Finite-Element Method Simulations of High-Q Nanocavities with 1D Photonic Bandgap

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ABSTRACT

High-Q optical resonances in photonic microcavities are investigated numerically using a time-harmonic finite-element method.

Keywords: optical microcavity, nanooptics, integrated optics, 3D Maxwell solver, finite-element method

1. INTRODUCTION

Optical microcavities allow to confine light to small volumes. High resonance Q-factors can be attained using the high reflectivity of multi-layer Fabry-Perot resonators, of total internal reflection and/or of photonic bandgap materials.[1] In this contribution we revisit a microcavity design proposed originally by Notomi, Kuramochi and Taniyama.[3] Notomi et al have shown that very high Q-factors can be reached with a size-modulated 1D stack design. In this case confinement to the cavity is obtained by total internal reflection in two dimensions, and by a photonic bandgap in the third dimension. Advantages of this design are its compactness and simplicity.

For an efficient design of microcavities and other integrated photonic components 3D simulations of Maxwell’s equations are needed. We have developed finite-element method (FEM) based solvers for the Maxwell eigenvalue and for the Maxwell scattering problems. The method is based on higher order vectorial elements, adaptive unstructured grids, and on a rigorous treatment of transparent boundaries. We perform a numerical analysis of the microcavity setup. Results on resonance wavelengths and Q-factors are generated using a resonance solver. The obtained values are confirmed by simulations of transmission spectra of light incident to the microcavities. Dependence of Q-factors and resonance wavelength on structural parameters are investigated. A focus of this contribution is on the numerical convergence of the obtained results.

2. INVESTIGATED SETUP

The investigated setup consists of a finite array of dielectric blocks, as depicted in Figure[1] The first and the last block of the array are merged to waveguides with same square shape as the blocks, but infinite in the third dimension (z-direction). The centers of the blocks are arranged periodically with a period of $a = 430 \text{ nm}$. Width and height of the waveguide and blocks (in x- and y-direction) are $W_x = 3a$ and $W_y = 0.5a$. The length of $2N_i + 1$ inner blocks is modulated symmetrically around a central block, $W_{x,n} = W_{x,0} + (|n|/N_i)^2(W_{x,N_i} - W_{x,0})$, with $W_{x,0} = 0.45a$, $W_{x,N_i} = 0.5345a$. The length of $2N_o$ outer blocks is constant $W_{x,n} = W_{x,N_i}$ ($n > N_i$), where the distance from the center block is denoted with $n$ (in number of blocks). The setup of Notomi et al corresponds to $N_i = 13$. The blocks consist of dielectric with refractive index $n = 3.46$, the surrounding is filled with vacuum ($n = 1.0$). Conceptually similar devices have also been investigated experimentally.[4]

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3. NUMERICAL RESULTS

3.1 Band diagram of the 1D periodic array

We start the numerical investigation by computing the band diagram of the 1D periodic array of dielectric blocks in vacuum. The unit cell of the computation is periodic in the z-direction with a period \( a \), transparent boundary conditions (perfectly matched layers, PML) apply in the x- and y-directions, the width of the blocks in the z-direction is \( W_z = 0.5345a \). Computation of modes with even symmetry is selected by reducing the symmetric computational domain to the half space \( x > 0 \) and applying corresponding boundary conditions at the symmetry plane. Figure 2 (left) shows a part of the band structure of the 1D photonic crystal. A band gap appears for dimensionless frequencies between \( \tilde{\omega} \approx 0.246 \) and \( \tilde{\omega} \approx 0.329 \). Dimensionless frequency \( \tilde{\omega} \) is defined as \( \tilde{\omega} = (\omega a)/(2\pi c_0) \), with time-harmonic frequency \( \omega \) and vacuum speed of light \( c_0 \). Dimensionless magnitude of Bloch vector \( \tilde{k} \) is defined as \( \tilde{k} = ka/(2\pi) \), with Bloch vector \( k \). For \( a = 430 \text{ nm} \) the bandgap corresponds to a wavelength range between approximately 1307 nm and 1748 nm. In Figure 2 (left) only modes below the light cone are displayed. Modes above the light cone have complex eigenfrequencies, which corresponds to leakage to the transversal directions.

Figure 2 (right) shows numerical convergence of the simulated lowest Bloch-mode at \( \tilde{k} = 0.5 \): Finite-element simulations have been performed for the same physical parameters and for different numerical parameters with increasing numerical accuracy. In this case the polynomial degree of the finite-element ansatz functions, \( p \), has been varied between \( p = 1 \) and \( p = 7 \) for a fixed spatial mesh discretizing the geometry of the unit cell. The computed value of \( \tilde{\omega} \) for \( p = 7 \), \( \tilde{\omega}_{p=7} \approx 0.24644 \), is taken as quasi-exact value, and the relative error of the

![Figure 1](image-url)

Figure 1. Top: Geometry of a size-modulated 1D stack microcavity with a central block of width \( W_{z,0} \), \( 2 \times N_i = 2 \times 13 \) size-modulated blocks of widths \( W_{z,n} \) and \( 2 \times N_o = 2 \times 5 \) blocks of constant width \( W_{z,N_i} \). Blocks and incoming/outgoing waveguides consist of dielectric material, the structure is surrounded by air, waveguides extend to infinity. The structure is mirror-symmetric at the planes \( x = 0 \), \( y = 0 \), therefore the computational domain can be reduced to one quarter of the whole structure. Bottom: Field distribution on resonance (pseudo-color representations), from top to bottom: intensity in a \( x-z \)-cross-section, intensity in a \( y-z \)-cross-section, \( \Re(E_y) \) in a \( x-z \)-cross-section, \( \Re(E_x) \) in a \( y-z \)-cross-section, \( \log(E_x^2) \) in a \( x-z \)-cross-section, \( \log(E_y^2) \) in a \( y-z \)-cross-section,
computed values of $\tilde{\omega}$ for $p = 1 \ldots 6$, $\Delta \tilde{\omega}_p = |\tilde{\omega}_p - \tilde{\omega}_{p=7}|/\tilde{\omega}_{p=7}$ is plotted as function of the number of unknowns of the discrete problem. Computation times on a standard workstation range between below a second and few minutes for the plotted values. High accuracy with relative errors better than 0.1% is obtained for $p \geq 3$. The solvers used for the band diagram simulations and for the further simulations throughout this contribution are part of the FEM program package JCMsuite which is developed by Zuse Institute Berlin and JCMwave.

3.2 Transmission of waveguide modes through a finite 1D periodic array

For simulating transmission through a finite array of blocks / a finite 1D photonic crystal at specific wavelength $\lambda_0$, we first compute the fundamental propagation mode of the waveguide at $\lambda_0$ using a FEM propagation modesolver. The obtained mode field is applied as input data to one of the boundaries of the 3D computational domain (left boundary in Fig. 1), such that the mode propagates in direction of the center of the waveguide. We then compute the scattered light field in the setup corresponding to this excitation using higher-order finite-elements. In post-processes we extract energy fluxes through interfaces and field distributions in several cross-sections from
the 3D light field distribution. Transmission $T$ is defined as ratio of the energy flux of the outgoing light field at the back side of the array to the energy flux of the incoming waveguide mode through the waveguide cross section.

Figure 3 shows a transmission spectrum for 800 incident waveguide modes with vacuum wavelengths between $\lambda_0 = 1075$ nm ($\tilde{\omega} = 0.4$) and $\lambda_0 = 2150$ nm ($\tilde{\omega} = 0.2$). In perfect agreement with the band structure simulations transmission is greatly suppressed in the frequency range between $\tilde{\omega} \approx 0.246$ and $\tilde{\omega} \approx 0.329$ which corresponds to a bandgap of the 1D periodic structure (cf Figure 2).

3.3 Direct simulation of high-Q cavity resonances

We use an eigenmode solver for directly simulating the resonance properties (resonance wavelength and Q-factor) of size-modulated 1D stack cavities: Given the geometrical setup as described in Section 2 one computes an electric field distribution $E$ and a complex eigenfrequency $\omega$ which satisfy Maxwell’s time-harmonic wave equation without sources,

$$\nabla \times \mu^{-1} \nabla \times E = \omega^2 \varepsilon E$$,

electric permittivity and magnetic permeability are denoted by $\varepsilon$ and $\mu$, respectively. Transparent boundary conditions (PML) take into account the specific geometry of the problem where waveguides are modelled to extend to infinity in the exterior domain. When the eigenmode $(E, \omega)$ is computed, the respective Q-factor is deduced from the real and imaginary parts of the complex eigenfrequency, $Q = \Re(\omega)/(2 \Im(\omega))$, the resonance wavelength $\lambda_0$ is given by $\lambda_0 = 2\pi c_0/\Re(\omega)$. Figure 1 shows visualizations of a typical field distribution obtained with the resonance solver.

Direct simulation of a resonance requires a single computation only. In contrast, deducing the resonance properties from a transmission or reflection spectrum generated with a time-harmonic solver requires several computations at various wavelengths. Especially for high-Q resonances, where the choice of wavelengths for a transmission scan is not clear a-priori, direct computation of resonances simplifies the simulation task and reduces computational effort. Time-domain solvers for simulating 3D high-Q resonances typically suffer from very long computation times and slow convergence rates.

We have performed simulations for different cavity setups. Figure 4 shows the dependence of Q-factor and resonance wavelength on the number of modulated blocks, $N_i$, of the 1D stack cavity setup (see Section 2). For these simulations, the number of outer blocks is fixed to $N_o = 4$. With increasing number of modulated blocks, the resonance wavelength is pulled from the band-edge (at a wavelength of 1748 nm) more and more.

Figure 4. Dependence of resonance wavelength $\lambda_0$ (left) and Q-factor (right) on number of modulated blocks, $N_i$. For all simulations, $N_o = 4$. Results are displayed for finite-element degree $p = 3$ and $p = 4$. 
inside the band-gap. At the same time, the Q-factor increases nearly exponentially for the investigated range of \( N_i = 1 \ldots 15 \). Figure 4 shows results for different numerical resolutions, i.e., for finite-element degree \( p = 3 \) and \( p = 4 \). As can be seen from these results, for higher numbers of modulated blocks, i.e., for higher Q-factors, influence of numerical resolution on the results gets more significant, up to a level of relative deviations of the order of ten percent.

Figure 5 shows the dependence of Q-factor and resonance wavelength on the number of outer, unmodulated blocks, \( N_o \), of the 1D stack cavity setup (see Section 2). For these simulations, the number of inner blocks is fixed to \( N_i = 13 \) which corresponds to the setting of Notomi et al.\(^3\) For these simulations, fourth-order finite-elements (\( p = 4 \)) have been used. With increasing number of unmodulated blocks, the resonance wavelength is changed only on a sub-nanometer scale. The Q-factor increases exponentially for \( N_o < 6 \) and reaches a plateau of \( Q \approx 3 \times 10^6 \) for \( N_o > 7 \). We expect that radiation losses to the surrounding air limit high-Q performance in this case.

For evaluating numerical errors of high-Q resonance simulations using the resonance mode solver we again show a numerical convergence study: The geometry setting is fixed to to \( N_i = 13, N_o = 5 \). Finite-element polynomial degree \( p \) is varied between \( p = 1 \) and \( p = 5 \), and Q-factor, resonance wavelength and numerical effort are recorded. Figure 6 (left) shows how the relative error of Q-factor and resonance wavelength converge with number of unknowns \( N \), where the solution at highest resolution (\( p = 5 \)) has been taken as reference result (\( \lambda_{qe} = 1694.12 \) nm, \( Q_{qe} = 1.04 \times 10^6 \), \( N_{qe} = 978,570 \)). Computation times for the displayed results are 1 sec, 12 sec, 2 min, 9 min, respectively (on a workstation with 8 CPU cores). This demonstrates that resonances with Q-factors of about 1 million can be computed at accuracies of about 0.1\% (resonance wavelength) and 10\% (Q) within few minutes.

In principle, a wrong numerical realization of transparent boundary conditions can introduce errors which will not show up in a convergence study as shown in Figure 6 (left). We realize transparent boundary conditions with the PML method, i.e., by a coordinate transform to complex space, by FEM discretization with higher-order elements (same order \( p \) as in the interior domain), and by truncation at a variable distance from the boundary to the interior computational domain. For a fixed setting of \( p = 4 \) we have further investigated dependence of the results on varied number of PML segments. Figure 6 (right) shows that convergence of the results with PML discretization parameter is very fast. This indicates that the main contribution to the numerical errors as shown in Figure 6 (left) are caused by discretization of the electromagnetic field in the interior domain. Typical settings for the results displayed in Figure 6 (left) and Figure 4-5 are about seven PML segments. The setting of further
PML parameters is done adaptively. More detailed studies should also consider influence of these parameters on numerical accuracy.

We note that an evaluation of the significant differences between the numerical results of Notomi et al. and our numerical results requires further investigations. Notomi et al. have reported results from a finite-difference time-domain method yielding significantly higher Q-factors (by about two orders of magnitude) for the same physical setting.

### 3.4 Light scattering response of a high-Q cavity

An alternative possibility of computing the resonance properties of a cavity is to investigate its scattering response to incident light fields. Using the same approach as in Section 3.2 we perform FEM light scattering simulations where the incident light fields are waveguide modes at fixed frequencies/wavelengths. From the near field solutions we deduce the energy stored in the central part of the cavity, and the energy flux transmitted through the device.

For these simulations we again investigate the modulated stack cavity with $N_i = 13, N_o = 5$. As numerical discretization parameter we choose a polynomial degree of the finite-element ansatzfunctions of $p = 4$. Figure 7 (left) shows the (normalized) energy $E$ stored in the cavity as a function of the wavelength of the incident waveguide mode. For automatic determination of the wavelengths of the incoming waveguide modes, $\lambda_{in}$ we use a self-adaptive bisection algorithm. In this example we used a search range of $\Delta\lambda \approx 3$ nm and 14 bisections, resulting in a final wavelength-resolution of $\delta\lambda \approx 10^{-4}$ nm. With a typical simulation time of about 10 min for a single-wavelength simulation, this results in a total computation time for the frequency scan of about 8 hrs.

We fit a Lorentzian distribution to the data points and deduce a resonance wavelength of $\lambda_0 \approx 1694.7345$ nm and a Q-factor of $Q \approx 1.14 \times 10^6 \left(\frac{\lambda_0}{FWHM}\right)$. Both are in very good agreement with the results from the resonance mode solver within the ranges of numerical error (see Section 3.3), as expected from the convergence study.

We have also recorded the total transmission through the device by integrating the energy fluxes over the incoming and outgoing facets of the device. Figure 7 (right) shows the transmission peak corresponding to the resonance. Here the total transmission reaches a maximum of $T \approx 0.31$. 

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**Figure 6.** Convergence of numerical results for high-Q ($10^6$) resonance simulation using a resonance solver: Dependence of relative errors of Q-factor and resonance wavelength, $\Delta Q = |Q_N - Q_{qe}|/Q_{qe}$ and $\Delta \lambda = |\lambda_N - \lambda_{qe}|/\lambda_{qe}$, on number of unknowns of the FEM problem, $N$. Geometry setting: $N_i = 13, N_o = 5$. Left: Finite-element degree $p$ varied between $p = 1$ and $p = 4$. Right: Number of segments discretizing the solution in the PML region varied between 1 and 7.
4. CONCLUSION

Size-modulated stack microcavities have been investigated numerically using time-harmonic finite-element solvers. The results have been validated by convergence analysis. Well converged results for cavities with Q-factors larger than $10^6$ have been obtained. Dependencies of resonance wavelength and quality factor on geometrical parameters have been investigated.

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