Model-Based Parameter Estimation (MBPE) for Metallic Photonic Crystal Filters

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Abstract **–** An efficient method for the accurate computation of the response of photonic crystal filters is obtained when Model-Based Parameter Estimation (MBPE) is combined with accurate field solvers. In this paper, MBPE is combined with Multiple Multipole Program (MMP) and the Method of Auxiliary Sources (MAS) and the results are compared with results obtained from a commercial field solver. When metals are present in photonic crystal filters, strong material dispersion at optical frequencies cause nonlinearity of the filter response. It is demonstrated that MBPE is still useful although it is originally designed for linear systems.

Keywords – Model-Based Parameter Estimation; PhC filters; MMP, MAS.

I. INTRODUCTION

Photonic Crystals (PhCs) consist of dielectric or metallic structures [1] arranged on a regular lattice like the atoms in a natural crystal. Mainly because of the Photonic Band Gap (PBG) - that is observed when the contrast between the materials used for fabricating the PhC is high enough - PhCs are very promising for integrated optics. In fact, the PBG is the photonic counter part to the electronic band gap of semiconductors. By doping PhCs one can easily introduce resonators (point defects) and waveguides (line defects) in a PhC. By combining both one can obtain useful components such as filters. PhC filters may be embedded in PhC waveguides but also in classical waveguides. The simplest PhC filter is a PhC slab illuminated by a plane wave. Such filters are currently intensively studied to determine their limitations and practical value. The main problem is that no simple design rules are available. Therefore, efficient numerical methods for the analysis and optimization of PhC filters are highly desirable. Model-Based Parameter Estimation (MBPE) [2 - 4] is an auxiliary technique that may be added to any field solver for obtaining the entire frequency response from the calculation of the response in a small number of frequency points. This means that the field solver only computes the filter for m discrete (real or complex) frequency points s_k (k=1…m) and MBPE then provides a very fast approximation for any desired frequency s.

Model-Based Parameter Estimation - also called Cauchy method [5] - was originally designed for linear PhC filters: The frequency response of linear filters is known to be best represented by a fraction of two polynomials (Cauchy formula) and MBPE takes advantage of this representation.

In the following it is demonstrated that MBPE is also useful and efficient for PhC filters made of dispersive materials, namely, PhC filters that include metal with strongly frequency-dependent complex permittivity at optical frequencies. As a particular case, filter analysis in the optical frequency range is considered. The electrodynamic problem of the PhC filter structure - containing silver rods - was solved by using the frequency domain solvers Multiple Multipole Program (MMP) [6], [7], [10], [11] and the Method of Auxiliary Sources (MAS) [8], [9].

II. MODEL-BASED PARAMETER ESTIMATION (MBPE)

Most EM phenomena require essentially a continuous representation of the system response over a specific frequency range. The computation of the observables (S parameters, transmission and reflection coefficients, field strengths in certain points of space, etc.) with sufficient resolution can be expensive especially when sharp resonances are present. MBPE allows us to obtain the system response over the entire frequency range by using a relatively small number of frequency samples.

The main concept of MBPE is the following. In the frequency domain, the response of a linear system may be optimally represented by Cauchy's method, i.e.,

$$F(s) = \frac{N(s)}{D(s)} + Error(s) = \frac{\sum_{i=0}^{n} N_i s^i}{\sum_{i=0}^{d} D_i s^i} + Error(s), \qquad (1)$$

where F is the response of the system and s the complex frequency that also may be limited to the radian frequency $i\omega$. The error of this approximation depends on the maximum orders n and d of the power series expansions in the nominator N and denominator D as well as on the method that determines the parameters N_i and D_i.

A simple technique to compute the parameters is to multiply equation (1) by D and rewrite equation (1) in a set of m frequency points s_k:

$$F(s_k)\sum_{i=0}^{d} D_i s_k^i - \sum_{i=0}^{n} N_i s_k^i = Error(s_k)\sum_{i=0}^{d} D_i s_k^i = E_k, \qquad (2)$$
$$k = 1,..,m$$

where E is an unknown error vector. When F is known in $m \geq n + d + 1$ points s_k, equation (2) is a linear system of m equations. One then can evaluate the parameters D_i and N_i in such a way that the square norm of the error vector is minimized. Before this is done, one should note that not all parameters are independent because nominator and denominator in equation (1) may be scaled with an arbitrary factor. For this reason, one of the parameters may be set equal to 1. It is reasonable to set D_d=1. One then obtains,

$$F(s_k)\sum_{i=0}^{d-1} D_i s_k^i - \sum_{i=0}^{n} N_i s_k^i = -F(s_k)s_k^d + E_k = R_k + E_k, \quad (3)$$
$$k = 1,..,m$$

where R is a known, right-hand-side vector. Note that equation (3) can be solved in such a way that the error vector E is zero when $m=m_0=n+d+1$, because one then obtains a square matrix system. This does not imply that $Error(s)$ becomes zero as well. Especially when the sample values $F(s_k)$ are only approximately known – which is always the case in practice – it is more reasonable to work with an overdetermined system of equations with $m > m_0$. Reasonable overdetermination implicitly provides smoothing of "noise" and "ripples" caused by inaccurate Maxwell solvers. When highly accurate codes such as MMP and MAS are used, very weak overdetermination (with overdetermination factors m/m_0 around 1.1) is sufficient. This obviously reduces the number of frequency points required. Since the time-consuming part of the MBPE is the computation of the sample values by the Maxwell solver, weak overdetermination saves computation time.

The most difficult problem is to determine the required maximum orders n and d of the power series of the nominator and denominator. Both depend very much on the size of the frequency range of interest, the desired accuracy, and the complexity of the system. Since metals within Metallic Photonic Crystals (MPhCs) and Metallo-Dielectric Photonic Crystals (MDPhCs) are strongly dispersive at optical frequencies, MPhC and MDPhC filters are non-linear and may be linearized only over a sufficiently short frequency interval. Therefore, it is reasonable to limit the maximum orders n and d by a value of typically not higher than 10 and to subdivide the frequency interval into two or more parts when the MBPE approximation is not accurate enough.

The algorithm block scheme of the MBPE procedure used for the PhC filter analysis is presented in Fig. 1. The MBPE procedure is adaptive and starts with small orders, i.e., n and d values and with a small number of test points according to the overdetermination factor specified by the user. It then increases the order by 1 and compares the resulting MBPE approximations. When the differences

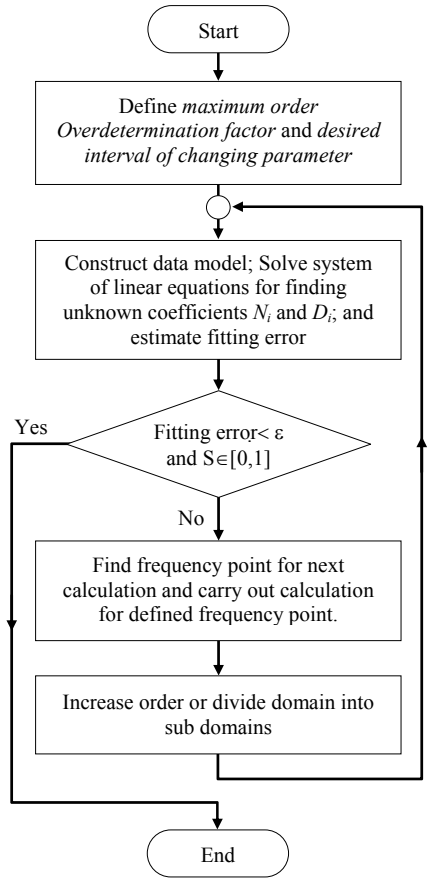


Fig. 1. MBPE procedure for PhC filters analysis.

between the two approximations are below a user-defined error bound over the entire frequency range and when all *S* parameters are within the range 0…1, the MBPE approximation is good enough and the procedure stops. Otherwise, it inserts new test points within the frequency range as follows: If an *S* parameter is out of the range, it inserts the new test point at the frequency where the biggest distance from the range 0…1 is encountered. Otherwise, it searches for the maximum difference between the current and previous MBPE approximation and sets the new test point at the corresponding frequency. The evaluation of the filter response, e.g., the *S* parameters, in the new test point is then performed by the field solver, for example, MMP or MAS. When the number of test points is high enough, the MBPE order is increased – provided that the user-defined maximum order is not yet reached. As soon as the maximum order is reached, the frequency interval is split into two intervals with half the length of the original interval and a separate MBPE approximation is started for each interval. This procedure is recursively continued if required.

One is often interested in the frequency dependence of several characteristic values, for example, the S parameters. Usually, the field solver can simultaneously evaluate all parameters with almost the same numerical costs as for a single parameter. Therefore, it is reasonable to implement an MBPE procedure that simultaneously evaluates the frequency response of several observables, for example, all S parameters. All that needs to be done for such a multi-parameter MBPE is to define the maximum fitting error over all model parameters – typically the sum of the square errors of all model parameters. Beside this, the procedure outlined in Fig. 1 remains the same.

To demonstrate how MBPE works for dispersive materials, we consider the problem of coupled metallic nanoparticles [11 - 13]. The first test system contains only two circular cylinders made of silver with a radius of 25 nm and a surface-surface separation of 5 nm (see Fig. 2), illuminated by an H-polarized plane wave. H-polarization is chosen, because plasmon resonances are obtained for this case. The electrodynamic problem was solved by the MAS. The MBPE procedure was started in 30 sample points and the overdetermination factor was set equal to 1.1. For the system response over the wavelength range 100 nm to 350 nm the adaptive MBPE algorithm requires only 63 frequency points for a maximum fitting error below 1%. In Fig. 2 the Scattering Cross Section (SCS) for the system is shown and Fig. 3 illustrates the field distribution at plasmon wavelengths. The Drude model is used for the frequency dependence of the permittivity of silver [10],

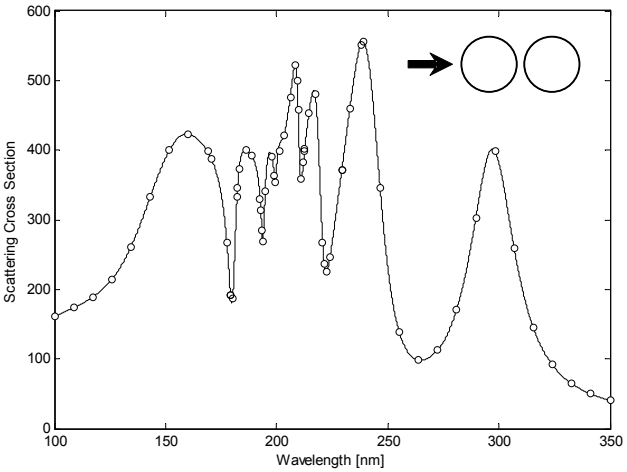
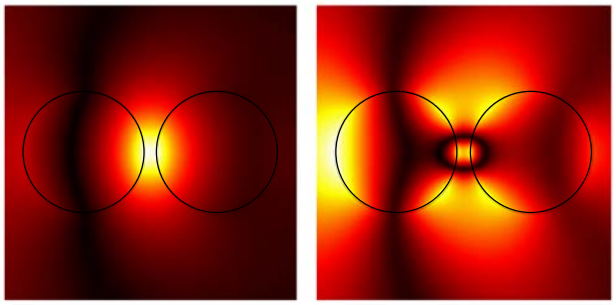


Fig.2. SCS for two intersecting cylinders made of silver with a radius of 25 nm at a surface-surface separation of 5 nm. The field is evaluated in 68 sample points marked by circles.



α) λ = 297 nm b) λ = 239 nm

Fig. 3. Near-Filed around coupled circular nanoparticles illuminated by an H-polarized plane wave incident from the left side.

$$\varepsilon(\nu) = 1 + \frac{i\tau\omega_p^2}{2\pi\nu(1 - i2\pi\tau\nu)}, \tag{4}$$

with $\tau = 1.45 \times 10^{-14} s$ and $\omega_p = 1.32 \times 10^{16} s^{-1}$. Note that this frequency dependence is only approximate and not very accurate. For more realistic results, experimental values should be used [14]. The value used here just serves as a demonstration how the MBPE can handle dispersive materials. Furthermore, this allows us to compare the results with time-domain solvers that only can handle dispersive materials described by simplified mathematical models such as the Drude model. Figure 4 illustrates the real and imaginary part of the permittivity of the Drude model for silver together with the different MBPE domains. The second and third domains are small

compared with other ones although the frequency dependence of the material properties is rather smooth everywhere. The reason for this is that plasmon resonances occur when the real part of the permittivity is close to -1, i.e., the adaptive MBPE has correctly located the critical frequency range. Note that the number of plasmon resonances depends on the material characteristics and on the geometry. Therefore it is usually not possible to precisely foresee the locations of the resonances.

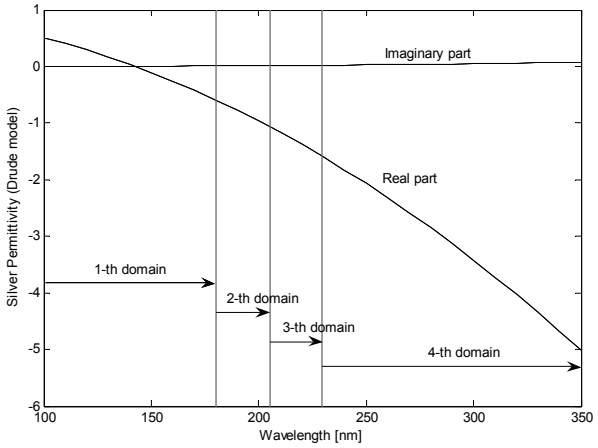


Fig.4. Frequency dependence of the permittivity of silver (Drude model). The vertical grey lines indicate the MBPE domains obtained from the automatic procedure. In each domain a Cauchy approximation of order 10 was used.

III. 2D METALLIC PHC SLAB

The PhC filter structure considered in the following consists of a 2D PhC with 5 layers of circular silver wires arranged on a square lattice. This structure extends to infinity in x direction and is finite in y direction, as illustrated in Fig. 5. The wire radius is 73.3 nm and lattice constant is 820 nm. E_z polarization is considered because metallic PhCs have a fundamental band gap for this polarization.

Numerical methods can take advantage of the periodic symmetry in x direction in different ways.

1) The MMP code introduces fictitious boundaries that separate a single "fundamental" cell from its neighbors as illustrated in Fig. 5. Along these boundaries, periodic (Floquet) boundary conditions are imposed [11]. It is then sufficient to compute the field in a single cell. Since this cell extends still to infinity in y direction, two additional fictitious boundaries are introduced that separate three areas: a) the upper half space with incident plane wave plus reflected zero and higher order Rayleigh expansions, b) the PhC area, and c) the lower half space with transmitted zero and higher order Rayleigh expansions. The areas a) and c) are modeled as for arbitrary gratings, whereas area b) has a finite size. Within b) the field is approximated by standard MMP expansions as an ordinary scattering problem.

Taking care of the periodic symmetry by means of periodic boundary conditions has the advantage of generality and simplicity in the implementation, i.e., any frequency-domain code that can handle simple scattering problems can handle periodic structures such as gratings and PhCs as soon as periodic boundary conditions are implemented. Within MMP, not only multipoles but a big library of analytic solutions of Maxwell's equations is available. All of these functions may then not only be applied for modeling scattering problems but also for modeling PhCs. For example, the field inside the wires is approximated by Bessel expansions rather than by multipoles.

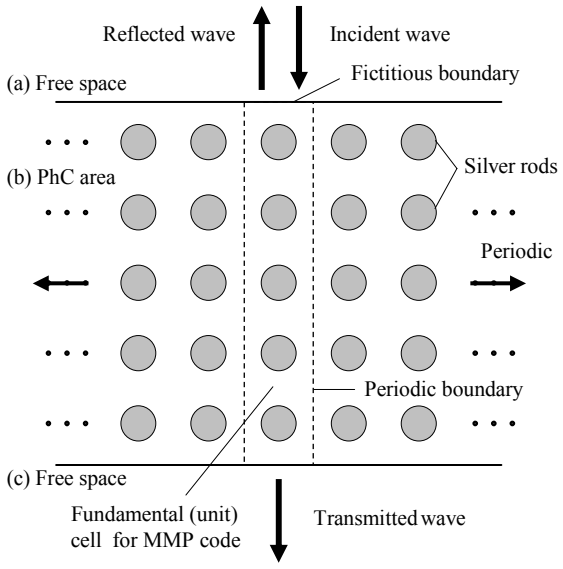


Fig. 5. The PhC filter structure for MMP code.

2) The Method of Auxiliary Sources (MAS) uses an approximation of the scattered field by a set of auxiliary sources, i.e., monopole sources, distributed along auxiliary lines that are always outside the physical area of the scattered field. Here, the periodic symmetry is taken into account by using periodic arrays of monopole sources as illustrated in Fig. 6. Thus, the periodic boundary conditions are automatically satisfied by the periodic expansions. Since only one type of relatively simple expansions – monopoles – is used, the implementation of a periodic set of expansions is not too difficult, but for an efficient implementation, a careful numerical analysis is

required. The functions describing the fields of auxiliary sources have the form

$$F_n(|\vec{r}_n - \vec{r}|) = \sum_{m=-\infty}^{\infty} \alpha \, \mathrm{H}_0^{(1)}(k\sqrt{(x - x_n - md)^2 + (y - y_n)^2}), \tag{5}$$

where d - is the period of the structure; α=1 for diffraction lattices and $\alpha = (-1)^m$ for waveguides with non-homogeneous filling. Now, the singularities are singled out in an explicit form. When the bad convergence of equation (5) is improved by use of the Poisson formula, an efficient algorithm is obtained. The amplitudes of each monopole array are computed in such a way that Floquet conditions are automatically met, i.e., no periodic boundary conditions are required. For the calculation of the reflected ($y>y_n$) and transmitted ($y<y_n$) fields for the 0 and p-th harmonic one has,

$$g_p = \frac{2\pi}{d} p, \quad h_p = \frac{2\pi}{d}\sqrt{D^2 - (p + D\cos\theta)^2}, \tag{6}$$
$$D = \frac{d}{\lambda}, \quad (p = 0, \pm 1, \pm 2, ...),$$

$$E_0(x, y) = \sum_{n=1}^{N} a_n \frac{\exp\left(ik\cos\theta(x - x_n)\right)}{k|\sin\theta|} \exp\left(ik|\sin\theta||y - y_n|\right), \tag{7}$$

$$E_p(x, y) = \sum_{n=1}^{N} a_n \frac{\exp\left(i(k\cos\theta + g_p)(x - x_n)\right)}{h_p} \exp\left(ih_p|y - y_n|\right) \tag{8}$$

where $\theta \in (0, \pi)$, is the incident angle of the plane wave; $\{a_n\}$, n=1..N are the amplitudes of the auxiliary sources, that must be calculated by imposing standard continuity conditions on the surface of the wires within one period in x direction.

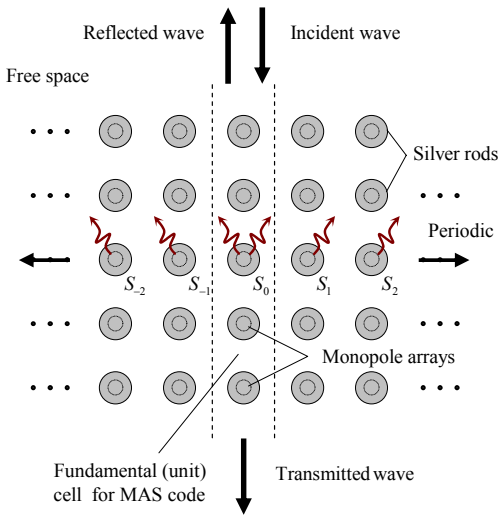


Fig. 6. The PhC filter structure for MAS code.

3) For time-domain methods such as FDTD and FIT [15] the appropriate handling of periodic symmetries becomes simple only for a vertically incident plane wave. One then may introduce electric or magnetic walls in y direction for separating the "fundamental" cell used in the MMP model.

Furthermore, absorbing boundary conditions may be imposed in the areas a) and c) for absorbing the reflected and transmitted waves (see Fig. 7). Consequently, FDTD (and FIT) codes discretize only a finite rectangular area b) like MMP. For the more general case of an obliquely incident plane wave, FDTD becomes more complicate and requires a complex formulation for taking the periodic boundary conditions accurately into account. Incidentally, material dispersion causes additional problems for time-domain codes. In order to avoid the time-consuming evaluation of convolution integrals, material models for dispersive materials are simplified, for example, by the Drude model given above. Despite of its inaccuracy, it is used for the following test case in order to obtain a comparison of MMP-MBPE and MAS-MBPE with commercial FDTD and FIT codes.

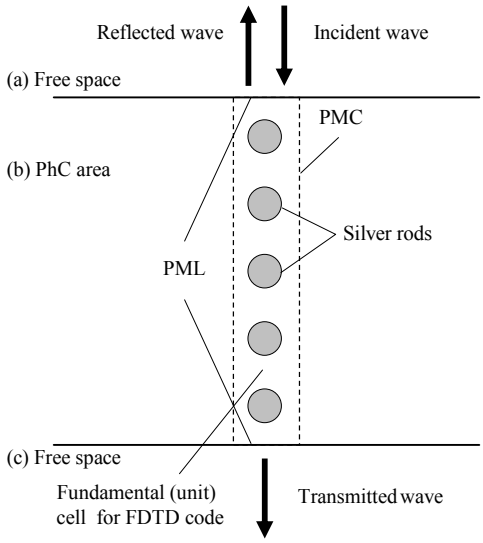


Fig. 7. The PhC filter structure for FDTD code.

IV. NUMERICAL TEST CASE: 2D METALLIC PHC SLAB

Figures 8 and 9 show the transmission characteristics of a PhC filter obtained with the three different methods outlined above. Excellent agreement is observed at sufficiently low frequencies (λ = 1.0 μm to 3.0 μm) (Fig. 8). The maximum difference between MMP brute-force, MMP-MBPE and MAS-MBPE is 0.02 % (there is no observable difference between curves plotted on graphs) and between MMP and FIT it is 0.1 %. For MMP-MBPE

and MAS-MBPE only 20 points were computed by MMP and by MAS, the remaining points were interpolated by MBPE (see Fig. 8, points with triangles). The total computation time for these MBPE solutions was below 1 minute on a PC and 5 minutes for the less accurate FIT solution.

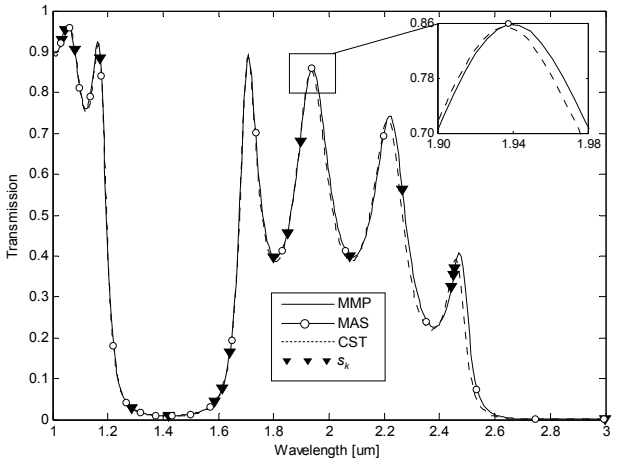


Fig. 8. MMP-MBPE, MAS-MBPE, and CST Microwave Studio (FIT) results of the test case at low frequency range. Only 20 frequency points s_k were computed and the remaining points were interpolated by MBPE.

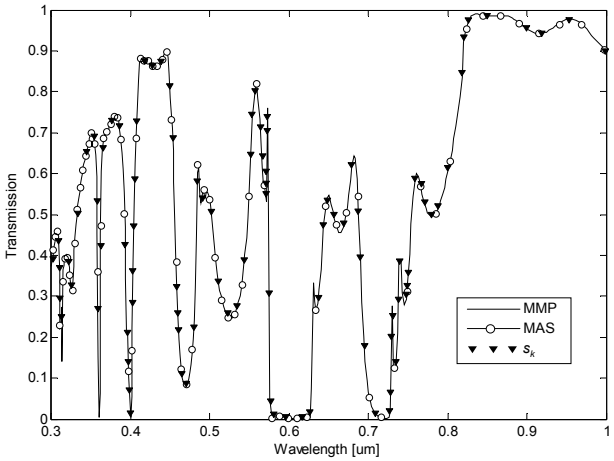


Fig. 9. MMP and MAS results with and without MBPE techniques. The maximum difference between MMP brute-force, MMP-MBPE and MAS-MBPE results is less then 0.02 %. Only 145 frequency points s_k were computed and the remaining points were interpolated by MBPE.

Excellent agreement between MMP and MAS is also observed for higher frequencies (λ = 0.3 μm to 1.0 μm) that cannot be handled correctly with the commercial FIT code (see Fig. 9). Only 145 frequency points were computed and the remaining points were interpolated by MBPE for higher frequency interval, while at least 2000 frequency points were required for getting a smooth curve using MMP or MAS without MBPE technique, i.e. the speed-up factor provided by the MBPE is more than 10.

Note that the computation time for FDTD and FIT codes for the more general case with oblique incidence and more accurate material models would strongly increase the computation time of the time domain codes, whereas it does not increase the computation time of the MMP-MBPE and MAS-MBPE solutions. The near field distribution for PhC filter is shown in Fig. 10.

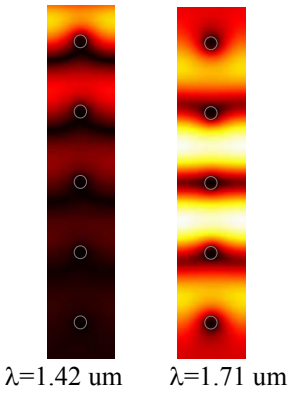


Fig. 10. Near-Filed for PhC filter.

The wavelength dependence of the permittivity (according to the Drude model with solid line and measurement fitting with doted line) is presented in Fig. 11 together with MBPE sample points where the field was evaluated. For long wavelength (λ = 1.0 μm to 3.0 μm) it was sufficient to use 20 sample points and the MBPE domain was not subdivided by the adaptive algorithm.

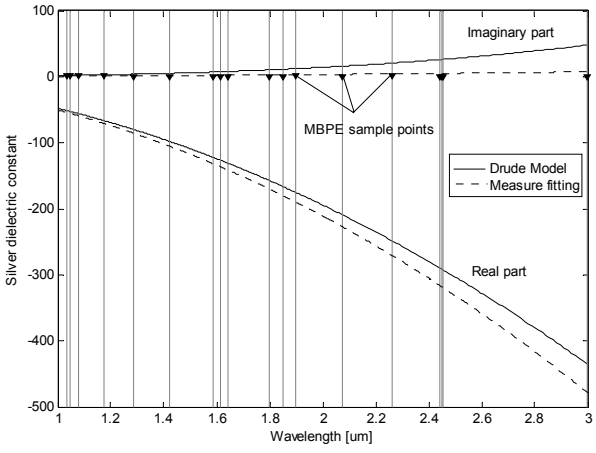


Fig. 11. Silver dielectric constant – Drude model. With vertical grey lines the MBPE sample point locations is plotted.

V. CONCLUSIONS

Adaptive MBPE algorithms may be added to any frequency domain field solver. These algorithms drastically reduce the numerical effort for the accurate computation of the filter response also when dispersive materials are present. It can simultaneously evaluate the frequency response of several observables. For the metallic photonic filter test case, excellent agreement between the MMP-MBPE and MAS-MBPE solutions is observed even at high frequencies, where the commercial FIT solver fails. This solver is outperformed by MMP-MBPE and MAS- MBPE even when simplified models are considered that cause no problems for FDTD and FIT.

VI. ACKNOWLEDGMENT

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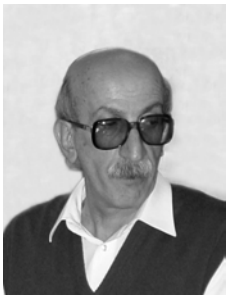

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