FEM AND ITS GENERALIZATION FOR THE DIFFRACTION BY POLYGONAL PROFILE GRATINGS

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ABSTRACT

For the numerical computation of efficiencies for optical gratings, there exists a huge variety of algorithms. Dealing with a boundary value problem for an elliptic partial differential equation, the application of finite element methods (FEM) is natural too. However, the oscillatory nature of the electromagnetic fields requires some modifications. The resulting FEM program can be used as a part of an algorithm to design optimal gratings.

THE FINITE ELEMENT METHOD (FEM)

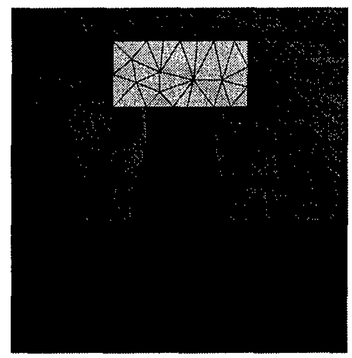
The variational form of the boundary problems is well known and its coerciveness is well established (cf. e.g. [6,1,3]). For example the variational equation for $u(x,y) = v(x,y) \cdot exp(-\mathrm{i}\alpha x)$ with v the unknown third component of the amplitude of the scattered magnetic field in the case of TM polarization is

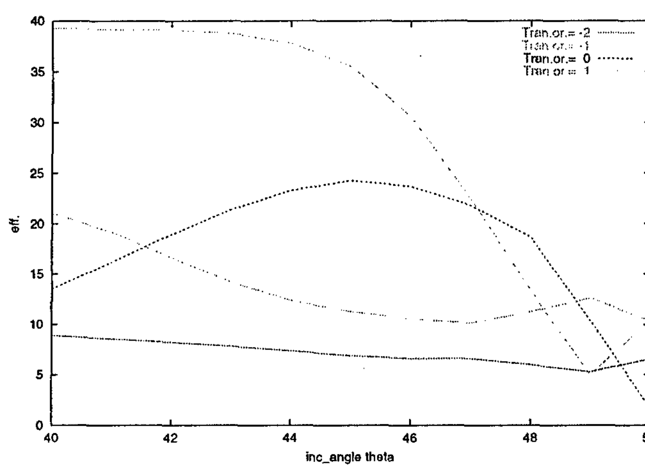
$$\int_\Omega \frac{1}{k^2}\{\nabla + \mathrm{i}(\alpha,0)\}u \cdot \overline{\{\nabla + \mathrm{i}(\alpha,0)\}\varphi} - \int_\Omega u\overline{\varphi} + \frac{1}{(k^+)^2}\int_{\Gamma+}(T_\alpha^+ u)\overline{\varphi}$$
$$+\frac{1}{(k^-)^2}\int_{\Gamma-}(T_\alpha^- u)\overline{\varphi} = -\frac{1}{(k^+)^2}\int_{\Gamma+}(2\mathrm{i}\beta e^{-\mathrm{i}\beta b})\overline{\varphi}, \quad \varphi \in H_p^1(\Omega). \qquad (1)$$

The domain Ω is the rectangular cross section of the grating profile taken over one period and $\Gamma^\pm$ stand for the upper resp. lower boundary sides. The symbol k stands for the piecewise constant refractive index taking the constant values k^+ resp. k^- above resp. below the grating. The number α is the product of k^+ times the sine of the incidence angle, ∇ is the gradient, and $T_\alpha^\pm$ a hypersingular boundary integral operator. The test function φ runs through all periodic (w.r.t. to the first variable x) functions in the Sobolev space $H^1(\Omega)$. A variational equation similar to (1) holds for the TE polarization. For the case of conical diffraction (incident plane wave with direction not in the plane perpendicular to the grooves of the grating), a coupled system of two such variational equations is to be solved.

To get the FEM solution, the domain is split into triangles/rectangles. An approximation of the magnetic field is sought in form of a continuous piecewise linear/bilinear function, and the test functions in (1) are replaced by the piecewise linears/bilinears. Substituting the numerical solutions for u over $\Gamma^{\pm}$ into well-known integral representations, we get the reflected and transmitted energy and the efficiencies of the reflected and transmitted modes. In contrast to popular alternative methods, the FEM needs no Rayleigh expansion, no slicing of blaze gratings, and no solution of big dense systems of integral equations. The convergence of the method is well established.

Example :	*cover material* :	Air
	coating material :	Photoresist
	substrate material :	SiO_2
	polarization :	TM
	period :	588 grooves/mm
	incidence angle :	47.5°





The figures show a coarse FEM grid of a coated lamellar grating profile with overetching, the isolines of the real part of the solution u, and the efficiencies of the transmitted modes of order -2, -1, 0, and 1 depending on the incidence angle in the interval $[40°, 50°]$.

GENERALIZED FEM

Unfortunately, due to a mismatch of the frequency of the solution and the discrete frequency of the approximate solution, the FEM deteriorates with large wave numbers. Even if the function can be approximated in the space of piecewise linears with high accuracy, the error of the FEM solution of Eq. (1) may be large. To overcome this so-called "pollution effect", we have first implemented a generalized FEM for the case of lamellar (binary) gratings which is a finite difference scheme over uniform rectangular gratings (cf. [2,4]). Further, we have tested the partition of unity method together with mortar techniques (cf. [5]), and we have implemented a new generalized FEM based on trial functions the restrictions of which to the triangles of the triangulations are solutions of the partial differential equation. These solutions are generated by an FEM over a fine uniform grid in the subtriangle. For a fixed accuracy, these methods reduce the storage requirements and, in some cases, the computing times essentially. In the table we present results for a coated echelle grating (wave length 160 nm, 166 grooves per mm, width of MgF2 coating 25 nm, blaze angle 80°, apex angle 90°, cover material Air, grating material Al, TE polarization, incidence angle 80°).

degrees of freedom	memory for solver	efficiency of order 74 (refl.)
105 785	0.35 GB	37.931045
263 624	0.70 GB	67.384460
559 800	1.98 GB	68.390312

OPTIMZATION OF GRATINGS (SYNTHESIS PROBLEM)

The mentioned methods for the numerical solution of the direct diffraction problem can be used as a part of an algorithm to design optimal gratings. We have implemented a code (cf. [4]) to minimize several objective functions including efficiencies and phase shifts. On a set of coated lamellar grids containing a certain number of rectangular pieces with prescribed material properties, we determine an optimal grating by a gradient descent method. The latter is based on the efficient computation of the gradients by generalized FEM.

ACKNOWLEDGEMENT

The authors gratefully acknowledge the support of the German Ministry of Education, Research and Technology under Grant No. 03-ELM3B5.

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