Proceedings

Maurizio Ferrari

Marian Marciniak

Giancarlo C. Righini

Tomasz Szoplik

Stefano Varas

Editors

IFN CNR

Micro- and nano-photonic materials and devices

Proceedings of MINAP 2012 – Final Conference of the MP0702 COST Action (Trento, Italy, 16-18 January 2012)

Editors:

Maurizio Ferrari, Marian Marciniak, Giancarlo C. Righini, Tomasz Szoplik, Stefano Varas

CNR

National Research Council, Italy

Editors

Maurizio Ferrari, *Institute of Photonics and Nanotechnology (IFN – CNR, Trento, Italy)*

Marian Marciniak, *National Institute of Telecommunications (Warsaw, Poland)*

Giancarlo C. Righini, *Nello Carrara Institute of Applied Physics (IFAC – CNR, Firenze, Italy)*

Tomasz Szoplik, *Warsaw University (Warsaw, Poland)*

Stefano Varas, *Institute of Photonics and Nanotechnology (IFN – CNR, Trento, Italy)*

Organizers

The Conference MINAP 2012 was promoted by the COST Action MP0702 and organized by IFN – CNR in close collaboration with Fondazione Bruno Kessler (FBK, Trento) and IFAC – CNR.

Web site of Conference: http://minap2012.fbk.eu

Conference Sponsors:

Printed by Bel Studio (Warsaw, Poland) on behalf of the Institute of Photonics and Nanotechnology (IFN – CNR, Trento, Italy) - January 2012.

ISBN: 978-83-7798-020-0

Table of Contents

Simulation of photonic crystal nanocavities using a bidirectional eigenmode propagation algorithm: a comparative study.

Jiří Petráček[1], Jaroslav Luksch[1], Bjorn Maes[2], Sven Burger[3], Pavel Kwiecien[4], Ivan Richter[4]
[1] Institute of Physical Engineering, Brno University of Technology
Technická 2, 616 69 Brno, Czech Republic, e-mail: petracek@fme.vutbr.cz
[2] Micro- and Nanophotonic Materials Group, University of Mons, Faculty of Science,
Avenue Maistriau 19, B-7000 Mons, Belgium
[3] Zuse Institute Berlin (ZIB), Takustraße 7, D– 14 195 Berlin, Germany
[4] Department of Physical Electronics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Břehová 7, 115 19 Praha 1, Czech Republic

ABSTRACT
A new implementation of bidirectional eigenmode expansion and propagation algorithm for the modeling of three-dimensional waveguide structures is presented. The eigenmodes, which are used for expansion of unknown field, are searched numerically using a full vector finite-difference or finite-element modesolver. The technique is applied to the modeling of high-*Q* one-dimensional photonic crystal nanocavity and its results are compared with results obtained by three other independent techniques.

Keywords: eigenmode expansion, numerical modeling, photonic crystals, high-*Q* nanocavities

1. INTRODUCTION

Currently, as photonic and/or plasmonic nanostructures are becoming very attractive components for photonics devices, among other important experimental and technological aspects, new modeling activities are of high interest in connection towards their direct application to realistic 3D problems to be solved and optimized. Clearly, such demands necessitate very efficient and reliable computational methods. One possibility is to perform rigorous simulation in the frequency domain using analytical modal techniques, such as the bidirectional eigenmode propagation [1] (BEP, also known as the mode matching method), which are based on the expansion of the unknown field into a set of the orthogonal waveguide modes. This approach is particularly advantageous for the structures composed of longitudinally uniform waveguides ("sections"). In principle, the modal methods can deal with the structures of arbitrary length (the number of the sections can influence only the total computational time) and readily provide device characteristics such as transmission, reflection or radiation loss. Recently, this approach has been extended to 3D structures [2,3]. Waveguide modes have been calculated using the finite-difference technique under the semi-vector approximation [2] or in the full-vector formulation [3].

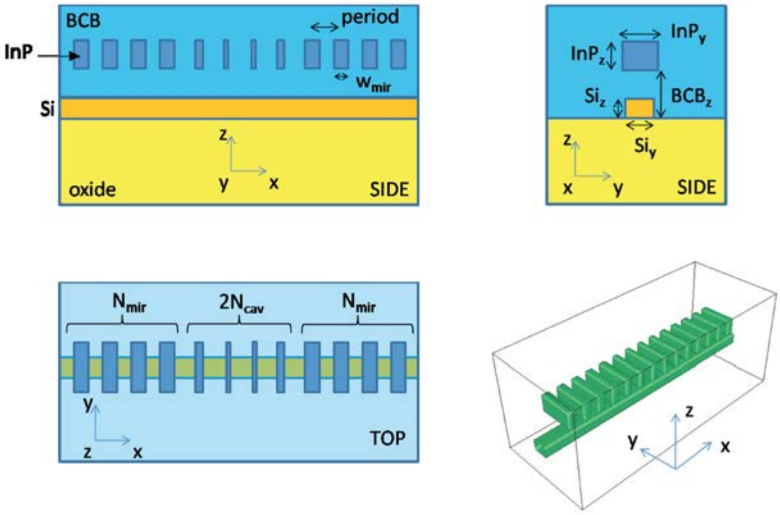

Figure 1. The photonic crystal cavity device coupled to a waveguide. The cavity is formed by the InP sections, the waveguide functions as input/output coupler. The 3D view only shows the Si and InP sections. The structural parameters are described in the text.

In this work, we briefly report about simulation of photonic crystal nanocavities using our own implementation of full-vector BEP for 3D structures. Moreover, we present comparison with other established techniques. Short description of the all techniques is the following.

- Bidirectional eigenmode expansion and propagation algorithm (BEP) was implemented at Brno University of Technology. We have used two different full vector techniques for searching of eigenmodes: a freely available finite-difference modesolver [4] and/or a finite-element commercially available software COMSOL Multiphysics. The techniques were effectively combined with the propagation algorithm of numerically-stable scattering matrices where the interface matrices were determined from overlap integrals of modal fields [2,3,5]. Resonance wavelength and *Q* factor are calculated from eigenvalues of reflectivity matrix.
- The finite-difference time-domain (FDTD) method, using a freely available software package [6].
- The time-harmonic, higher-order 3D finite element (FE) solver JCMsuite with adaptive meshing has been used to compute resonance modes and corresponding complex eigenfrequencies of the cavity [7]. From the complex eigenvalues, resonance wavelength and *Q* factor are derived [8].
- Aperiodic rigorous coupled wave analysis (aRCWA). This is Fourier expansion scheme which uses in-house robust 3D tool which effectively combines both 2D mode solver (based on 2D periodic RCWA tool in a combination with the isolating boundary conditions, either complex coordinate transforms or PMLs [9,10]), with the help of both ASR technique [11] and/or the application of structural symmetries [12], again combined with advanced “grating-oriented” schemes of scattering matrix formalism. Altogether, this efficient tool has been already successfully applied to both subwavelength [13] and plasmonic 3D nanostructures [14]. Resonance wavelength and *Q* factor are calculated from transmission spectra.

For the simulation we used a hybrid cavity structure which research has been conducted within the European Action COST MP0702. Note, that the full results of the study will be published elsewhere [15]. Here, the cavity serves as an example of novel and promising structure used for presentation of BEP and comparison of the numerical techniques. The structure, which is illustrated in Fig. 1, consists of a size-modulated 1D stack cavity coupled with the waveguide. It has been shown that such stack cavities (a simple periodic array of dielectric blocks) can reach ultrahigh *Q* factors provided widths of the blocks (i.e. here the widths of InP sections in *x* direction) are properly modulated near the cavity center [16].

2. RESULTS

Referring to Fig. 1, we used the following parameters for the calculation: InP_y = 0.7 μm, InP_z = 0.35 μm, Si_z = 0.22 μm and BCB_z = 1.0 μm. Refractive indices in various materials are 3.46 (Si), 1.45 (silicon oxide), 3.17 (InP) and 1.54 (benzocyclobutene, BCB).

Center positions of the InP sections are regularly spaced with period a = 0.35 μm. We use 10 unmodulated ‘mirror’ sections (N_{mir} = 10) with width w_{mir} = 0.2 μm. The number of modulated sections on each side of the center is N_{cav} and we consider modulation of section widths of the form

$$w(i) = (0.15\,\mu\text{m})\left[1 + \frac{(i-1)^2}{3N_{\text{cav}}^2}\right], \quad i = 1 \ldots N_{cav} \tag{1}$$

We searched for the fundamental cavity quasi-TE mode (electric field parallel with *y*). In Fig. 2, we show cavity characteristics and compare results of BEP, FDTD and FE techniques. (Note, that in the scale of the graphs the FD and FE based BEP techniques provide identical results. Therefore we present results of the FE based BEP only.) It is seen that the different methods generate results which give the same qualitative picture; showing their good applicability. However, results differ significantly on an absolute scale. This demonstrates that accurate computation of 3D resonators remains a challenging problem.

As the second alternative modal technique, we have applied the aRCWA method based on the free-space Fourier harmonic expansions, rather than on waveguide eigenmode expansions, as in the BEP case. Figure 3 hence shows, as an example here, the convergence *Q* factor behavior of BEP and aRCWA techniques for N_{cav} = 11. As can be seen, although *Q* factor values are not again directly comparable, similar agreement as reached with other two methods has been obtained. Note that the mode numbers in the two figures are, in fact, not directly comparable due to the different nature of the expansion modes. Furthermore, as was expected, the effectively needed number of modes is much larger in aRCWA as compared to waveguide modes applied directly to BEP. The origin of these discrepancies will be discussed and further investigated.

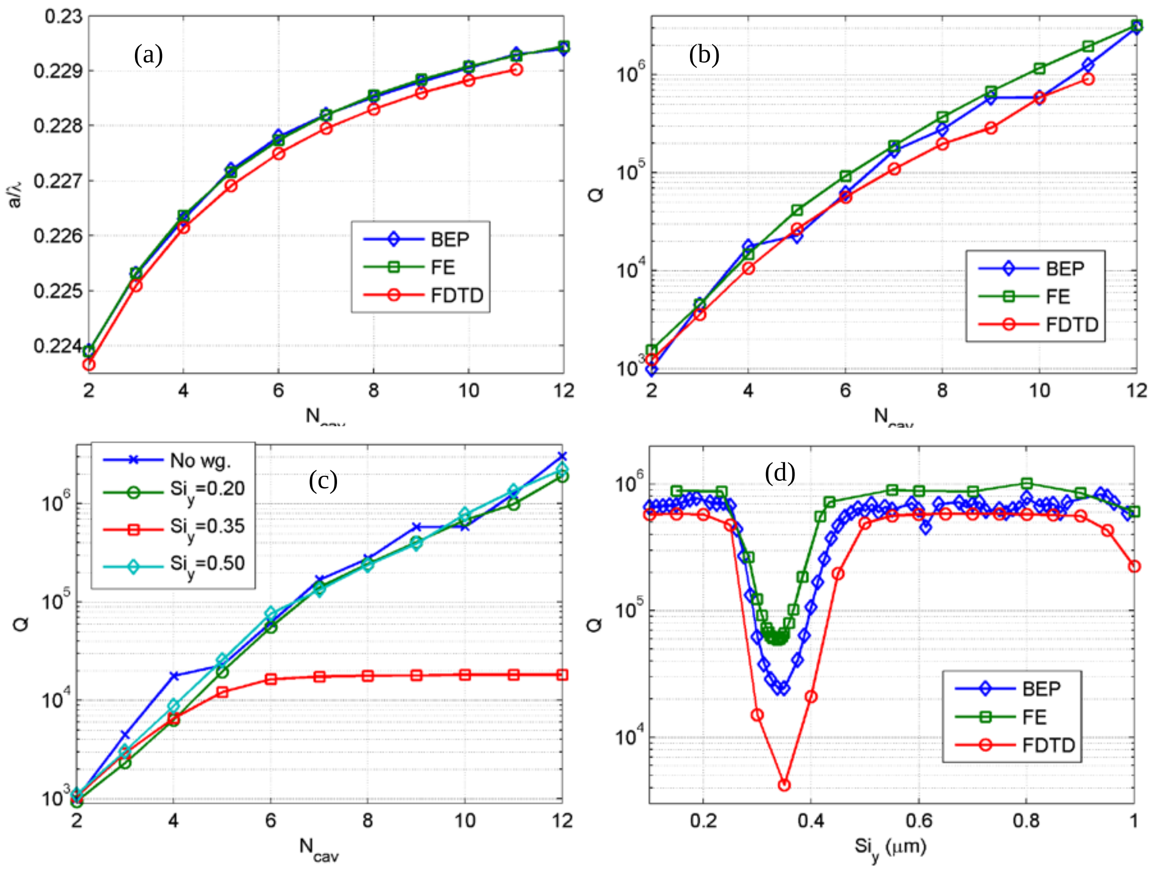

*Figure 2. Q-factor and normalized resonance frequency a/λ provided by three numerical techniques for the cavity shown in Fig. 1. (a) and (b) show results for single cavity without waveguide. (c) BEP results for single cavity (*No wg.*) and hybrid cavity with various values of* $\mathrm{Si_y}$ *(in* μm*). (d) Hybrid cavity with* $N_{\mathrm{cav}} = 10$.

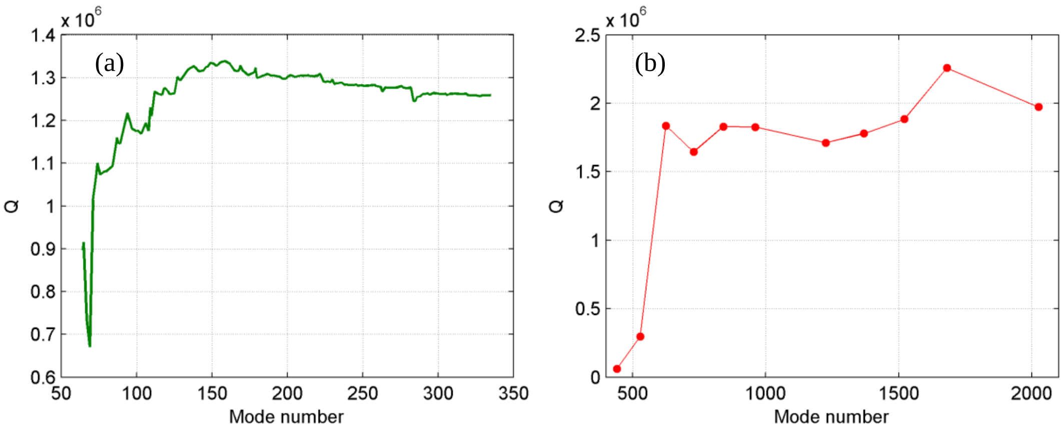

Figure 3. Convergence behavior of BEP (a) and (b) aRCWA . The structure is as in Fig. 1 with $\mathrm{Si_y} = 0.50$ μm *and* $N_{\mathrm{cav}} = 11$.

3. CONCLUSIONS

In summary, we have developed a bidirectional eigenmode expansion algorithm for the modeling of 3D waveguide structures. The technique has been applied to the novel and promising structure, high-*Q* one-dimensional photonic crystal nanocavity, which research has been conducted within the European Action COST MP0702. Simulations results have been compared with results obtained by three other independent techniques. The all techniques have appeared efficient in providing the important cavity characteristics, with their advantages and disadvantages. Presented results indicate that accurate computation of 3D resonators remains a challenging problem which should be further investigated.

ACKNOWLEDGEMENTS

The work was conducted within the European Action COST MP0702. J.P., J.L, P.K. and I.R. acknowledge supports of this work by Ministry of Education, Youth, and Sports of the Czech Republic under contracts OC09005 and OC09038, and by Czech Science Foundation under contract P205/10/0046.

REFERENCES

[1] G. Sztefka, H.-P. Nolting: Bidirectional eigenmode propagation for large refractive index steps, *IEEE Photon. Technol. Lett.*, vol. 5, no. 5, pp. 554-557, May 1993.
[2] K. Jiang, W.-P. Huang: Finite-difference-based mode-matching method for 3-D waveguide structures under semivectorial approximation, *J. Lightwave Technol.*, vol. 23, no. 12, pp. 4239-4248, Dec. 2005.
[3] J. Mu, W.-P. Huang: Simulation of three-dimensional waveguide discontinuities by a full-vector mode-matching method based on finite-difference schemes, *Opt. Express*, vol. 16, no. 22, pp. 18152-18163, Oct. 2008.
[4] A. B. Fallahkhair, K. S. Li, T. E. Murphy: Vector finite difference modesolver for anisotropic dielectric waveguides, *J. Lightwave Technol.*, vol. 26, no. 11, pp. 1423-1431, May 2008.
[5] P. Bienstman, R. Baets: Optical modelling of photonic crystals and VCSELs using eigenmode expansion and perfectly matched layers, *Opt. Quantum Electron.*, vol. 33, no. 4-5, pp. 327-341, Apr. 2001.
[6] A.F. Oskooi, D. Roundy, M. Ibanescu, P. Bermel, J. D. Joannopoulos, S. G. Johnson: MEEP: A flexible free-software package for electromagnetic simulations by the FDTD method, *Computer Physics Communications*, vol. 181, pp. 687–702, Jan.2010.
[7] J. Pomplun, S. Burger, L. Zschiedrich, F. Schmidt: Adaptive finite element method for simulation of optical nano structures, *Phys. Stat. Sol. (b)*, vol. 244, pp. 3419-3434, Oct. 2007.
[8] S. Burger, J. Pomplun, F. Schmidt, L. Zschiedrich: Finite-element method simulations of high-Q nanocavities with 1D photonic bandgap, *Proc. SPIE*, vol. 7933, p. 79330T, Jan. 2011.
[9] E. Silberstein, P. Lalanne, J.-P. Hugonin, Q. Cao: Use of grating theories in integrated optics, *JOSA A*, vol. 18, no. 11, pp. 2865-2875, Nov. 2001.
[10] J.-P. Hugonin, P. Lalanne: Perfectly matched layers as nonlinear coordinate transforms: a generalized formalization, *JOSA A*, vol. 22, no. 9, pp. 1844-1849, Sep. 2001.
[11] J. Čtyroký, P. Kwiecien, I. Richter: Fourier Series-Based Bidirectional Propagation Algorithm With Adaptive Spatial Resolution, *J. Lightwave Technol.*, vol. 28, no. 20, pp. 2969-2976, Oct. 2010.
[12] Z. Y. Li, K. M. Ho: Application of structural symmetries in the plane-wave-based transfer-matrix method for three-dimensional photonic crystal waveguides, *Phys. Rev. B*, vol. 68, no. 24, pp. 245117-1, Dec. 2003.
[13] P. Kwiecien, I. Richter, J. Čtyroký: Comparison of 2D and 3D Fourier modal methods for modeling subwavelength-structured silicon waveguides, *Proc. SPIE*, vol. 8306, p. 83060Y, Oct. 2011.
[14] P. Kwiecien, I. Richter: Efficient three dimensional aperiodic rigorous coupled wave analysis technique, *Proc. ICTON 2011* (13th International Conference on Transparent Optical Networks, June 2011, Stockholm, Sweden), pp. 1-5, June 2011.
[15] B. Maes, J. Luksch, J. Petráček, S. Burger: Numerical method comparison for high-Q optical nanocavities. Under preparation.
[16] M. Notomi, E. Kuramochi, H. Taniyama: Ultrahigh-Q Nanocavity with 1D Photonic Gap, *Opt. Express*, vol. 16, no. 15, pp. 11059-11102, Jul. 2008.