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Direct and Inverse Problems for Diffractive Structures – Optimization of Binary Gratings

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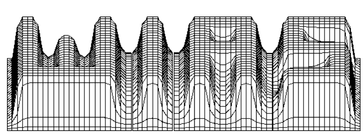

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Abstract

The goal of the project is to provide flexible analytical and numerical tools for the optimal design of binary and multilevel gratings occurring in many applications in micro–optics. The direct modeling of these diffractive elements has to rely on rigorous grating theory, which is based on Maxwell's equations. We developed efficient and accurate direct solvers using a variational approach together with a generalized finite element method which appears to be well adapted to rather general diffractive structures as well as complex materials. The optimal design problem is solved by minimization algorithms based on gradient descent and the exact calculation of gradients with respect to the geometry parameters of the grating.

1 Introduction

Diffractive optics is a modern technology in which optical devices are micromachined with complicated structural features on the order of the length of light waves. Exploiting diffraction effects, these devices can perform functions unattainable with conventional optics and have great advantages in terms of size and weight. The current applications in micro–optics are far–reaching, including high–power laser beam shaping and splitting, solar cell design, image processing and optical document security. Therefore the optimal design of microoptical devices has received considerable attention in the engineering community and has stimulated several mathematical investigations.

One of the most common geometrical configurations for diffractive optical structures is a periodic pattern embedded into a thin–film layer system, such as the multilevel diffraction grating shown in Fig. 1. The pattern is usually created using tools from semiconductor industry. In most applications the grating is illuminated by an incoming time–harmonic plane electromagnetic wave whose length is comparable to the period of the grating. In this situation geometrical optics approximations to the underlying electromagnetic field equations are not accurate, hence, the mathematical modeling has to rely on Maxwell's equations or related partial differential equations.

The electromagnetic theory of gratings has been studied extensively since Rayleigh's time. In particular, during the last decade significant progress has been made concerning the direct diffraction problem, i.e. the calculation of the reflection and transmission coefficients of the propagating wave components of the diffracted field. Several approaches and numerical methods have been proposed for obtaining rigorous solutions to the problem, including modal expansion, differential and integral

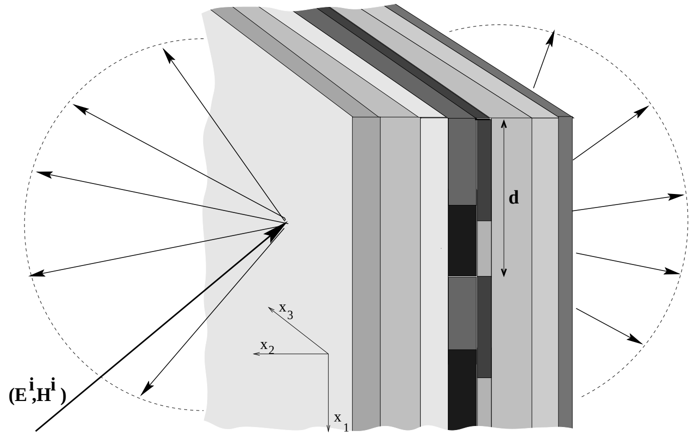

Figure 1: Multilevel diffraction grating

methods, analytical continuation, and variational methods. The latter approach turned out to be sufficiently flexible to overcome the difficulties associated with non–smooth grating profiles and the highly oscillatory nature of waves and interfaces. The variational method also leads to effective formulas for the gradient of cost functionals arising in optimal design problems, so that gradient–based minimization algorithms can be used to find gratings with specified optical functions.

2 Mathematical Model

Consider a periodic diffraction grating formed by a periodic pattern of nonmagnetic materials (of permeability μ) with different dielectric constants ϵ; see Fig. 1. If the coordinate system is chosen such that the grating structure is periodic in x_1–direction and invariant in x_3–direction, then the diffraction problem is determined by the function $\epsilon(x_1, x_2)$ which is say d–periodic in x_1. This function is assumed to be piecewise constant and complex valued with $0 \le \arg \epsilon < \pi$. The material above and below the grating is assumed to be homogeneous with dielectric constants $\epsilon = \epsilon^+ > 0$ and ϵ^-, respectively. The grating is illuminated by an incoming plane electromagnetic wave

$$\mathbf{E}^i = \mathbf{p}\, e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3} e^{-i\omega t} \ , \quad \mathbf{H}^i = \mathbf{q}\, e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3} e^{-i\omega t}$$

from the top with the angles of incidence $\theta, \phi \in (-\pi/2, \pi/2)$. In our applications the wavelength $\lambda = 2\pi c/\omega$, c denoting the speed of light, is comparable to the period d. For notational convenience we will change the length scale by a factor of $2\pi/d$ so that the grating becomes 2π–periodic: $\epsilon(x_1 + 2\pi, x_2) = \epsilon(x_1, x_2)$. Note that this is equivalent to multiplying the frequency ω by $d/2\pi$. Then the wave vector of the incident field is expressed in terms of the angles of incidence as

$$\mathbf{k} = (\alpha, -\beta, \gamma) = k^+(\sin\theta\cos\phi, -\cos\theta\cos\phi, \sin\phi) \qquad \text{with } k^+ = \omega(\mu\epsilon^+)^{1/2} \ .$$

Note that $(\mathbf{E}^i, \mathbf{H}^i)$ satisfy the time–harmonic Maxwell equations if the constant amplitude vectors $\mathbf{p}$, $\mathbf{q}$ fulfil the relations $\mathbf{p} \cdot \mathbf{k} = 0$ and $\mathbf{q} = (\omega\mu)^{-1}\mathbf{k} \times \mathbf{p}$. Thus the incoming field is determined by two of their components, for example, p_3 and q_3. The total fields then also satisfy Maxwell's equations, together with transmission conditions for their tangential components at the interfaces and a radiation condition at infinity.

In the following we mainly restrict ourselves to the case $\gamma = 0$, i.e. the so–called classical diffraction problem, where $\phi = 0$ so that the wave vector $\mathbf{k}$ lies in the x_1–x_2 plane. In that case the resulting electromagnetic field can be split into the cases of TE and TM polarization, where either the electric field or the magnetic field is parallel to the x_3–axis. In both cases Maxwell's equations can be reduced to transmission problems for a scalar Helmholtz equation

$$\Delta v + k^2 v = 0$$

in $\mathbb{R}^2$, where $k = \sqrt{\omega^2 \epsilon \mu}$ is the refractive index and the function v stands for the x_3–component of the total electric or magnetic field, and is α quasi–periodic in x_1: $v(x_1 + 2\pi, x_2) = \exp(2\pi\alpha i) v(x_1, x_2)$. For TE polarization the solution and its normal derivative $\partial_n v$ have to cross the interfaces continuously, whereas in TM polarization $\epsilon^{-1}\partial_n v$ has to be continuous. Moreover, the diffracted field can be expanded as an infinite sum of plane waves,

$$v = \sum_{n \in \mathbb{Z}} A_n^{\pm} \exp(i(n+\alpha)x_1 + i\beta_n^{\pm}|x_2|) \ , \quad x_2 \to \pm\infty,$$

with the unknown Rayleigh amplitudes $A_n^{\pm}$. Here we have used the notation

$$\beta_n^{\pm} = \sqrt{(k^{\pm})^2 - (n+\alpha)^2}, \ n \in \mathbb{Z} \, ,$$

where k^- denotes the refractive index of the homogeneous medium below the grating structure. Since $\beta_n^{\pm}$ is real for at most a finite number of indices n, we see that only a finite number of plane waves in the sum propagate into the far field, with the remaining evanescent modes decaying exponentially as $x_2 \to \pm\infty$. The number of propagating modes and the direction of propagation for each mode is determined by the frequency of the incident wave, the refractive index of the material, and the period of the structure. The Rayleigh coefficients A_n^+ (resp. A_n^-) corresponding to these propagating modes are called the reflection (resp. transmission) coefficients. From an engineering point of view, these coefficients are the key feature of any grating since they indicate the energy and phase shift of the propagating modes. In particular, the ratio of the energy of a given propagating mode to the energy of the incoming wave is called the efficiency of the mode. The reflected and transmitted efficiencies in the TE case are given by

$$e_n^{TE,\pm} = (\beta_n^{\pm}/\beta)|A_n^{\pm}|^2$$

and in the TM case by

$$e_n^{TM,+} = (\beta_n^{+}/\beta)|A_n^{+}|^2 \ , \quad e_n^{TM,-} = (k^+/k^-)^2(\beta_n^{-}/\beta)|A_n^{-}|^2.$$

The exact computation of these quantities is the main goal of the direct diffraction problem. More details can be found in [8], [3], whereas the general case of the so–called conical diffraction problem ($\gamma \neq 0$) has been studied in [7]. In that case the invariance of the diffractive structure in x_3–direction allows us to reduce Maxwell's equations to a system of two–dimensional Helmholtz equations, which are coupled via transmission conditions at the interfaces.

3 Optimal Design of Binary Gratings

A major part of the motivating applications in diffractive optics is associated with the inverse problems of optimal interface shape design or profile reconstruction from scattered fields. There have been a number of papers from the engineering community that are concerned with the optimal design of periodic gratings; see [10]. By far the greatest activity has been in optimization for ray–tracing and phase–reconstruction techniques which are valid within the domain of Fourier optics. A few of these papers are devoted to optimization problems using rigorous diffraction theory. However, the optimization procedures are usually only based on the values of certain cost functionals, i.e., they require the solution of a large number of direct problems and are therefore computationally expensive. Sometimes the approximation of gradients by simple difference quotients is used, which is, however, very unefficient for a large number of parameters. More advanced methods to find optimal solutions utilize, besides the values of cost functionals, also its gradients or even properties of higher order differentials. The simplest example are descent–type algorithms, which are computationally efficient if explicit gradient formulas are available.

Let us consider the model problem of designing a binary grating on top of a multilayer stack in such a way that the propagating modes have a specified intensity or phase pattern for a chosen range of wavelengths or incidence angles. Assume that the period of the grating and the number of transition points and of thin–film layers are fixed (cf. Fig. 2). Typical minimization problems involving the diffraction efficiencies or Rayleigh coefficients are the following.

To realize prescribed values $c_n^{TE,\pm}, c_n^{TM,\pm}$ of certain reflection and transmission efficiencies, the functional

$$\begin{aligned} &\sum \left(|e_n^{TE,+} - c_n^{TE,+}|^2 + |e_n^{TM,+} - c_n^{TM,+}|^2\right) \\ &+ \sum \left(|e_n^{TE,-} - c_n^{TE,-}|^2 + |e_n^{TM,-} - c_n^{TM,-}|^2\right) \to \min \end{aligned} \tag{1}$$

can be used.

The optimal design of a grating providing a given phase shift φ between the nth reflected TE and TM mode can be performed using the functional

$$-e_n^{TE,+} - e_n^{TM,+} + |A_n^{TE,+} - \exp(i\varphi) A_n^{TM,+}|^2 \to \min \quad . \tag{2}$$

Note that the efficiencies are functions of the transition points, the thicknesses of layers and the height of the grating, so that the minimum has to be taken over some compact set in the (finite dimensional) parameter space reflecting, e.g., technological constraints on the design of the grating and the thin–film layers. Obviously many other functionals are possible and have been investigated, especially if a corresponding optimization over a range of wavelengths or incidence angles is required.

To find local minima of these cost functionals via gradient descent methods, we must calculate the gradient of Rayleigh coefficients. Explicit gradient formulas based on the solution of the direct problem and its adjoint will be outlined in the next section.

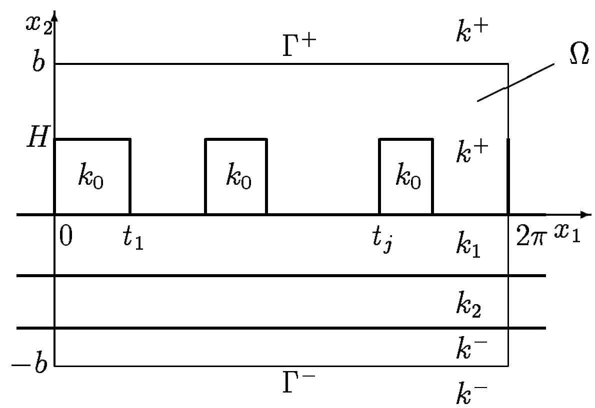

Figure 2: Problem geometry

4 Analysis

The direct diffraction problems admit variational formulations in a bounded periodic cell, enforcing implicitely the transmission and radiation conditions. If we introduce two artificial boundaries $\Gamma^\pm = \{x_2 = \pm b\}$ lying above resp. below the grating structure, denote by Ω the rectangle $(0, 2\pi) \times (-b, b)$ (cf. Fig. 2), and define the 2π-periodic function $u = v \exp(-i\alpha x_1)$, then the diffraction problem for TE polarization can be transformed to a variational problem for u in the rectangle Ω (cf. [2], [3]):

$$\begin{aligned} B_{TE}(u,\varphi) \;&:=\; \int_\Omega \nabla_\alpha u \cdot \overline{\nabla_\alpha \varphi} - \int_\Omega k^2\, u\, \bar\varphi + \int_{\Gamma^+} (T_\alpha^+ u)\, \bar\varphi + \int_{\Gamma^-} (T_\alpha^- u)\, \bar\varphi \\ &=\; -\int_{\Gamma^+} 2i\beta p_3 \exp(-i\beta b)\, \bar\varphi \;, \quad \forall \varphi \in H_p^1(\Omega) \;. \end{aligned}$$

Here $\nabla_\alpha = \nabla + i(\alpha, 0)$, and $H_p^1(\Omega)$ denotes the Sobolev space of functions which are 2π-periodic in x_1. The non-local operators on the artificial boundaries are defined by

$$(T_\alpha^\pm u)(x_1, \pm b) = -\sum_{n\in\mathbb{Z}} i\, \beta_n^\pm\, \hat u_n^\pm\, \exp(inx_1) \;,$$

where $\hat{u}_n^{\pm}$ are the Fourier coefficients of u on $\Gamma^{\pm}$. Similarly, the TM diffraction problem can be formulated as

$$B_{TM}(u,\varphi) := \int_{\Omega} \frac{1}{k^2}\, \nabla_\alpha u \cdot \overline{\nabla_\alpha \varphi} - \int_{\Omega} u\, \bar{\varphi} + \frac{1}{(k^+)^2} \int_{\Gamma^+} (T_\alpha^+ u)\, \bar{\varphi}$$

$$+\frac{1}{(k^-)^2} \int_{\Gamma^-} (T_\alpha^- u)\, \bar{\varphi} = -\frac{1}{(k^+)^2} \int_{\Gamma^+} 2i\beta q_3 \exp(-i\beta b)\, \bar{\varphi} \ , \quad \forall\, \varphi \in H_p^1(\Omega) \ .$$

The sesquilinear forms B_{TE} and B_{TM} are strongly elliptic, i.e., coercive modulo compact operators on $H_p^1(\Omega)$. This leads to existence, uniqueness and regularity results for the variational equations in all cases of physical interest; see [3]. In particular, the TE and TM diffraction problems are uniquely solvable for all but a sequence of countable frequencies ω_j, $\omega_j \to \infty$, and the solution is unique for all frequencies if one of the materials is absorbing. While the solution to the TE problem is always sufficiently smooth ($u \in H_p^2(\Omega)$), the TM solution may have singularities at the corner points of the grating. More precisely, near corners one has $u = r^\lambda f + g$, where r denotes the distance to the corner point, the exponent λ with $0 < \mathrm{Re}\ \lambda < 1$ is determined by the refractive index of the grating material and f, g are some smoother functions. In particular, if two materials with optical indices k_1 and k_2, respectively, meet at some corner, then λ is the solution with minimal positive real part of the equation

$$\left(\frac{\sin(\pi\lambda/2)}{\sin(\pi\lambda)} \right)^2 = \left(\frac{k_1^2 + k_2^2}{k_1^2 - k_2^2} \right)^2 \ .$$

Hence, the partial derivatives of u are not square integrable on the grating profile, in general.

A detailed solvability and regularity theory of the conical diffraction problem, which is also based on a variational formulation, can be found in [7].

The variational approach leads to effective formulas for the gradient of cost functionals arising in the optimal design of binary and multilevel gratings. As an example, we present a formula for the partial derivatives of the Rayleigh coefficients with respect to the transition points t_j of a binary profile (cf. Fig. 2) in the TM case:

$$D_j A_n^{\pm} = \frac{(-1)^{j-1}}{2\pi} \exp(-i\beta_n^{\pm} b)((k_0)^2 - (k^+)^2) \int_{\Sigma_j} gr(u) \cdot \overline{gr(w_\pm)}\, dx_2 \ ,$$

where Σ_j denotes the vertical segment at t_j, u is the solution of the direct TM problem, $w_\pm$ solves the adjoint problem

$$B_{TM}(\varphi, w_\pm) = \int_{\Gamma^\pm} \varphi \exp(-inx_1) dx_1 \ , \quad \forall \varphi \ ,$$

and

$$gr(u) = \frac{1}{k^+ k_0} \left(\frac{k_0}{k^+}\, \partial_{x_1,\alpha} u|_+ \, , \ \partial_{x_2} u|_+ \right) \ ,$$

where the plus sign denotes the one-sided limit as the interface is approached from the region above. Similar formulas are valid for the derivatives with repect to the height and the layer thicknesses. Note that the above gradient formula is only well–defined if the TM solution has mild singularities at the corners of the grating profile; see [5] for an approach in case of arbitrary singurities and more general non-smooth material interfaces, which also extends to conical diffraction [6].

5 Numerical Methods

The direct and adjoint diffraction problems have the form: Find $u \in H_p^1(\Omega)$ satisfying the equation

$$a(u, \varphi) = (f, \varphi) \ , \quad \text{for all } \varphi \in H_p^1(\Omega) \ ,$$

where $a(u, \varphi)$ is a strongly elliptic sesquilinear form, and (f, φ) stands for a linear and continuous functional on the function space $H_p^1(\Omega)$. The strong ellipticity implies that finite element approximations for all invertible problems under consideration lead to a uniquely solvable linear system of equations if the meshsize is sufficiently small. Moreover, the approximate solutions converge to the corresponding exact solution in the norm of the function space with optimal order.

Due to the rectangular geometry of binary gratings it is quite natural to choose piecewise bilinear functions as finite elements on a uniform rectangular partition of $\Omega = (0, 2\pi) \times (-b, b)$. This leads to a linear system with a block–tridiagonal matrix. The nonlocal boundary terms in the sesquilinear forms imply that the first and the last block of the main diagonal are fully occupied matrices, whereas the remaining blocks are sparse.

The computation of the nonlocal terms in the sesquilinear forms can be performed very efficiently with an accuracy comparable with the computer precision. Since the traces of the finite element functions on $\Gamma^{\pm}$ are piecewise linear periodic functions with uniformly distributed break points, it is possible to use recurrence relations for the Fourier coefficients of spline functions and convergence acceleration methods.

If e.g. the artificial boundary Γ^+ is divided into m subintervals of equal length and the basis of hat functions $\{\varphi_j\}$ is used, then the form

$$\int_{\Gamma^+} (T_\alpha^+ \varphi_p) \, \overline{\varphi_q} \; dx_1 \ , \quad p \, , q = 0, ..., m-1$$

corresponds to an $m \times m$ circulant matrix with the eigenvalues

$$\tau_0 = -2i\pi \, \beta \ , \quad \tau_p = -4i\pi \left(\frac{\sin(\pi p/m)}{\pi}\right)^4 \sum_{r=-\infty}^{\infty} \frac{\beta_{rm+p}^+}{m(r+p/m)^4} \ .$$

Thus one only has to expand

$$\frac{\beta_{rm+p}^+}{m} = \sqrt{\left(\frac{k^+}{m}\right)^2 - \left(\frac{\alpha}{m} + r + \frac{p}{m}\right)^2}$$

with respect to powers of $|r + p/m|$ and to use fast computation of the generalized Zeta function.

Usual FE approximations of the Helmholtz equation involve besides the approximation error also the so–called pollution error which increases together with the wavenumbers and enlarging domains. Roughly speaking, the pollution error is caused by the well–known fact that the discretization of the Helmholtz equation with the wave number k results in an approximate solution possessing a different wave number k_h. In one–dimensional problems, for example, the usual piecewise linear FE solution of the equation $u'' + k^2 u = 0$ on a uniform grid has the discrete wave number

$$k_h = \frac{1}{h} \arccos \frac{2(3 - (kh)^2)}{6 + (kh)^2} = k - \frac{k^3 h^2}{24} + O(k^5 h^4) \ .$$

It turns out that this "phase lag" leads to suboptimal error estimates.

In the one–dimensional case it is possible to construct a generalized FEM without pollution by modifying the evaluation of the sesquilinear form. However, in higher dimensions it is not possible to eliminate the pollution in the FE error by any modification of the evaluation of the sesquilinear form. Therefore, we extended an approach by Babuška et al [1] to design a so–called GFEM with minimal "phase lag" for piecewise uniform rectangular partitions; see [4] for the details.

The method was used to evaluate the reflection and transmission efficiencies of binary gratings on multilayer systems of different geometries and materials and it turned out to be robust and reliable in both the TE and TM case. Compared with the usual FEM the obtained results were accurate already for rather poor discretizations. In Fig. 3 we compare the numerical values of some reflection and transmission efficiencies versus the square root n of total number of grid points computed with the usual FEM and the GFEM on quadratic meshes for a binary grating with one groove per period situated on a layer. In each case the GFEM results differ already for $n = 40$ only by 2% from the corresponding values for $n = 200$, whereas the FEM results converge rather slowly to these values.

The sparse structure of the matrix can be used to apply efficient direct or iteration methods for solving linear systems. We used a block version of the so–called sweep method, which utilizes the block–tridiagonal structure of the matrix and additionally the circulant properties of the dense blocks. Since the matrices of the discretized variational problems are nonsymmetric, we also applied preconditioned GMRES-type and BiCGstab methods as iterative solvers. The corresponding equations with averaged wave numbers k are good candidates for preconditioners, which can be inverted very efficiently using FFT.

In the case that the grating is situated on top of a multilayer stack (cf. Fig. 2), one can reduce the integration domain Ω used in the FE solution by taking into account that the solution is smooth within the layers. We introduce a new artificial boundary, $\widetilde{\Gamma}^-$ say, into the first layer and new nonlocal boundary operators which model the layer system below $\widetilde{\Gamma}^-$ together with the radiation condition for $x_2 < -b$.

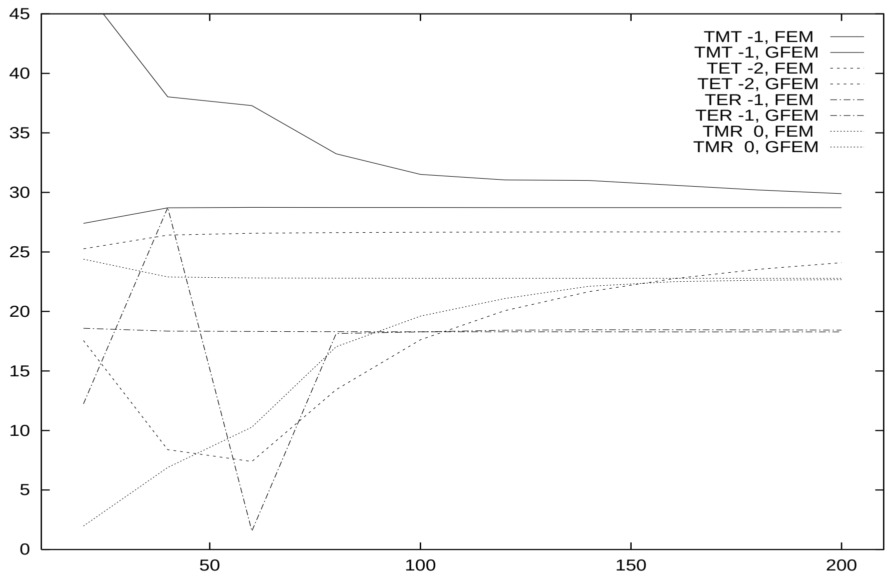

Figure 3: Comparison of efficiencies computed with FEM and GFEM

Combining the GFEM in the reduced domain with Rayleigh series expansions in the layer system then leads to a considerable reduction of the computational complexity; see [4] for a detailed presentation.

After having solved the linear system corresponding to the GFE discretization of the variational equations, the diffraction efficiencies are determined from the Fourier coefficients of the solution on the artificial boundaries. A stable recursive algorithm is used for the computation of the transmission efficiencies and the solutions on the layer interfaces, which appear in the gradient formulas.

6 Some Optimization Results

The GFEM and the gradient formulas were integrated into a computer program to find the optimal design of binary gratings with desired phase or intensity pattern for a given range of incidence angles or wavelengths. The optimal design problems were treated as nonlinear optimization problems with linear constraints, and we implemented a projected gradient algorithm and an interior point method for their numerical solution. Several numerical examples including polarisation gratings, high reflection mirrors and beam splitters successfully demonstrated the efficiency of the algorithm.

As a first example, we provide the optimization results for some beam splitters. The illuminating unpolarized wave with $\lambda = 0.633\mu$m is normally incident from a dielectric medium with optical index $\nu = 1.5315$. Recall that the optical index of a material with permittivity ϵ is defined by $\nu = (\epsilon/\epsilon_0)^{1/2}$, where ϵ_0 denotes the permittivity of the vacuum. Choosing the period $d = 1.266\mu$m, three diffraction orders propagate with angles $0°$ and $\pm 30°$. Such beam splitters with large diffraction angles are useful in, e.g., optical clock signal distribution. The goal is

a) to maximize the efficiencies of the orders ± 1

b) to obtain maximal and equal efficiencies of all three orders

by optimizing the height H and the fill factor f of the grating with one groove per period. Using the cost functional (1), the following results have been obtained (cf. Fig. 4):

a) $H = 0.734\mu\text{m}$, $f = 0.72$, b) $H = 0.43\mu\text{m}$, $f = 0.58$.

Further applications in laser design are discussed in [9].

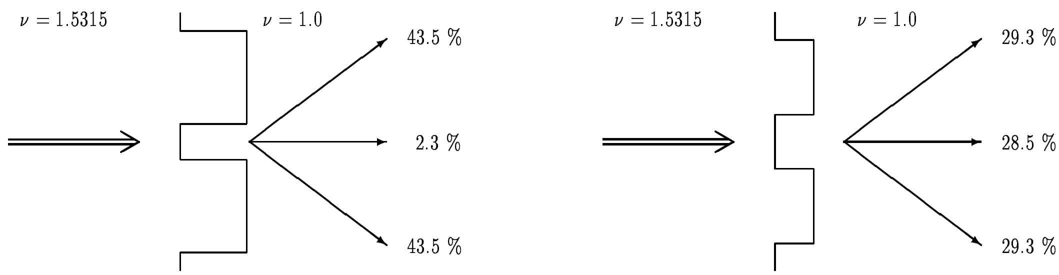

Figure 4: Optimal design of an 1–to–2 and an 1–to–3 beam splitter

The next example concerns the design of a zero–order copper grating ($\nu = 12.7 + 51.1i$) as circular polarizer for a CO_2 laser with $\lambda = 10.6\mu\text{m}$ such that in the range of incident angles $\theta \in (29^\circ, 31^\circ)$ the efficiencies of the reflected TE and TM polarized wave are maximal and the phase difference between them is close to $\pi/2$. Here one has to minimize the functional (2) extended over the range of incident angles, which possesses many local minima. One of the reasonable geometries is $d = 3.0\mu\text{m}$, $H = 1.65\mu\text{m}$, and the fill factor is 0.24. Table 1 contains the computed values.

7 Conclusion

We focused on optimal design problems for binary and multilevel gratings, using exact formulas for the gradients of cost functionals and a fast and reliable method for the numerical solution of direct problems. The method is based on a variational formulation and combines a finite element method in the grating structure with Rayleigh series expansions in the layer system below the grating. The approach is not restricted to rectangular profiles, but allows the numerical treatment of rather general diffraction structures, together with a rigorous convergence analysis.

Table 1: Zero order efficiencies and phase difference for circular polarizer

θ	TE	TM	phase
29.0	97.50	95.72	90.72
29.2	97.50	95.72	90.58
29.4	97.51	95.72	90.45
29.6	97.51	95.72	90.32
29.8	97.52	95.72	90.18
30.0	97.52	95.72	90.04
30.2	97.53	95.72	89.91
30.4	97.53	95.72	89.77
30.6	97.54	95.72	89.63
30.8	97.54	95.72	89.49
31.0	97.55	95.72	89.35

We proposed a generalized finite element method (GFEM) with minimal pollution, which provides highly accurate numerical results in the computation of diffraction efficiencies. So far the extension of this method to more general (e.g., polygonal) grating profiles remains an open problem.

To solve optimal design problems for binary gratings by gradient descent, explicit formulas for the gradients with respect to the parameters of the grating profile and the thicknesses of layers have been developed. These formulas involve the solutions of direct and adjoint diffraction problems and reduce considerably the computational costs compared to simple difference approximations of the gradients.

We expect that this approach is also applicable to the inverse problem of profile reconstruction from far field data. Another challenging direction of future research is the efficient solution of direct and inverse problems for non–periodic and three–dimensional diffractive structures.

References

[1] I. Babuška, F. Ihlenburg, E. Paik, S. Sauter, A generalized finite element method for solving the Helmholtz equation in two dimensions with minimal pollution, Comp. Meth. Appl. Mech. Eng., **128**, 325-359 (1995).

[2] G. Bao, D.C. Dobson, J.A. Cox, Mathematical studies in rigorous grating theory, J. Opt. Soc. Amer., **A 12**, 1029–1042 (1995).

[3] J. Elschner, G. Schmidt, Diffraction in periodic structures and optimal design of binary gratings. Part I: Direct problems and gradient formulas, Math. Meth. Appl. Sci., **21**, 1297–1342 (1998).

[4] J. Elschner, G. Schmidt, Numerical solution of optimal design problems for binary gratings, J. Comp. Physics, **146**, 603–626 (1998).

[5] J. Elschner, G. Schmidt, Diffraction in periodic structures and optimal design of binary gratings. Part II: Gradient formulas for TM polarization, Weierstrass Institute, Berlin, Preprint No. **538** (1999).

[6] J. Elschner, G. Schmidt, Conical diffraction by periodic structures: Variation of interfaces (submitted).

[7] J. Elschner, R. Hinder, F. Penzel, G. Schmidt, Existence, uniqueness and regularity for solutions of the conical diffraction problem, M^3AS (to appear).

[8] R. Petit (ed.), Electromagnetic Theory of Gratings, Springer Verlag, Berlin, Topics in Current Physics, Vol. **22** (1980).

[9] H.–J. Rostalski, J. Guhr, B. Kleemann, J. Elschner, G. Schmidt, M. Ferstl, E. Pawlowski, R. Steingrüber, G. Bostanjoglo, R. Motzkus, Use of a multilayer dielectric diffraction grating as the resonator mirror of a neodymium–doped yttrium aluminium garnet laser, J. Mod. Opt., **45**, 1523-1535 (1998).

[10] J. Turunen, F. Wyrowski (eds.), Diffractive Optics for Industrial and Commercial Applications, Akademie Verlag, Berlin (1997).