Design Criteria and 3D FEM Modeling of Air Hole Photonic Crystal

Alessandro Massaro, Vito Errico, Roberto Cingolani, Adriana Passaseo and Massimo De Vittorio.

National Nanotechnology Laboratory of CNR-INFM , Distretto Tecnologico-ISUFI, Università del Salento, Via Arnesano, 73100 Lecce- Italy.

ABSTRACT

This work presents a detailed numerical Finite Element Method FEM modeling for passive optical components such as photonic crystals (PhCs). The accurate modeling characterizes the PhCs structures by considering the field resonance and the radiation behavior of the periodic pattern. The frequency responses at each side of the photonic crystal are evaluated by considering the 3D periodic structure enclosed in a black box with six input/output ports. This scattering matrix approach (SMA) is useful in order to evaluate in plane and vertical PhCs the resonance of the photonic crystal. Through the analysis of all the frequency responses we characterize the passband regions and the stopband regions of the PhC slab.

Keywords: Photonic Crystal, FEM Method, Numerical Simulation.

INTRODUCTION

Photonic crystals PhCs [1]-[4] are actually used in many optical applications as biosensors, optical resonators and wavelength filters. By using a numerical modeling it is possible to design and to characterize the PhCs structures regarding a specific application. After a first step of general characterization it is necessary to optimize the structure in order to predict the fabrication error effects in the frequency response or in the radiation aspect. Photonic crystal slab (PhCS) produced by thin film-based on standard technology suffers from manufacturing imperfections resulting in degradation of the absorption/diffraction response. Geometrical imperfections like roughness at layer boundaries, non perfect hole radius and slow variation of the lattice period may change the frequency response. The high sensitivity of the scattering parameters to the variation of the geometrical imperfections requests an accurate modeling which considers an error margin in the final characterization. For this purpose the numerical finite element method (FEM) is able to highlight physical phenomena not easily predictable by theories, and provides, in perspective, design criteria for the 3D photonic crystals. The 3D FEM modeling [5]-[6] is based on the definition of the unit cell (see Fig.1) as a three-dimensional photonic crystal slab. The unit cell is completely characterized by the scattering parameters, by the radiated field and by the Q factor evaluation. The scattering S matrix is defined by setting all the six PhCS sides of the unit cell (shown in Fig.1) as wave ports. Wave ports are typically placed at this side-interface in order to provide a window that couples the model device to the external world. The electro-magnetic (EM) simulator assumes that the structure is excited by the natural field patterns (modes) associated with these cross-sections. The 2D field solution generated for each wave port is the exact modal boundary conditions at those ports for the 3D problem. The simulator generates a solution by exciting each wave port individually. The frequency response of the analyzed PhCS cell is obtained by setting all the six sides (Fig. 1 b)) of the unit cell as input-output ports. In this way the boundary conditions are represented by the wave ports and the transmission and reflection on each port are characterized by the scattering parameters. The general scattering S_{ij} parameter is found by driving port j with an incident wave and evaluating the reflected wave amplitude coming out from port i . The incident waves on all ports except the j^{th} port are set to zero, which means that all ports should be terminated in matched loads to avoid reflections. Thus, the S_{ij} is the reflection coefficient seen looking into port i when all other ports are terminated in matched loads. The excitations on the ports are all the modes that the unit cell may guide. Instead the radiated field is evaluated by considering the radiation pattern above the PhCS. Finally the total Q-factor is calculated by the ratio between the energy stored in the PhCS and the power lost through the six unit cell sides. In this work we analyze different photonic crystal geometries, including pillar structure, in order to define a generic design FEM criteria. The 3D FEM model highlights the difference between the theoretical 1D and the 3D design and also predicts the real behaviour of the dielectric periodic structure.

1.1 FEM Modeling: examples of 3D Photonic Crystal

As first example we start with the design of a simple 1D photonic crystal structure. In order to obtain an high reflectivity around a preferred wavelength of $\lambda_0=1.55 \mu\text{m}$, we consider a grating of air ($n_1=1$), and GaAs ($n_2=3.408$) layers with thickness d_1 and d_2 respectively. The relationships between the refractive indices and thicknesses are the following: $n_1 d_1 = \lambda_0/4$ and $n_2 d_2 = \lambda_0/4$. The first 3D FEM model of this grating takes into account six rectangular air holes in GaAs slab (see Fig. 2): the grating period is d_1+d_2 , the dimension of the rectangular air holes are ($w \times d_1 \times h$) $0.1137\mu\text{m} \times 0.3875\mu\text{m} \times 0.1137\mu\text{m}$, the dimension of the GaAs ($n=3.408$) slab are $0.1137\mu\text{m} \times 3.1209\mu\text{m} \times 0.1137\mu\text{m}$. In Fig. 2 is shown the expected bandgap (stopband) region around $\lambda_0=1.55 \mu\text{m}$ which corresponds to a high reflection on port 1 and to a low transmission at port 2 by exciting the structure from port 1 (low S_{21} parameter and high S_{11} parameter). By considering 6x6 rectangular hair holes (as reported in Fig. 3) the scattering inside the unit cell will change the frequency responses: the S_{11} parameter is high around $\lambda_0=1.55 \mu\text{m}$, moreover S_{21} presents a minimum near λ_0 but is not equal to zero, so the bandgap is not well defined as in the previous case. We observe from the six port of Fig. 3 that part of signal coming from port 1 couples to port 6 (see S_{61} parameter); moreover the parameter S_{66} characterizes also the effect of the slab thickness regarding the grating resonance. The bandgap region will appear again by considering a central defect region (as reported in Fig. 4): in this case the bandwidth and the central wavelength of the stopband are changed and the S_{66} parameter is equal to zero. As second example we analyze the circular photonic crystal of Fig. 1 a). The circular GaAs PhC slab is designed with air holes having radius of 119 nm, period $a=350\text{nm}$, slab thickness = 200nm; the six central holes (radius = 84nm) are shifted of 35nm from the center. In Fig. 5 and Fig. 6 we show some whispering gallery modes WGM configuration, and other modal profiles with field confinement in the central cavity region for different working wavelengths. In a first step we model the PhCS structure by considering a working wavelength around $\lambda_0 = 1.28 \mu\text{m}$, which corresponds to the ground state emission wavelength of the InAs/InGaAs quantum dots (QDs) embedded in a GaAs slab. The radius and the position of air holes are chosen in order to obtain a cavity mode. By using the six port model it is possible to verify the cavity coupling by the S_{63} and S_{66} (represented in Fig. 7) at $\lambda_0 = 1.28\mu\text{m}$: in particular the S_{63} parameter represents the coupling of the in plane signal with port 6, and the S_{66} parameter represents the z-vertical resonance of the cavity. It is also possible to predict a fabrication error by evaluating the variation of the scattering parameter with a geometrical parameter. In Fig. 7 we show an example of S_{63} variation with the inner holes radius. In complex 3D structure it is necessary, for the high computational cost, to divide the structure in more cells, and each unit cell must be coupled to other ones. In this case, for a complete characterization, it is important to define the impedances characteristics Z_0 (in order to evaluate the reflection at the port), and the effective propagation constants $\beta(\omega)=(n_{\text{eff}}\omega)/c$ (in order to evaluate the matching condition) at each port. In Fig. 8 we show some of these quantities concerning the 3D unit cell of the circular PhC slab.

1.2 FEM: Radiation Field and Q factor

Another important aspect in the modeling of the PhCs is the radiation field, which is evaluated in the space surrounding the device, by enclosing the PhC unit cell in a spherical surface. In order to observe the near field, we excite the port 1, 2, 3 and 4 of Fig. 1 b) by the fundamental mode calculated by the effective refractive index method related to the corresponding wave port. The near-field region is the region closest to the source (PhCs unit cell). The electric field $E(x,y,z)$ external to the region bounded by a closed surface may be written as

$$\mathbf{E}(x, y, z) = \int_S ((j\omega\mu_0 \mathbf{H}_{\text{tan}})G + (\mathbf{E}_{\text{tan}} \times \nabla G) + (\mathbf{E}_{\text{normal}} \nabla G)) dS \quad (1)$$

where S represents the radiation boundary surface, j is the imaginary unit, $\mathbf{H}_{\text{tan}}$ is the component of the magnetic field which is tangential to the surface, $\mathbf{E}_{\text{normal}}$ is the component of the electric field that is normal to the surface, G is the free space Green's function, given by

$$G = \frac{e^{-jk_0|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \quad (2)$$

where k_0 is the free space wave number, $\mathbf{r}$ and $\mathbf{r}'$ represent field points and source points on the surface, respectively. As example we show in Fig. 9 and Fig. 10 the radiation pattern of the E_x (tangential component) and E total field for different number of concentric air holes lines. In particular we observe many radiation E_x lobes by increasing the number of the concentric lines. Moreover only two main lobes are observed about the E total field radiation pattern in the case of nine concentric lines.

Concerning the Q-factor evaluation, we use a different approach. All the structure is embedded in an absorbing material, so it is possible to calculate the ratio between the energy stored (given by the PhCs resonance) and the power loss (flowing outside the structure through the absorbing layer). It is possible to absorb the wave at the radiation boundary, essentially by ballooning the boundary infinitely far away from the structure. At radiation boundary surfaces, the second-order radiation boundary condition is used

$$(\nabla \times \mathbf{E})_{\text{tan}} = jk_0 \mathbf{E}_{\text{tan}} - \frac{j}{k_0} \nabla_{\text{tan}} \times (\nabla_{\text{tan}} \times \mathbf{E}_{\text{tan}}) + \frac{j}{k_0} \nabla_{\text{tan}} (\nabla_{\text{tan}} \cdot \mathbf{E}_{\text{tan}}) \quad (3)$$

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 the free space. The accuracy of the approximation depends on the distance between the boundary and the object from which the radiation emanates. The Q factor is evaluated as

$$Q = 2\pi \text{freq} \frac{U}{P} \quad (4)$$

where U is the energy stored inside the PhCs, P is the power lost through the absorbing material, and freq is the working frequency. In Fig. 11 we show the 3D Q factor FEM model: all the PhC is embedded in absorbing layers in order to evaluate the total Q factor. Regarding the circular PhC above described we evaluate a total Q factor of 50000 with an $\lambda_0/2$ air layer below the PhC structure (enhancement of the vertical cavity resonance).

2 FEM: Complex Photonic Crystal Structures (DBRs Pillars)

The FEM unit cell approach can be used also for complex PhCs such as pillar structures. If the single pillar behaves as a Distributed Bragg Reflector (DBR), the FEM unit cell will characterize the reflectivity or the transmittivity of the single DBR. As example we propose a GaN microcavity embedded between two Distributed Bragg Reflectors (DBRs) consisting of AlGaIn/GaN multilayers, on sapphire substrate, properly designed to enhance the cavity resonance around $\lambda_0=400\text{nm}$. In Fig. 12 we show the comparison of the reflectivity between a square and pillar type DBR with a GaN cavity: we consider in the simulation five GaN/AlGaIn couples and seven GaN/AlGaIn couples above and below the central GaN microcavity respectively. The layer thicknesses satisfies the condition $n_i d_i = \lambda_0/4$ where n_i and d_i refers to the refractive index and to the thickness of each layer; the GaN cavity satisfies the condition $n_{\text{GaN}} d_{\text{GaN}} = \lambda_0/2$. Also in this case the FEM modeling highlights the importance of the 3D geometry regarding the DBR frequency response.

3 Conclusion.

The FEM modeling is an important step in the design of photonics crystals. The goal of the modeling is to analyze the effect of the 3D geometry on the frequency response. The SMA approach, the radiation field and the quality factor evaluation provide the real behavior of a PhCs structure by exciting the periodic pattern from different directions. The concept of a six port unit cell can be extended to a cascade of different unit cells including pillar geometries. The input/output relationships provide a direct approach about the PhCs frequency behavior.

4 Figures and captions.

Fig.1:a) Circular photonic crystal, b)SMA: six ports unit cell which encloses the circular photonic crystal PhC.

Fig.2: S_{21} and S_{11} parameters of a 3D FEM grating model..

Fig.3: 6x6 periodic pattern: scattering parameters.

Fig.4: 6x6 periodic pattern with central defect region: scattering parameters.

Fig.5: 2D FEM simulation: Whispering Gallery Modes of the 2D circular photonic crystal.

Fig.6: 2D FEM simulation: modal cavity resonances of the 2D circular photonic crystal.

Fig. 7: 3D FEM: Circular photonic crystal. Above: S_{66} parameter; below: example of sensitivity analysis of the S_{63} parameter.

Fig.8: Circular photonic crystal. Left: impedances characteristics Z_0 at ports 5 and 6. Right: effective propagation constants at ports 1 and 6.

Fig.9: Circular photonic crystal of Fig. 1 a). Left: E_x field radiation pattern of a circular PhC with a pattern of five concentric lines. Right: E_x field radiation pattern of a circular PhC with a pattern of nine concentric lines

Fig.10: Circular photonic crystal of Fig. 1 a). Left: E_{total} field radiation pattern of a circular PhC with five concentric lines. Right: E_{total} field radiation pattern of a circular PhC with nine concentric lines.

Fig.11: 3D FEM Q factor modeling: the PhC slab structure is completely embedded by absorbing layers.

Fig.12: Reflectivity S11 parameter: comparison between square and pillar Distributed Bragg Reflector DBR. The side dimension of the square block is 2 μm , the pillar radius is 0.5 μm . Inset left: 3D square and pillar DBR model. Inset right: numerical modal profile at waveport 1.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the help of the technician Epifani Gianmichele.

REFERENCES

1. T. Asano, B.S. Song, Y. Akahane, and S. Noda, " Ultrahigh-Q nanocavities in two-dimensional photonic crystal Slab", IEEE J. of Selected Topics in Quantum Electron. 12(6), 1123-1134 (2006).
2. Yoshie, A. Scherer, J. Hendrickson, G. Khitrova, H.M. Gibbs, G. Rupper, C. Ell, O.B. Shchekin, D.G. Deppe, " Vacuum rabi splitting with a single quantum dot in a photonic crystal nanocavity," Nature 432, 200-203 (2004).
3. T. Yoshie, O.B. Shchekin, H. Chen, D.G. Deppe, A. Scherer, "Quantum dot photonic crystal laser," Electron. Lett. 38, 967-968 (2002).
4. V. Errico, T. Stomeo, A. Salhi, M. De Giorgi, A. Passaseo, M. De Vittorio, "Quantum dot nano-cavity emission tuned by a circular photonic crystal lattice", Microelectron. Eng. 84, 1570-1573 (2007).
5. A.Massaró, L.Pierantoni, and T.Rozzi, " Q-factor evaluation, design and accurate EM performance of multilayer dielectric filter, "Int. J. Numer. Model. 19(6), 521-537 (2006).
6. T. Fujisawa, and M. Koshiba, "Finite-element mode solver for nonlinear periodic optical waveguides and its application to photonic crystal circuits," IEEE J. Lightw. Technol. 23(1), 382-387 (2005).