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Ph.D. Thesis booklet

Simulation of electromagnetic wave propagation in linear and nonlinear structured dielectrics

Tamás Szarvas

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

Budapest University of Technology and Economics

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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 geometry of the structure. In case of the size of the structure is in the range of the wavelength or even finer (photonic crystals and electromagnetic metamaterials), new light propagation phenomena arise, which cannot be observed in bulk crystals. Such phenomenon is for instance the presence of a band structure in 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 unavoidable [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. With periodic poling quasi phase matching can be obtained in nonlinear processes [6]. Nonlinear second harmonic wave generation 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 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 and hence amplification of the second harmonic fields in two dimensions.

Objectives

One purpose of my Ph.D. thesis is the determination of the geometry of special, monolithic, T-shaped grating structures by optimization of those geometrical parameters to achieve the desired optical properties. The targeted optical devices to be created via optimization could be a broadband mirror, a bandpass filter, or dichroic short- and longpass filters. Another goal is the development of numerical methods for the simulation of wave propagation in spatially structured second harmonic crystals. The method(s) should describe Second Harmonic Generation (SHG) in a homogeneous crystal, in two-dimensional periodically poled crystals, in materials structured both in the linear and nonlinear susceptibilities. It is desired to include the presence of backward SHG, to handle pump depletion, and to describe SHG in macroscopic scale.

Scientific achievements

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

1. I have determined the structure parameters for a number of basic optical devices derived from a T-shaped surface relief grating via numerical optimization. Aimed first at a mirror, I have optimized the initial grating structure to achieve the widest high reflection plateau in the near-infrared range subject to the constraint for the narrowest widths of the bottom and top layers constituting the T-shaped ridges. Second, a bandpass filter was designed; its parameters were determined for a center wavelength of 1550 nm. Finally, two kinds of dichroic beamsplitters were realized: a short- and a longpass one. [P1]

2. I have extended the linear Finite Difference Frequency Domain (FDFD) method to second order nonlinear media, showing that second harmonic generation can be simulated with the NonLinear Finite Difference Frequency Domain (NL-FDFD) method. I have worked out the general formulation for the two-dimensional case with 3m symmetry of the d_{ijk} tensor, and also for the three-dimensional case with arbitrary symmetry of the d_{ijk} tensor. I have simulated a homogeneous nonlinear crystal and a 1D periodically poled lithium niobate crystal and the obtained conversion efficiencies were shown to compare remarkably well with the analytical values. I have examined two-dimensional resonant waveguide grating 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 the Second Harmonic Wave (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 in a new method called PseudoSpectral Frequency Domain (PSFD) method. I have worked out the NonLinear PseudoSpectral Frequency Domain (NL-PSFD) method and compared it to the NL-FDFD method. I have introduced the implementation of an oblique incidence source for the PSFD method. I have calculated the conversion efficiency and the angle of the generated SHW of a tilted nonlinear quasi phase matched grating in two variants: by normal incidence on a slanted structure and by oblique incidence on the same structure but oriented in the axial direction, and validated the results by direct comparison to each other and to the analytical solution. [P3]

4. I have introduced a specific method derived from the NL-PSFD method for large volume simulation, where the linear susceptibility tensor may show special spatial structure or be homogeneous. I have shown that in this method the core matrix, instead of being scaled up to a large sparse matrix (like in the FDFD and PSFD methods), can be kept in the same size as the simulation area. The resulting matrix equation in the obtained NL-PSFD-SYLV method was shown to be of Sylvester type and has been solved by iteration using the modified conjugate gradient method. I have simulated a real, two-dimensional nonlinear photonic crystal of periodically poled cylinders in a centered rectangular lattice, where the nonlinear interaction occurs non-collinearly via the first Fourier component of the second order nonlinear tensor. I have calculated the angle of incidence of the fundamental wave for phase matching as well as the expected angle of the generated SHW. From the simulational result I have determined the direction of propagation of the SHW and also the conversion efficiency, both of which agree with the theoretical expectations. [P3]

List of publications

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).

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[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).