PROCEEDINGS OF SPIE

Opto-Ireland 2005

Photonic Engineering

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Dublin, Ireland

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Published by
SPIE—The International Society for Optical Engineering

Volume 5827

**The International Society
for Optical Engineering**

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Please use the following format to cite material from this book:

Author(s), "Title of Paper," in *Opto-Ireland 2005: Photonic Engineering*, edited by Brian W. Bowe, Gerald Byrne, Aidan J. Flanagan, Thomas J. Glynn, Jonathan Magee, Gerard M. O'Connor, Ronan F. O'Dowd, Gerard D. O'Sullivan, John T. Sheridan, Proceedings of SPIE Vol. 5827 (SPIE, Bellingham, WA, 2005) page numbers.

ISSN 0277-786X
ISBN 0-8194-5812-0

Published by
SPIE—The International Society for Optical Engineering
P.O. Box 10, Bellingham, Washington 98227-0010 USA
Telephone 1 360/676-3290 (Pacific Time) · Fax 1 360/647-1445
<http://www.spie.org>

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Printed in the United States of America.

Finite difference time domain method (FDTD) to predict the efficiencies of the different orders inside a volume grating

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ABSTRACT

Different electromagnetic theories have been applied in order to understand the interaction of the electromagnetic radiation with diffraction gratings. Kogelnik's Coupled Wave Theory, for instance, has been applied with success to describe the diffraction properties of sinusoidal volume gratings. Nonetheless the predictions of Kogelnik's theory deviate from the actual behaviour whenever the hologram is thin or the refractive index is high. In these cases, it is necessary to use a more general Coupled Wave Theory (CW) or the Rigorous Coupled Wave Theory (RCW). Both of these theories allow for more than two orders propagating inside the hologram. On the other hand, there are some methods that have been used long in different physical situations, but with relatively low application in the field of holography. This is the case of the finite difference in the temporal domain (FDTD) method to solve Maxwell equations. In this work we present an implementation of this method applied to volume holographic diffraction gratings.

Keywords: Holography; Volume gratings, diffraction gratings.

1. INTRODUCTION

During the last years there has been an increasing interest in studying materials for data storage applications¹. In particular, photopolymers are considered one of the most interesting materials² for holographic data storage applications. Their acceptable energetic sensitivity, a variable spectral sensitivity depending on the sensitizer dye used, good resolution, high diffraction efficiency and good signal/noise ratio, imply that these materials have great potential in developing holographic memories, but it's their low price, easy preparation and self-processing properties make them even more attractive for use on a large scale in read only WORM (write once read many) type memories. Therefore, it is important to completely understand these materials, both experimentally and theoretically. In addition, the mechanism of hologram formation in these materials and the interaction of the electromagnetic radiation with the recorded hologram must be understood if these materials are to be implemented.

Although there is a great understanding of how light propagates inside different periodic structures, the field of study of electromagnetic theories to accurately predict the behavior of waves inside volume holograms is still interesting. A usual way to calculate the efficiencies of the different orders that propagate in the volume grating is to solve Maxwell equations for the case of an incident plane wave on a medium which the relative dielectric permittivity varies in^{3,4}. Although the idea seems clear and precise, there are in the literature a great number of models that allow solving the problem.

The most popular Theory in holography that has provided an analytical solution for the efficiency of the first and zero order is the Coupled Wave Theory of Kogelnik⁵. During decades researchers in the field of Holography have used the analytical expressions deduced by Kogelnik to estimate the theoretical predictions of phase and amplitude, transmission and reflection volume holograms. Kogelnik assumed that only two orders propagated in the hologram, orders zero and +1, and obtained analytical solutions for the efficiencies of the first and zero order when a plane wave impinges on a diffraction grating with a sinusoidal variation of its electro-optical properties (relative dielectric permittivity and

conductivity). The highly predictive character of the expressions derived by Kogelnik made his work one of the most cited by holographic researchers. Nonetheless Kogelnik's theory assumed some approximations that make it inaccurate for some cases, such as dielectric gratings that are not sinusoidal or for thin gratings (outside the Bragg regime). In these cases more rigorous theories are needed, such as the rigorous coupled wave theory proposed by Moharam and Gaylord⁶. Since the first introduction of the Rigorous Coupled Wave Theory (RCWT) to predict the efficiency of the different orders that propagate inside a hologram, a lot of advances have been done in the research of electromagnetic theory applied to periodic structures⁷⁻¹¹. The Rigorous Coupled Wave Theory has been applied with success to volume holograms¹² photonic band structures¹³, diffractive lenses¹⁴, etc. Nonetheless, in lots of applications the finite size of the gratings should be taken into consideration¹⁵. Moreover the RCW is usually studied for the incidence of a perfect plane wave into the grating, if gratings have limited spatial aperture and are illuminated by finite-width beams other methods are needed. In this work we discuss on a finite difference time domain (FDTD) method to solve Maxwell's equations in the periodic medium. The FDTD method has raised much attention for application in engineering problems in the last decades¹⁶⁻²⁰. It has also received attention in optics²¹⁻²². Although the method was included by H. Ichikawa²³ in the study of dielectric gratings, his approach didn't include some advancements in the theory of the FDTD that improve the performance of the algorithm.

Parallel to the improvements in the electromagnetic theory applied to periodic structures, the application and models of photopolymer materials for the recording of high quality diffraction elements has also seen important developments. New theoretical models that permit a deeper understanding of the mechanism of hologram formation in photopolymer materials have been proposed. Since the polymerisation driven diffusion (PDD) model proposed by Zhao et al.²⁴ several new models have been presented which give a clearer understanding of the hologram formation mechanisms in photopolymers²⁵⁻³². For example, the non-local polymerisation driven diffusion (NPDD) model proposed by Sheridan and co-workers²⁹⁻³¹, explains more experimental facts, such as the cut-off of diffraction efficiency for high spatial frequencies. Based on the ideas of a non-local behavior of the photopolymer, but using a finite-difference method to solve the basic diffusion equations, instead of a Fourier expansion of the monomer and polymer concentrations, S. Wu and E. N. Glysts³² analyzed mechanism of hologram formation in photopolymer materials. A finite difference approach to solve Maxwell equations seems also the adequate method to be combined with the finite difference method of solution of the diffusion equation.

2. THE FDTD METHOD FOR TE POLARIZATION

In this section we will explain the basic assumptions of the FDTD method to study the propagation of light inside a phase sinusoidal transmission grating (figure 1), where the relative permittivity in the hologram can be expressed as:

$$\epsilon_r = \epsilon_{r0} + \epsilon_{r1} \cos(Ky) \quad (1)$$

ϵ_{r0} is the average dielectric constant, ϵ_{r1} the amplitude of the relative permittivity and $\mathbf{K}$ is the grating vector, which is related to the period of the interference fringes, Λ , as follows:

$$|\mathbf{K}| = 2\pi/\Lambda \quad (2)$$

For TE polarization the electric field is assumed to be polarized in the z direction, whereas the periodic structure is supposed to lie in the xy plane. In this case Maxwell equations can be expressed in the form:

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu_0} \left(-\frac{\partial E_z}{\partial y} \right) \quad (3)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_z}{\partial x} \right) \quad (4)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) \quad (5)$$

Where μ_0 is the magnetic permeability of the freespace and ϵ is the dielectric permittivity of the periodic medium which is related to the free space permittivity and the relative dielectric permittivity of equation (1) by:

$$\epsilon = \epsilon_0 \epsilon_r \quad (6)$$

Fig.1 Dielectric grating and axis conventions for TE polarization.

The finite difference expressions of equations (3)-(6) are¹⁶:

$$H_x|_{i,j}^{n+1/2} = H_x|_{i,j}^{n-1/2} + \frac{\Delta t}{\mu_{i,j}\Delta} (E_z|_{i,j-1/2}^n - E_z|_{i,j+1/2}^n) \quad (7)$$

$$H_y|_{i,j}^{n+1/2} = H_y|_{i,j}^{n-1/2} + \frac{\Delta t}{\mu_{i,j}\Delta} (E_z|_{i+1/2,j}^n - E_z|_{i-1/2,j}^n) \quad (8)$$

$$E_z|_{i,j}^{n+1} = E_z|_{i,j}^n + \frac{\Delta t}{\epsilon_{i,j}\Delta} \left(H_y|_{i+1/2,j}^{n+1/2} - H_y|_{i-1/2,j}^{n+1/2} + H_x|_{i,j-1/2}^{n+1/2} - H_x|_{i,j+1/2}^{n+1/2} \right) \quad (9)$$

Where Δt is the time increment, Δ the lattice space increments in the x and y directions, μ_{ij} and ϵ_{ij} stands for the value of the magnetic permeability and the dielectric permittivity at cell i,j of the grid. For the case studied μ_{ij} is constant in all points with value μ_0 and ϵ_{ij} is obtained by using expression (1) where the y values are calculated by:

$$y = n\Delta \quad (10)$$

n, being an integer.

3. TOTAL AND SCATTERED FIELD. CONNECTING CONDITION

The total-field/scattered-field formulation will be used to implement the FDTD method. The approach is based on the linearity of Maxwell's equations¹⁶. The electric and magnetic field can be decomposed as follows:

$$\vec{E}_{tot} = \vec{E}_{inc} + \vec{E}_{scat} \quad (11)$$

$$\vec{H}_{tot} = \vec{H}_{inc} + \vec{H}_{scat} \quad (12)$$

$\vec{E}_{inc}$ and $\vec{H}_{inc}$ are the incident field values that would exist in vacuum if there were no materials in the space. $\vec{E}_{scat}$ and $\vec{H}_{scat}$ correspond to the scattered field values, that is the fields that result from interaction between the incident field and the materials that will be modelled.

The grid is divided in two zones region 1 and region 2. In region 1, the total-field region, the values of the total electric and magnetic fields are calculated by means of the Yee algorithm described in section 2. In region 2, the scattered-field region, the values of the scattered electric and magnetic fields are now calculated.

In figure 2 the two dimensional grid used for the simulation of the dielectric grating is presented, where regions 1 and 2 are depicted. The region where the ABC that will be explained in section 4 is also presented in the figure.

Fig.2 Divission of the grid in total and scattered field regions. The ABC zone is also presented.

As can be seen in the figure there is a limiting interface between regions 1 and 2. In the nearest points to this interface, care must be taken if the total field or scattered field values are calculated by using the finite difference expression, since this expression involves simultaneously the evaluation of a total field value and a scattered field one. As explained by Taflove et al.¹⁶ in the limiting surface the input values of an incident plane wave can be calculated. To do this the electric and magnetic field values of a one-dimensional wave can be obtained by using the finite difference process. If the electric field value is known at m_{0-2} , for instance, the magnetic and electric field values are calculated by using the finite-difference expressions:

$$E_{inc}|_{m_0-2}^n = E_0 \sin\left(\frac{2\pi}{\lambda} n\Delta t\right) \quad (13)$$

$$H_{inc}|_{m+1/2}^{n-1/2} = H_{inc}|_{m+1/2}^{n-1/2} + \frac{\Delta t}{\mu_0 \Delta \left[\frac{v_p(0)}{v_p(\phi)} \right]} \left(E_{inc}|_m^n - E_{inc}|_{m+1}^n \right) \quad (14)$$

$$E_{inc}|_m^{n+1} = E_{inc}|_m^n + \frac{\Delta t}{\epsilon_0 \Delta \left[\frac{v_p(0)}{v_p(\phi)} \right]} \left(H_{inc}|_{m-1/2}^{n+1/2} - H_{inc}|_{m+1/2}^{n+1/2} \right) \quad (15)$$

Where the factor $\left[\frac{v_p(0)}{v_p(\phi)} \right]$ is included to correct the values in order to take into account propagation of a wave forming

an angle ϕ with the x axis. Figure 3 shows how the values of the fields at the different points of the limiting surface can be calculated. On the other hand in figures 4 and 5 two numerical simulations corresponding to a plane wave forming an angle of 20° with the x axis and another forming an angle of 45° are presented. Since no media exist in the grid, it is interesting to observe how the waves are confined in the total field region, no electric field is presented in the scattered field zone.

Fig 3. Implementation of the connecting condition

Fig 4. Confinement of plane waves in the total field region for a plane wave forming an angle of 20° with the x axis.

Fig 5. Confinement of plane waves in the total field region for a plane wave forming an angle of 45° with the x axis.

4. IMPLEMENTING THE ABSORBING BOUNDARY CONDITION

One of the problems associated with FDTD codes is that the grid used for the simulation has a finite size. This implies that in order to simulate open regions some artificial tricks must be introduced¹⁶. That is, we want to find a suitable boundary condition to simulate the extension to infinity of the outer perimeter of the grid. Several absorbing boundary conditions (ABC's) are used in the literature. In this case we have decided to use an artificial absorbing medium situated in the perimeter of the computational space. To analyze the effect of this artificial medium we will firstly consider Maxwell's equations for TE polarization for lossy media:

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left(-\frac{\partial E_z}{\partial y} - \sigma^* H_x \right) \quad (16)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left(\frac{\partial E_z}{\partial x} - \sigma^* H_y \right) \quad (17)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right) \quad (18)$$

Where ε and μ are the dielectric permittivity and magnetic permeability of the medium, and σ and σ^* correspond to the electric conductivity and magnetic loss of the medium. We now assume that the lossy medium is the free-space with some lossy properties added to it. Therefore, $\varepsilon = \varepsilon_0$ and $\mu = \mu_0$. Now, if the following condition is satisfied:

$$\frac{\sigma}{\varepsilon_0} = \frac{\sigma^*}{\mu_0} \quad (19)$$

no reflection occurs when a plane wave coming from free-space impinges normal to the lossy medium artificially created. Therefore, light is absorbed by the artificial medium with no reflection

Now the finite-difference expressions of equations (16)-(18) are:

$$H_x|_{i,j}^{n+1/2} = e^{-\frac{\sigma^* \Delta t}{\mu_0}} H_x|_{i,j}^{n-1/2} + \frac{1}{\sigma^* \Delta} \left(1 - e^{-\frac{\sigma^* \Delta t}{\mu_0}} \right) (E_z|_{i,j-1/2}^n - E_z|_{i,j+1/2}^n) \quad (20)$$

$$H_y|_{i,j}^{n+1/2} = e^{-\frac{\sigma^* \Delta t}{\mu_0}} H_y|_{i,j}^{n-1/2} + \frac{1}{\sigma^* \Delta} \left(1 - e^{-\frac{\sigma^* \Delta t}{\mu_0}} \right) \left(E_z|_{i+1/2,j}^n - E_z|_{i-1/2,j}^n \right) \quad (21)$$

$$E_z|_{i,j}^{n+1} = e^{-\frac{\sigma^* \Delta t}{\epsilon_0}} E_z|_{i,j}^n + \frac{1}{\sigma^* \Delta} \left(1 - e^{-\frac{\sigma^* \Delta t}{\mu_0}} \right) \left(H_y|_{i+1/2,j}^n - H_y|_{i-1/2,j}^n + H_x|_{i,j-1/2}^{n+1/2} - H_x|_{i,j+1/2}^{n+1/2} \right) \quad (22)$$

To analyze the effects of the medium artificially created, we will study the propagation of a wave generated by a sinusoidal source. Figures 6-8 show the numerical simulations for a wave generated by a sinusoidal source of wavelength $\lambda = 0.633$ nm. The space increment was chosen to be $\Delta = \lambda/10$ and the time increment as $\Delta t = \Delta/c$, where c is the speed of light in free space. In figure 6 the simulation was stopped for a number of time steps of $n = 46$, whereas in figures 7 and 8 the final time step was 306. In figure 7 no ABC was implemented and the effect of the reflected waves from the boundaries can be clearly observed, whereas in figure 8 no interference between forward and backward waves is seen, due to the implement of the ABC governed by equations 16-18.

Fig 6. Numerical simulation of a wave generated by a sinusoidal source of wavelength $\lambda = 0.633$ nm. The number of time steps was $n = 46$;

Fig 7. Numerical simulation of a wave generated by a sinusoidal source of wavelength $\lambda = 0.633$ nm. The number of time steps was $n = 306$. No ABC is included.

Fig 8. Numerical simulation of a wave generated by a sinusoidal source of wavelength $\lambda = 0.633$ nm. The number of time steps was $n = 306$. An ABC is included.

5. NUMERICAL SIMULATIONS FOR A TRANSMISSION DIFFRACTION GRATING

In this section the numerical results using the implementation of the FDTD code explained in the preceding sections will be shown for the analysis of a transmission diffraction grating of 1200 lines/mm. The refractive index modulation was chosen to be of $n_1 = 0.025$ which corresponds to typical values of the refractive index modulation for some materials, such as photographic emulsions, used to record holographic gratings. Figure 9 shows the situation after a plane wave has impinged onto the grating. In order to observe the output fields a region just near the grating was chosen. Finally it is expected that the interference of two plane waves, the transmitted plane wave and the diffracted one, must be observed in this region.

Fig 9. Situation after a plane wave has impinged onto the grating.

Fig 10. Numerical simulation of the output fields for a transmission grating of 1200 lines/mm after a plane wave has incided onto the medium at Bragg angle. No grating is presented.

Figure 10 show the numerical simulated output fields for a transmission grating of 1200 lines/mm after a plane wave has incided onto the medium at Bragg angle. No grating is presented in this case, and it can be seen that the plane wave is transmitted without diffraction. Figures 11-13 show now the numerical simulated output fields for gratings of different thickness, where the interference of the transmitted and diffracted waves is observed in all cases.

Fig 11. Numerical simulation of the output fields for a transmission grating of 1200 lines/mm after a plane wave has incided onto the medium at Bragg angle. A grating of $1.5\ \mu\text{m}$ thick and $n_1 = 0.025$ is presented in this case.

Fig 12. Numerical simulation of the output fields for a transmission grating of 1200 lines/mm after a plane wave has incided onto the medium at Bragg angle. A grating of $4.7\ \mu\text{m}$ thick and $n_1 = 0.025$ is presented in this case.

Fig 13. Numerical simulation of the output fields for a transmission grating of 1200 lines/mm after a plane wave has incident onto the medium at Bragg angle. A grating of $7.9\ \mu\text{m}$ thick and $n_1 = 0.025$ is presented in this case.

6. CONCLUSIONS

In this work an implementation of the finite difference time domain (FDTD) method to solve Maxwell equations for holographic transmission gratings has been presented. The algorithm presented extends the ideas of total-scattered field and absorbing boundary conditions to improve the computation of the output electric fields. In particular, an ABC corresponding to an artificial absorbing medium with the same dielectric permittivity and magnetic permeability of the free space has been analyzed for the proposed code. The results presented show that the implemented ABC is adequate for the present algorithm. Numerical results have also been presented for the simulation of the electromagnetic radiation inside a transmission diffraction grating of 1200 lines/mm and a refractive index modulation of $n_1 = 0.025$. The results show that the expected interference pattern caused by the transmitted and the diffraction orders is present at the output of the grating. These preliminary results also show that the implementation of an FDTD code with ABC for diffraction gratings permits the evaluation of the electric field for every instant of time and can be applied to more complex structures and situations.

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