (membrane-type PhC) as [19]

$$Q = 2\pi f \frac{U}{P} \quad (5)$$

where U is the energy stored inside the CPhCS, P is the power lost through the absorbing material, and f is the working frequency. The whole structure is embedded in an absorbing material, so it is possible to calculate the ratio between the energy stored (given by the CPhCS resonance) and the power loss (flowing outside the structure through the absorbing layer). As FEM boundary condition, we consider radiation boundary surfaces in which the second-order radiation boundary condition is used [19]

$$(\nabla \times \mathbf{E})_{\text{tan}} = jk_0 \mathbf{E}_{\text{tan}} - \frac{j}{k_0} \nabla_{\text{tan}} \times (\nabla_{\text{tan}} \times \mathbf{E}_{\text{tan}}) + \frac{j}{k_0} \nabla_{\text{tan}} (\nabla_{\text{tan}} \mathbf{E}_{\text{tan}}) \quad (6)$$

where $\mathbf{E}_{\text{tan}}$ is the tangential component to the surface of the electric field and j is $(-1)^{1/2}$. We observe that the second-order radiation boundary condition approximates free space; in this way, we do not consider the numerical error generated by the backscattering of the boundary condition. In order to estimate the part of the power that flows along the y -vertical direction or along the x - z in-plane directions, the total Q factor is decomposed into vertical $Q_{\perp}$ factor and in-plane $Q_{\parallel}$ factor as follows [20]:

$$\frac{1}{Q} = \frac{1}{Q_{\perp}} + \frac{1}{Q_{\parallel}} = \frac{P_{\perp}}{2\pi f U} + \frac{P_{\parallel}}{2\pi f U} \quad (7)$$

where $P_{\perp}$ and $P_{\parallel}$ represent power flow along the y -vertical direction and the x - z in-plane directions, respectively. In order to analyze the direction of the radiated power in a membrane-type CPhCS, $P_{\perp}$ is decomposed into $P_{\perp\uparrow}$ (power flowing in the positive y -direction) and $P_{\perp\downarrow}$ (power flowing in the negative y -direction through the substrate). In order to analyze the real behavior of the GaAs slab, the real and the imaginary parts of the refractive index are considered.

III. OPTIMIZATION AND NUMERICAL RESULTS

The slab thickness and the inner holes of the proposed CPhCS are optimized [14] in order to enhance the SH signal generated in the coupled cavity. In particular, the optimization is performed by tailoring different geometrical parameters, namely the inner hole position, the inner holes radius, the slab thickness, and the distances of the inner holes from the microcavity center.

The design and the optimization of the presented CPhCS are based on the following steps.

- 1) The outer holes radius R is fixed in order to obtain a low reflection at the input port 1 [Fig. 2(a)] at the fundamental wavelength $\lambda_0 = 1.55 \mu\text{m}$.
- 2) The inner holes radius r is fixed in order to couple the SH signal ($\lambda_{\text{SH}} = 0.775 \mu\text{m}$) inside the microcavity (the coupling efficiency is evaluated as ratio between the SH power localized inside the microcavity region and the total SH power).
- 3) The high coupling efficiency of the SH is obtained by tuning the slab thickness T and the inner holes distances d_1 and d_2 [see Fig. 2(b)].
- 4) The maximum SH conversion efficiency $\eta = P_0/P_{\text{SH}}$ (P_0 is the input pump source at $\lambda_0 = 1.55 \mu\text{m}$ and P_{SH} is the SH power evaluated in the central microcavity region) is

Fig. 3. Laser beam modeling. Power flow at the input section (arc-length) for $E_0 = 0.03 \text{ V/m}$. Inset: focused laser beam profile $w(z)$. Right inset: time evolution of the laser source in the CPhCS structure after some time steps.

performed by choosing the optimum input power P_0 for a dual-resonant mode (the resonant modes are the fundamental WGM and the SH mode) that exchange energy.

- 5) Finally, the quality factor of the SH mode, radiated above the microcavity, is increased through an air layer placed below the slab (3-D membrane-type CPhCS).

Concerning the modeling of the pump source, the laser beam is focused in a spot size of $w_0 = 10 \mu\text{m}$. Moreover, the pump wavelength is $\lambda_0 = 1.55 \mu\text{m}$, the pulse time delay is 40 fs, and the pulsewidth is 100 fs. In Fig. 3, the input power related to the pump signal and the initial electric field propagation in the CPhCS structure are shown. By considering the design point 1), we found for the CPhCS of Fig. 1 an outer hole radius of $R = 119 \text{ nm}$, and a lattice constant $a = 350 \text{ nm}$ that provide the band passing behavior around $\lambda_0 = 1.55 \mu\text{m}$. The design and the optimization of the SH generation are based on the points 2)–4). The geometrical parameters r , T , d_1 , and d_2 are obtained by considering a parametric analysis that considers simultaneously the SH coupling efficiency versus the parameters r , T , d_1 , and d_2 [see Figs. 4–6(a) and (b)]. From Fig. 6(a), we observe that a higher SH coupling efficiency (35%) is obtained by shifting the inner holes by a distance of $d_1 = 360 \text{ nm}$ from the center. Moreover, the tuning of d_2 [see Fig. 6(b)] provides a coupling efficiency of 50%. By analyzing Figs. 4–6, we conclude that the optimized CPhCS will be characterized by $r = 100 \text{ nm}$, $T = 200 \text{ nm}$, $d_1 = 360 \text{ nm}$, and $d_2 = 350 \text{ nm}$. In order to evaluate the optimum input power for a high-intensity SH converted signal, we evaluate (Fig. 7) the conversion efficiency $\eta = P_0/P_{\text{SH}}$ related to the point 4): the optimum parameter η (see working point of Fig. 7), which provides a low reduction of the SH power in the microcavity region with respect to the fundamental mode, is obtained for an input power P_0 as low as 7.5 kW/cm^2 .

In Fig. 8, the calculated spectra and the electric field profile of the fundamental signal and the SH signal are reported: the transmittivity is evaluated by the fast Fourier transform (FFT) of

Fig. 4. SH coupling efficiency versus the inner holes radius r . The efficiency is evaluated as ratio between the transmittivity of the SH mode ($\lambda_{sh} = 0.775 \mu\text{m}$) and the transmittivity of the fundamental TE mode ($\lambda = 1.55 \mu\text{m}$). The plot is obtained by fixing $a = 350$ nm, $R = 119$ nm, $d_1 = 360$ nm, and $d_2 = 350$ nm.

Fig. 5. SH coupling efficiency versus the slab thickness T . The plot is obtained by fixing $a = 350$ nm, $R = 119$ nm, $r = 100$ nm, $d_1 = 360$ nm, and $d_2 = 350$ nm.

the total signal (generated by the laser source) inside the cavity region [port 2 of Fig. 2(a)]. The high SH confinement minimizes the absorption effect of the GaAs material by providing an SH conversion efficiency of 50%. The SH signal emitted in the vertical y -direction above the microcavity region can be further enhanced by considering an air cavity below the CPhCS. In Fig. 9, we show how it is possible to obtain a total Q -factor as high as 35 000 by considering a cavity depth of $3(0.775)/2 = 1.1625 \mu\text{m}$. In order to prove the SH emission along the positive y -direction, we decompose (see Figs. 9 and 10) the total Q -factor into parallel ($Q_{//}$) and in-plane ($Q_{\perp}$) components: in particular, we observe from Fig. 8 that for an air cavity depth (air layer thickness arranged below the GaAs slab) of $3(\lambda_{sh})/2$, the major contribution is represented by $Q_{//}$ (which is characterized by a low in-plane power lost). The normalized power lost components related to the Q -factors are reported in Fig. 10, where they represent the regions where $P_{\perp}$ is flowing along the negative y -direction (region I where $P_{\perp} = P_{\perp\downarrow}$ is directed in the substrate region) and along the positive y -direction (region II where $P_{\perp} = P_{\perp\uparrow}$ is directed in the air region above the microcavity). The decomposition of the normalized components $P_{\perp\uparrow}$ and $P_{\perp\downarrow}$ and the SH 3-D radiation pattern are showed in Fig. 11: this figure proves the emission of the SH signal above the microcavity.

Fig. 6. SH coupling efficiency versus the inner holes distances (a) d_1 and (b) d_2 reported in Fig. 2(b). The plot (a) is obtained by fixing $a = 350$ nm, $R = 119$ nm, $r = 100$ nm, and $d_2 = 350$ nm. The plot (b) is obtained by fixing $a = 350$ nm, $R = 119$ nm, $r = 100$ nm, and $d_1 = 350$ nm.

Fig. 7. Dependence of SH conversion efficiency on fundamental input power P_0 : a conversion efficiency is obtained for a working input power of $P_0 = 7.5 \text{ kW/cm}^2$.

IV. CONCLUSION

In this paper, we predict the presence and the enhancement of an SH field generated by a focused laser beam at $\lambda_0 = 1.55 \mu\text{m}$ in a microcavity of a GaAs CPhCS. The SH mode ($\lambda = 0.775 \mu\text{m}$) enhanced in the microcavity can be used for

Fig. 8. In-plane transmittivity of CPhCS for different slab T thicknesses. Inset left: fundamental WGM mode profile and SH mode profile. Inset right: inner hole shift regarding the optimization. The transmittivity response is obtained for an input power of $P_0 = 7.5 \text{ kW/cm}^2$ at $\lambda_0 = 1.55 \text{ μm}$.

Fig. 9. 3-D frequency-domain FEM modeling: SH quality Q -factors (Q , $Q_{\perp}$, and $Q_{//}$) obtained by considering an air cavity below the CPhCS membrane type at different depths ($T = 200 \text{ nm}$).

Fig. 10. 3-D frequency-domain FEM modeling: normalized powers lost $P_{\perp}$, $P_{//}$, and $P_{//}$ versus the air cavity depth.

applications such as add-drop filtering and WDM. In this paper, we use different numerical tools: the time-domain approach that provides the transient analysis and coupling efficiency of the SH

Fig. 11. 3-D frequency-domain FEM modeling: power lost $P_{\perp}$ decomposed into $P_{\perp\uparrow}$ and $P_{\perp\downarrow}$ versus the air cavity depth. Inset: SH 3-D radiation pattern.

signal generated by the nonlinear process, and frequency-domain approach that provides the Q -factor of the whole membrane CPhCS type. Technological and experimental aspects are under study.

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