Statistical Investigations of high-Q Photonic Crystal Resonators

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***Abstract*—Manufacturing deviations of photonic crystal resonators are statistically investigated, since for a high quality factor of such structures small tolerances are mandatory. For this reason an extensive sequence of full-wave electromagnetic simulations is carried out and the results are analyzed in terms of appropriate stochastic distributions.**

***Index Terms*—Photonic crystals, Statistical analysis, Weibull distribution**

I. Introduction

Photonic crystal resonators which have a high quality factor are important structures in optoelectronics and photonics [1], [2]. Dependent on purpose and operating frequencies these are manufactured as a lattice of holes in a dielectric slab or vice versa as dielectric rods in a medium with lower refractive index. It is known from the literature that highest quality factors are not obtained with totally homogeneous lattices but with slight deviations in lattice constants, radii or even material which are subject to optimization [3]. However, for highest quality factors manufacturing tolerances have to be as small as possible. So, we study the sensitivity of the quality factor of the photonic crystal resonator by extensive stochastic parameter variations. Related studies with focus on the one dimensional Bragg reflectors have been performed purely analytically in [4].

II. Model Problem

The model problem under test is a quasi-two dimensional photonic crystal resonator cf. Fig. 1. It consists of 16 dielectric rods which are modeled to be lossless. The lattice constant is 8 microns, the rods' radii are 3 microns, and an electromagnetic eigenmode can be trapped into the 13 micron air-gap. The external quality factors Q of the trapped eigenmodes are finite, since some power can dissipate through the boundaries at z_{min} and z_{max}. The lateral boundaries are $\vec{E}_{tan} = 0$ at y_{min} and y_{max} and $\vec{H}_{tan} = 0$ at x_{min} and x_{max}. For our preliminary study we reduce the computational effort to one quarter of the resonator by applying symmetry conditions. That means that the computational model consists of eight rather than 16 dielectric rods. For simulation we use the commercially available code CST Microwave Studio [5] based on the finite integration technique. A discretization with a hexahedral mesh and 20 lines per wavelength yields 34668 degrees of freedom for this setup. In the reference simulation all the remaining eight dielectric rods have $\varepsilon_r = 10$ which yields a quality factor Q_0 =20,500 at a loaded eigenfrequency of f_0 = 8.2783 THz with CST's eigenmode solver. The residual of all eigenmode computations is less than 10^{-8}.

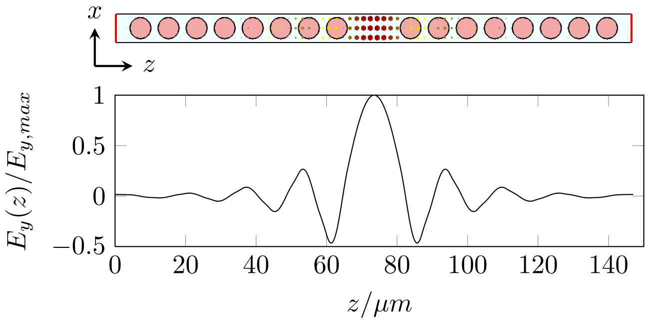

Figure 1: A two dimensional photonic crystal resonator bounded with 16 dielectric rods and electrical field distribution of the trapped eigenmode. Quality factors are finite since some power is able to radiate through the boundaries at z_{min}, z_{max}.

In the following, we allow for manufacturing tolerances such as geometrical imperfections or material impurities which are modeled by a slight shift in the relative dielectric constant ε_r of the rods rather than changing their geometry. Therefore, the relative permittivity for each of the eight dielectric rods is considered to be Gaussian-distributed with a mean permittivity of $\overline{\varepsilon_r} = 10$ and a standard deviation of $\sigma_\varepsilon = 1$. The parameter space of the eight independent Gaussian distributions is sampled by a Sobol minimum discrepancy sequence with 50,000 samples, using R's randtoolbox [6], [7]. From the parameter set we form 50,000 numerical models for simulation with CST, whose solution take some days of computational time on actual workstations.

III. Statistical Results

The relative frequency distribution of the computed quality factors Q is shown in blue in Fig. 2. The smallest and largest observed quality factors are Q_{min} =3,500 and Q_{max} =25,400 while the mean is $\overline{Q}$ =16,720 with a standard deviation of σ_Q =2,708. On the one hand it turns out that the mean $\overline{Q}$ is not as high as the initial Q_0 =20,500, on the other hand there are 3,106 samples or 6.2% of the overall samples which show a higher Q than Q_0. The ratio between smallest and highest Q is a factor larger than eight.

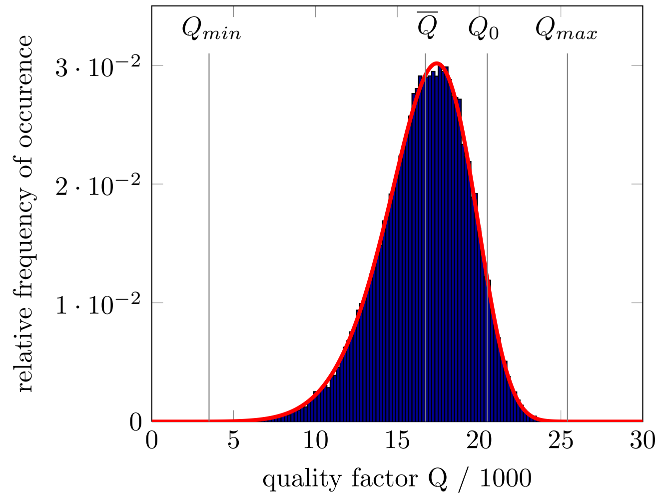

Figure 2: The relative frequency distribution of computed quality factors Q can be approximated by the Weibull distribution (1) (red line).

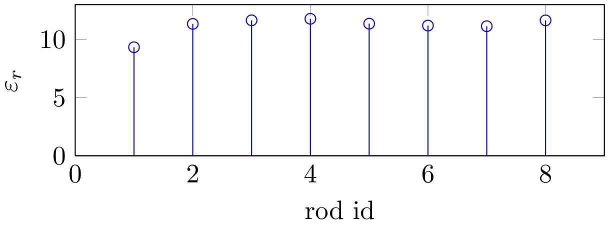

Figure 3: Parameter set for relative permittivity which yields the highest quality factor Q_{max}.

The parameter set which yields the highest quality factor Q_{max} is shown in Fig. 3. The Gaussian-like oscillating variation of the rods' relative permittivities agrees well with results from the literature [3] where a spatial Fourier transformation yields hints for an optimal confinement of a cavity's eigenmode.

The relative frequency distribution of the computed quality factors in Fig. 2 is transformed into a probability density function (PDF). It turns out that the PDF can be fairly matched by a Weibull distribution [8]. The Weibull distribution has the density function

$$f(Q;k,\lambda) = \frac{k}{\lambda}\left(\frac{Q}{\lambda}\right)^{k-1} \exp -(Q/\lambda)^k. \quad (1)$$

The PDF consists of the shape parameter k and the scale parameter λ. These parameters are determined by a numerical least-square matching of the relative frequency distribution in Fig. 2, and the resulting curve is plotted in red.

The question is how many simulations of different dielectric parameter sets are necessary, in order to get reasonable results. Therefore, the variation of the Weibull's distribution parameters k and λ for an increasing number of samples as well as the overall residual of the least-square fit is shown in Fig. 4. For more than 13,000 samples of the Sobol sequence there is no significant change in the parameters any more and the overall residual is less than $5 \cdot 10^{-5}$. However, the residual can still be reduced and so it depends on the accuracy demands posed on how many samples have to be considered.

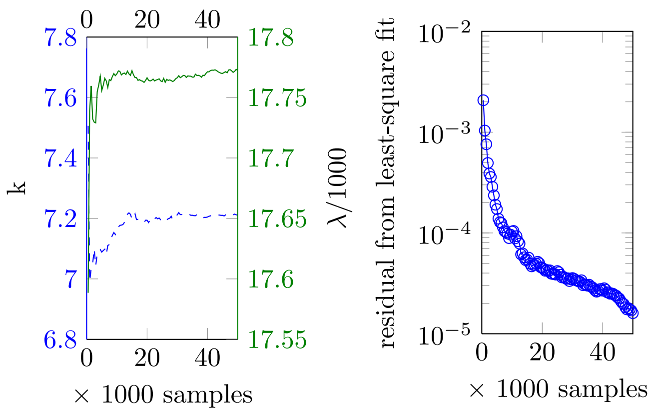

Figure 4: Left: Convergence of the Weibull distribution's parameters λ and k for an increasing number of samples. Right: Residual of the least-square fit in dependency on the number of samples.

IV. CONCLUSIONS

In our contribution we show a study on sensitivity of high quality factors from a photonic crystal resonator. It turns out that statistical variations of dielectric rods' permittivity lead to a distribution of quality factors, which can be modeled by the Weibull distribution. With an increasing quality factor also the sensitivity on possible manufacturing tolerances rises. Results from the full computational model without used symmetry will be presented at the conference.

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