MŰEGYETEM 1782

PhD Thesis booklet

Simulation of electromagnetic wave propagation in linear and nonlinear structured dielectrics

Tamás Szarvas

Supervisor: Zsolt Kis, PhD
Wigner Research Center for Physics
Department of Quantum Optics and
Quantum Informatics

Budapest University of Technology and Economics
2020

Introduction

Electromagnetic wave propagation in dielectrical media is influenced by several properties of the material, such as the linear and nonlinear susceptibility, the anisotropy, and the structure. In case of structure dimension is in the range of the wavelength or even finer (photonic crystals and electromagnetic metamaterials), new light propagation phenomenon arise, which cannot be observed in bulk crystals. Such phenomena are for instance the presence of band structure of the light dispersion relation in periodic one-, two-, and three-dimensional crystals, which is analogous with the band structure for electrons in solid crystals. [1,2] Analytical description of the electromagnetic wave propagation, diffraction and scattering is well described, but when the geometry is complex like in photonic crystals, numerical simulations become indispensable [3].

Photonic crystal based devices have been produced for a long time, such as multilayer dielectric mirrors, which are one-dimensional structures. Even though very good optical properties can be achieved using these multilayer dielectric structures, they have some drawbacks. Thermally driven motion of the optical elements gives rise to noise in high-precision interferometers [4], and it turns out that mirrors with multilayer dielectric coating exhibit higher thermal noise than the monolithic ones [5], which are created from the same material by micromachining in the scale of the wavelength. Not only the linear susceptibility can be periodically structured but the second order susceptibility as well: an example to such medium is the Periodically Poled Lithium Niobate (PPLN). With periodic poling quasi phase matching can be obtained in nonlinear processes [6]. Nonlinear Second Harmonic wave Generation (SHG) has been thoroughly examined in one dimension both analytically and numerically. Recently, the application of advanced domain poling techniques enabled the fabrication of two-dimensional (2D) patterns of the sign of the nonlinear coefficient in certain nonlinear crystals, such as $LiNbO_3$ and $LiTaO_3$ [7]. This method can be used to achieve quasi phase matching in SHG and hence amplification of the second harmonic fields in 2D.

Objectives

The purpose of my Ph.D. thesis is on the one hand, the determination of the geometry of a special monolithic, T-shaped grating structures by optimization of the structure dimensions for specific optical properties. The targeted optical devices to be created via optimization could be a broad band mirror, a band filter, or dichroic short- and longpass filters. On the other hand, the other main goal is the development of numerical methods for the simulation of wave propagation in materials with structured second order susceptibility based on linear methods. The methods should describe SHG in a homogeneous crystal, SHG in 2D periodically poled crystals, presence of backward SHG, SHG in materials structured both in the linear and nonlinear susceptibilities, SHG in macroscopic scale.

Scientific achievements

The major achievements of my Ph.D. research are summarized in the following points:

1. I have determined the structure parameters for a couple of specific optical mirrors which are obtained from a T-shaped Surface Relief Grating (SRG) via numerical optimization. First, I have optimized the initial structure to achieve the widest high reflection plateau in the Near-InfraRed (NIR) range subject to the constraint for the narrowest widths of the bottom and top layers constituting the T ridges. Second, a band-pass filter was examined and its parameters were determined. Finally, two kinds of dichroic beam splitters were realized: short- and longpass ones. These mirrors can be applied to steer the propagation of bichromatic laser fields, e.g. with wavelengths 1310 and 1550 nm, in experiments where the higher thermal noise of the more traditional multilayer dielectric mirrors is not acceptable. [P1]

2. I have extended the linear Finite Difference Frequency Domain (FDFD) method to second order nonlinear media, showing that Second Harmonic Generation (SHG) can also be simulated with the Non-Linear FDFD (NL-FDFD) method. For the case of 3m symmetry of the underlying crystal lattice (e.g. $\mathrm{LiNbO_3}$), the structure of the nonlinear tensor was shown to allow for a two dimensional simulation. In order to simulate SHG process in a two-dimensional structure, I introduced two Yee-meshes for the fundamental and second harmonic fields, respectively. The Maxwell's equations for the Fundamental Wave (FW) and Second Harmonic Wave (SHW) were discretized on the appropriate mesh. I have also worked out the general formulation for the three-dimensional case with arbitrary symmetry of the d_{ijk} tensor. Undepleted SHG was simulated in a homogeneous nonlinear crystal and the obtained conversion efficiency was shown to compare remarkably well with the analytical value. A similar result was obtained for SHG with pump depletion in a 1D Periodically Poled Lithium Niobate (PPLN) crystal as well. I also carried out true two-dimensional simulations to demonstrate the capabilities of the method in higher dimensions. For real two-dimensional structures of one- or fivefold cylinder arrays with periodic variation of both the linear and the nonlinear susceptibilities, I have shown that the reflection spectra, the normalized reflectivity power of SHW and also the E_z field structure calculated at the resonance frequency, are in good agreement with results reported in [8] using a semi-analytical method. [P2]

3. I showed how the pseudospectral method can be applied to the FDFD method resulting a new method called Pseudo Spectral Frequency Domain (PSFD) method.

This new method gives much more accurate approximation of the analytical derivatives compared to the standard FDFD method. In order to show this, the relative numerical phase velocity values obtained from simulation results were plotted together with the analytical curve for axial and diagonal directions of the simulational grid. Next the Non-Linear PSFD (NL-PSFD) method was presented and compared to NL-FDFD method by simulating a homogeneous nonlinear crystal. For comparison I have examined how the numerical coherence length and maximum conversion efficiency value depend on the sampling density. NL-PSFD method exhibits better accuracy in general, similar accuracy can be reached in NL-FDFD method by using 6-8 times finer grid. I have introduced the implementation of oblique incidence source for PSFD method. The correctness of this procedure is demonstrated by simulating a tilted nonlinear Quasi Phase Matched (QPM) grating in two ways: first, QPM grating was tilted and the wave vector of the FW was parallel to x axis of the simulation domain, second, FW has oblique incidence and QPM grating was parallel to the x axis of the simulation domain. I have calculated the conversion efficiency for both cases and compared them with each other and with the analytical solution as well: all three curves are shown, they overlap very well. The angle between the Poynting vector of SHW and the grating boundaries is compared for both cases together with the expected theoretical value, again, the simulation results provide identical solutions which agrees with the theoretical one. [P3]

4. I have introduced a specific method derived from NL-PSFD method for large volume simulation when only the second order nonlinearity is structured spatially. In this method the core matrix is not scaled up to a large sparse matrix (like in the FDFD and PSFD methods) but kept in the same size as the simulation area, the resulted matrix equation is Sylvester type, thus we denote the method as NL-PSFD-SYLV, and the solution is obtained by iterations with the modified conjugate gradient method. The efficiency of this method in large scale simulation is illustrated by simulation of a real, two-dimensional nonlinear photonic crystal. Nonlinear interaction occurs in non-collinear way, via the $\mathbf{G}_{01}$ Fourier component of $\chi^{(2)}(\mathbf{r})$. Phase matching criteria is calculated for the selected wavelength (1500 nm), and so the angle of incidence is determined for FW and the expected angle of generated SHW too. Direction of propagation of SHW is calculated from the Poynting vector and compared to the analytical results, after 10 μm of propagation, the wavefront takes the direction of phase matching condition. Conversion efficiency is also calculated from the Poynting vector, and compared to the analytical solution, where the numerical solution is in good agreement with the theoretical expectations. [P3]

List of publication

Major publications related to thesis points

[P1] T. Szarvas and Zs. Kis. ”Optimization of a T-shaped optical grating for specific applications.” *Optical Engineering*, **55**(7): 077103 (2016).

[P2] T. Szarvas and Zs. Kis, ”Numerical simulation of nonlinear second harmonic wave generation by the finite difference frequency domain method.” *Journal of the Optical Society of America B*, **35**(4): 731–740 (2018).

[P3] T. Szarvas and Zs. Kis, ”Application of pseudospectral method to the finite difference frequency domain method.” *Journal of the Optical Society of America B*, **36**(2): 333–345 (2019).

Further publications and conferences

[P4] T. Szarvas and Zs. Kis, ”Simulation of wave propagation in periodically structured dielectrics.” In ”Kvantumelektronika 2014: VII. Szimpózium a hazai kvantumelektronikai kutatások eredményeiről,” (2014).

[P5] T. Szarvas and Zs. Kis, ”Optimization of surface relief grating for band filter application by numerical simulation.” In ”17th International Conference on Transparent Optical Networks (ICTON),” (2015).

[P6] T. Szarvas and Zs. Kis, ”Optical simulation of monolithic grating structure.” In ”Mesterpróba 2015” (2015).

[P7] T. Szarvas and Zs. Kis, ”Simulation of second harmonic wave generation by extended Finite Difference Frequency Domain method.” In ”International OSA Network of Students (IONS) Balvanyos 2017,” (2017).

[P8] T. Szarvas and Zs. Kis, ”Simulation of electromagnetic wave propagation in structured dielectrics.” In ”Wigner Research Centre for Physics Seminar,” (2018).

[P9] T. Szarvas and Zs. Kis, ”Másodharmonikus keltés numerikus modellezése az FDFD módszer kiterjesztésével.” In ”Kvantumelektronika 2018: Szimpózium a hazai kvantumelektronikai kutatások eredményeiről,” (2018).

[P10] T. Szarvas and Zs. Kis, ”Simulation of nonlinear photonic crystals by modified finite difference frequency domain method.” In ”Frontiers in Optics / Laser Science,” (2018).

References

[1] I. A. Sukhoivanov and I. V. Guryev. *Photonic Crystals - Physics and Practical Modeling*. Springer Series in Optical Sciences (2009).

[2] A. R. McGurn. *Nonlinear Optics of Photonic Crystals and Meta-Materials*. Morgan & Claypool Publishers (2015).

[3] T. Rylander, P. Ingelström, and A. Bondeson. *Computational Electromagnetics*. Springer (2005).

[4] V. Braginsky, M. Gorodetsky, and S. Vyatchanin. "Thermodynamical fluctuations and photo-thermal shot noise in gravitational wave antennae." *Physics Letters A*, **264**: 1–10 (1999).

[5] G. M. Harry, A. M. Gretarsson, P. R. Saulson, et al. "Thermal noise in interferometric gravitational wave detectors due to dielectric optical coatings." *Classical and Quantum Gravity*, **19**: 897–917 (2002).

[6] R. Boyd. *Nonlinear Optics 3rd Edition*. Elsevier, Academic Press (2008).

[7] M. Manzo, F. Laurell, V. Pasiskevicius, et al. "Two-dimensional domain engineering in LiNbO3 via a hybrid patterning technique." *Optical Materials Express*, **1**(3): 365–371 (2011).

[8] L. Yuan and Y. Y. Lu. "Analyzing second harmonic generation from arrays of cylinders using Dirichlet-to-Neumann maps." *Journal of the Optical Society of America B*, **26**(4): 587–594 (2009).