ANALYSIS OF PERIODIC STRUCTURES USING RCWA

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Received 30 April 2012; accepted 03 May 2012

1. Introduction

The work is focused on the rigorous analysis of periodic structures that exhibit diffraction of electromagnetic (EM) waves in the visible domain considering both the polarisation states TE and TM. Based on this rigorous coupled wave analysis (RCWA) using Maxwell's equations a numerical simulation program has been developed and implemented. The transfer matrix method was implemented in the course of solving numerical problems. It was necessary to solve numerical problems of quasi-singular matrices, which are caused by exponentially growing amplitudes of evanescent waves. Diffraction efficiencies of various gratings (lamellar grating, volume phase grating, relief grating with sinusoidal profile) were calculated. An experimental method for determining the parameters of the surface grid was proposed and developed.

RCWA was first introduced by Magnusson and Gaylord [1] and then developed further by Moharam and Gaylord [2], enhanced with matrix formulation by Moharam *et al.* [3]. Later, several improvements were implemented by Li [4-5].

In Section 2 we briefly revise the basic formulae of RCWA applied to lamellar gratings for modelling wave propagation through such a periodic structure. In Section 3 transmission diffraction efficiency of various periodic structures is constructed. An inverse problem is formulated for determining the groove depth of relief surface grating.

2. Problem formulation

First, we formulate RCWA for a lamellar grating, which is infinitely extended in the *y* and *x* direction. It has a finite thickness in the *z* direction, thus, a planar monochromatic electromagnetic (EM) wave *o* with wavelength λ propagates in that direction in the plane *x-z* (Fig. 1).

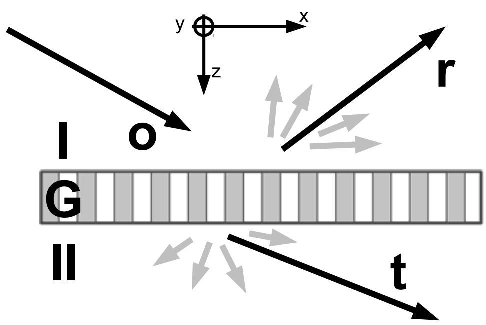


Fig. 1*: Scheme of the lamellar grating with diffracted planar electromagnetic wave*

The grating is periodic in the *x* direction with spatial period *p*. Because of the symmetrical geometry the vectors of the electric field for TE polarisation (vector of electric field lies in the plane *x-y*) and the magnetic field for TM polarisation (vector of magnetic field lies in the plane *x-y*) can be simplified as

$$\mathbf{E} = (0, E, 0) \tag{1}$$

$$\mathbf{H} = (0, H, 0) \tag{2}$$

Then starting from Maxwell's equations, Helmholtz equations can be derived for both TE (3) and TM polarisation (4).

$$\Delta E = -\varepsilon\mu k^2 E + \frac{1}{\mu}\frac{\partial E}{\partial x}\frac{\partial \mu}{\partial x} \tag{3}$$

$$\Delta H = -\varepsilon\mu k^2 H + \frac{1}{\varepsilon}\frac{\partial H}{\partial x}\frac{\partial \varepsilon}{\partial x} \tag{4}$$

All fields can be are expressed in Fourier series form

$$F(x,z) = \sum_s f_s(z)\mathrm{e}^{\mathrm{i}k_{xs}x} \tag{5}$$

where F stands for E or H and k_{xs} is the x-component of the wave vector given by Floquet's theorem

$$k_{xs} = k_{x0} + \frac{2\pi}{p}s \tag{6}$$

Relative permittivity, permeability and their inverse functions are Fourier decomposed in the same way.

Then the Helmholtz equations are solved in each region above (I), inside (G) and below (II) the thin grating. Solutions of Eq. (3), (4) are

$$f_s^I = r_s \mathrm{e}^{-\mathrm{i}k_{zs}^I z} \tag{7}$$

$$f_s^G = Q_{st}\left[q_t^1 \mathrm{e}^{-\mathrm{i}\sqrt{l_t}z} + q_t^2 \mathrm{e}^{\mathrm{i}\sqrt{l_t}z}\right] \tag{8}$$

$$f_s^{II} = t_s \mathrm{e}^{\mathrm{i}k_{zs}^{II} z} \tag{9}$$

where the matrix Q_{st} couples diffraction orders of the diffracted planar waves and l_t are the eigennumbers of Q_{st}. Using continuity of field vectors at interfaces between layers a transfer matrix M_{st} can be formulated which determines the amplitudes of the reflection and transmission coefficients r_s and t_s.

$$\begin{pmatrix} r_s \\ o_s \end{pmatrix} = M_{st}\begin{pmatrix} t_s \\ 0 \end{pmatrix} \tag{10}$$

Here a special renormalization method is implemented to avoid numerical instabilities caused by exponentially growing amplitudes [6].

3. Results

3.1 Diffraction on volume phase grating

Diffraction efficiencies (defined by the ratio of the intensity of the diffracted light beam to the incident beam intensity in the z direction) of a thick hologram is presented. The very first theoretical model of this phenomenon was made by Kogelnik [7]. Phase hologram can be treated as a binary grating with nonzero coefficients of the -1st, 0th and 1st orders of Fourier series of spatial permittivity and permeability, respectively. In Fig. 2 diffraction efficiency of volume phase grating versus angle of incidence is presented. The thickness of the simulated grating was 5 µm with spatial period 1075 nm. The main index of refraction of the grating is 1.2 with sinusoidal space modulation of 0.05. One can observe the maximum efficiency of the first diffracted order at Bragg's angle at point 0.31 which is theoretically also given by Eq. (11).

$$\sin\varphi_{Bragg} = \frac{\lambda}{2p} \tag{11}$$

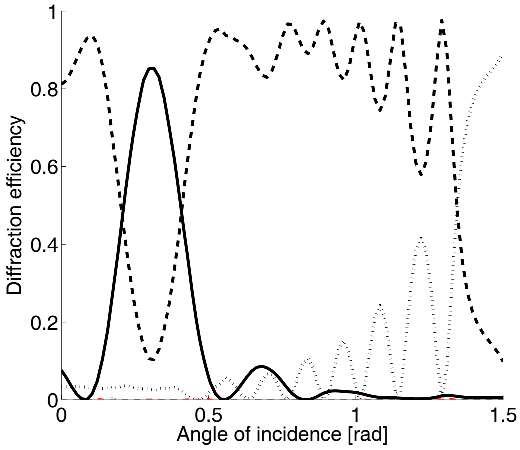
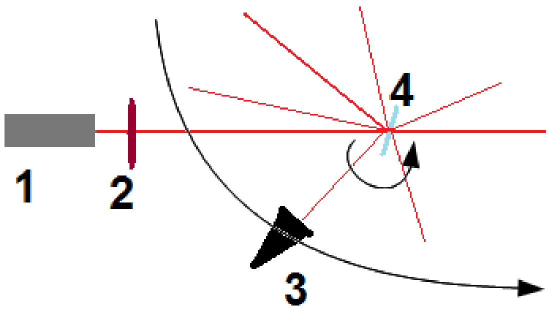


Fig. 2: *Diffraction efficiency of the 1st transmitted (continuous line), 0th transmitted (dashed line) and 0th reflected (dotted line) diffraction orders. Complementarity of orders can be observed. Wavelength of the incident planar EM wave is 650 nm*

3.2 Determining the groove depth of surface relief grating with sinusoidal profile

Relief gratings with arbitrary profile can be treated as a sandwich of lamellar gratings with different filling factors. Transfer matrix of such a structure is the product of transfer matrices of the sub-layers. We designed an experiment (Fig. 3) to obtain the groove depth of a surface relief grating.



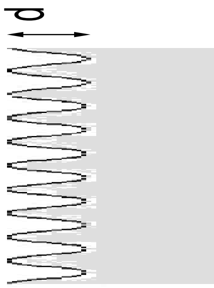


Fig. 3: *Scheme of the experiment: 1-laser, 2-polarisator, 3-photodetector, 4-grating Right: cross section of the grating, d – groove depth*

In this experiment we used a relief surface grating with sinusoidal profile (Fig. 3) with unkown groove depth. The spatial period of the grating was 1000 nm, the refractive index of the material was 1.37. The substrate below the grating was an absorbing layer. We used a laser beam TE polarised with wavelength 650 nm. The angle of incident (18°) was near the Bragg's angle so we measured the strongest intensity of the first diffracted order. Tab. 1 shows the intensities of the corresponding diffraction orders. The error of the intensity measurement was 0.5 mV.

Tab. 1 *Intensities of diffracted orders*

	Incident wave	0th reflected	0th transmitted	1st transmitted
Intensity [mV]	208.8	16.1	167.1	9.8

Then we constructed the diffraction efficiencies of the grating (Fig. 4) versus the groove depth using RCWA. Comparing these results to the measured data the groove depth of the grating can be inversely deduced, which is (186 ± 5) nm. We also measured the groove depth with AFM, (175 ± 5) nm.

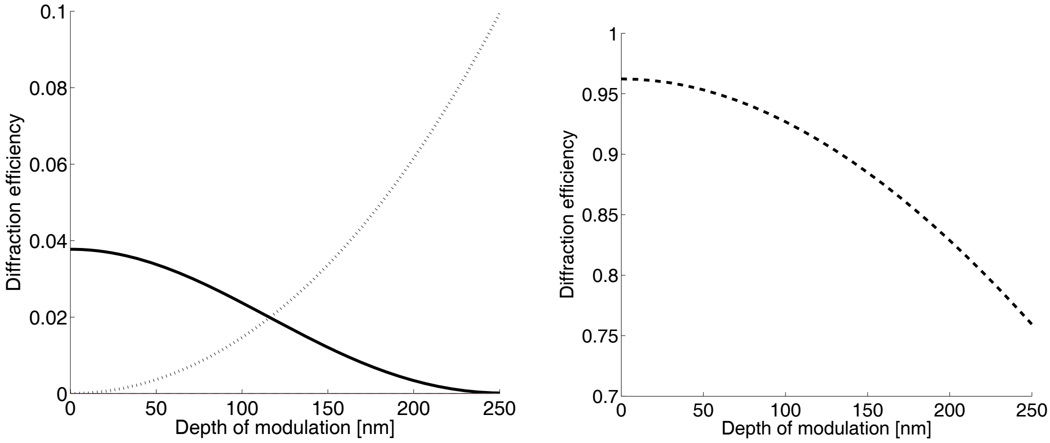


Fig. 4: *Diffraction efficiencies of the relief grating used in the experiment. Continuous line – 0th reflected, dashed line – 0th transmitted, dotted line – 1st transmitted order.*

3.3 Diffraction spectra of a subwavelength lamellar grating

Consider a binary lamellar grating (Fig. 1) with period 250 nm. The groove depth of the grating is 2000 nm and the filling factor is 0.5. The grating is made of material with relative permittivity 5. The substrate is made of the same material as the grating. Fig. 5 shows the transmittance and reflectance spectra for TE and TM polarisations for the normal incidence. One can observe that resonance peaks start to appear at a certain wavelengths. For our configuration this is below wavelength 360 nm for TE polarisation and 453 nm for TM polarisation. For larger wavelength, both transmission and reflection oscillates as a function of λ. These oscillations can be interpreted as Fabry-Perot resonances at thin dielectric layer with effective relative permittivity. This way it is possible to determine the minimal wavelength at which the grating starts to behave as a homogenous layer with an effective relative permittivity.

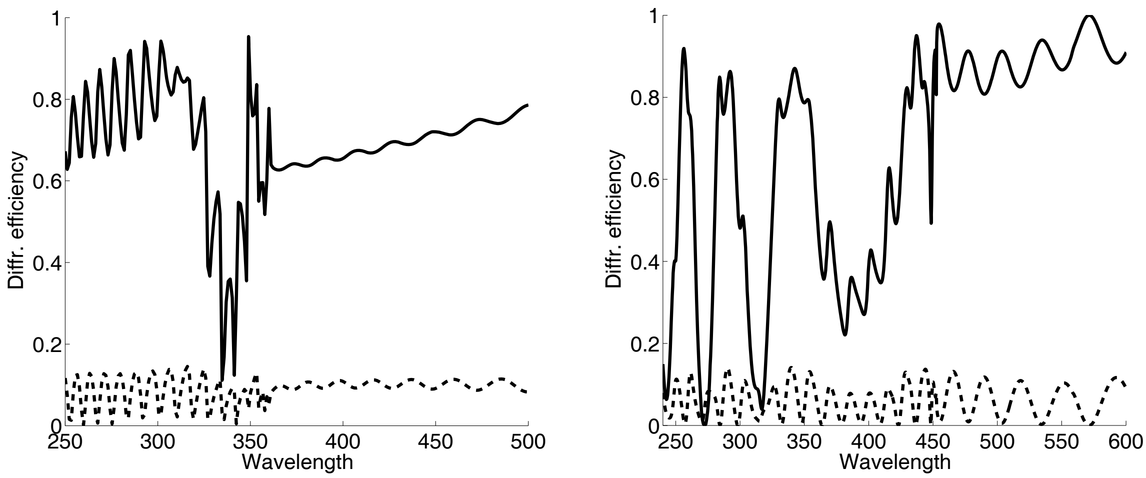


Fig. 5: *Transmittance (continuous line) and reflectance (dashed line) spectra of the 0th diffracted order for TE (left) and TM (right) polarisation. Please note that the 1st diffracted order of transmission is not showed.*

Conclusion

We showed that the numerical RCWA is very useful in the investigation of the electromagnetic response of periodic structures. Since this analysis is rigorous and vectorial, it can be used for modelling structures with subwavelength spatial period. RCWA enables us to calculate the frequency dependence of the transmissison and reflection of the electromagnetic wave propagation through periodic media, such as volume phase holograms, binary gratings and surface relief gratings.

The existence of the Bragg's angle was demonstrated for a thick phase grating. We constructed diffraction spectra of a subwavelength lamellar grating and showed the existence of resonant peaks. Investigation of effective parameters of periodic stuctures is demonstrated. It is also possible to obtain the groove depth of a surface relief grating constructing an inverse problem experiment.

Acknowledgement

This publication originates from the project „National Center for Research and Applications of Renewable Energy Sources“ (IMTS 26240120028) of Operational program Research and Development financed by European fund of Regional Development and the work was supported by the Slovak Republic grant agency VEGA, project No. 1/0879/11.

References:

[1] Magnusson R.; Gaylord, T. K.: Analysis of multiwave diffraction of thick gratings, *J. Opt. Soc. Am.* **67**, p. 1165–1170 (1997)

[2] Moharam, M.G.; Gaylord, T. K.: Rigorous coupled wave analysis of planar grating diffraction, *J. Opt. Soc. Am.* **71**, p. 811–818 (1981)

[3] Moharam, M. G.; Grann, E. B.; Pommet, D. A.; Gaylord, T. K.: Stable implementation of the rigorous coupled-wave analysis for surface relief gratings: enhanced transmittance matrix approach, *J. Opt. Soc. Am. A* **12**, p. 1068–1076 (1995)

[4] Li, L.: Convergence of the coupled-wave method for metallic lamellar diffraction Gratings, *J. Opt. Soc. Am. A* **10**, p. 2581–2591 (1993)

[5] Li, L.: Fourier modal method for crossed anisotropic gratings with arbitrary permittivity and permeability tensors, *J. Opt. A: Pure Appl. Opt.* **5**, p. 345–355 (2003)

[6] Pendry, J. B.; Mackinnon, A.; Roberts, P. J.: Universality classes and fluctuations in disordered systems, *Mathematical and Physical Sciences* **437**, p. 67–83 (1992)

[7] H. Kogelnik: Coupled wave theory for thick hologram gratings, *The Bell System Technical Journal* **48**, p. 2909-2947 (1969)