MATHEMATICAL STUDIES IN RIGOROUS GRATING THEORY

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Abstract

We consider the diffraction of a time harmonic wave incident on a grating (or periodic) structure. This paper is devoted to the study of mathematical issues that arise in the direct modeling, inverse, and optimal design problems. Particular attention is paid to the variational approach and finite element methods. For the direct problem, various results on existence, uniqueness, and numerical approximations of solutions are presented. Convergence properties of the variational method, and sensitivity to TM polarization are examined. Our recent work on inverse diffraction problems and optimal design problems is also discussed.

1 Introduction

The emergence of various high precision micromachining techniques - such as direct-write electron-beam lithography and reactive-ion-etch processing, x-ray lithography and LIGA processing, and single-point diamond machining - has permitted the fabrication of complex surface-relief profiles for use as high efficiency gratings and other diffractive structures. Devices with periods $0.25\mu m$ and aspect ratios greater than 3:1 are currently attainable and represent an example of reasonable bounds achievable using the most advanced of these techniques. Thus, in the practical application of diffractive optics technology for both imaging and nonimaging devices, there is increasingly a need for mathematical models and numerical codes both to provide rigorous solutions of the full electromagnetic vector-field equations for complicated grating structures, thus predicting performance given the structure, and to carry out optimal design of new structures. The former situation - determining rigorous solutions for a given structure - is referred to as the direct problem, while the latter case of optimal design is an example of the inverse problem.

The electromagnetic theory of gratings has been studied extensively since Rayleigh's time. The advent of computers has greatly accelerated activity in the area and has given rise to several approaches and numerical methods to yield rigorous solutions to the problem, including differential methods [1], [2], and [3], integral methods [1], analytical continuation [4]–[8], variational method [9], [10], and others. In light of the essential mathematical nature of the problem, it is noteworthy that by far the largest number of papers in the literature have come from the engineering community and proportionately few from applied mathematicians. Evidence of this is found in Petit's [1] and Cadilhac's [11], [12] remarks on the lack of existence and uniqueness theorems for the problem. Even more glaringly absent has been convergence analysis of the various numerical methods, although the more recent work by applied mathematicians in the analytic continuation method and the variational method has begun to rectify this.

For the inverse problem [13], by far the greatest activity has been in global optimization techniques for raytracing and phase reconstruction techniques. Much of the raytracing optimization work is done by vendors of commercial optical design codes. Phase reconstruction is used primarily to design phase-only diffractive devices, such as Dammann gratings, producing a desired far-field intensity distribution. The Gerchberg-Saxton algorithm [14] yields reasonably high efficiency and has been most widely used for this purpose, although Farn [15] recently has demonstrated a new dual-loop algorithm that yields both good efficiency and intensity shaping over orders. These phase reconstruction methods are valid within the domain of Fourier optics; attempts to extend the validity further, either into the near-field or to "fast" optics, mostly have been confined, at least in the engineering and optics community, to techniques based on simulated annealing [16]. There is a large and active group of applied mathematicians working in the area of inverse problems, but the specific applications generally lie outside optics. There have been a number of developments in this area which can be applied profitably to optics.

Here we draw on work done in this area at the Institute for Mathematics and Its Applications at the University of Minnesota since 1990 and address specifically the issues of existence and uniqueness of solutions and convergence of the variational method, as well as optimal design and inverse diffraction problems implemented by us. In particular, conditions that guarantee existence and uniqueness are discussed. Optimal rates of convergence can be obtained for TE polarization. In the TM polarization case, however, the convergence analysis is much more difficult. In fact, everyone active in the field is well acquainted with the situations (usually involving a complex index of refraction) where solutions for TM polarization converge much more slowly than TE polarization. We provide some insight into the nature of this phenomenon. For the inverse problem, we present our recent results on uniqueness, stability, and a new approach for optimal design. Many of these results have been published in the mathematical literature, but generally they have not yet received much exposure in the optics community, and thus we attempted to include a comprehensive list of references.

The reader is referred to [1] for various aspects of electromagnetic theory of gratings up to the early 80s. A description of mathematical problems which arise in industrial applications may be found in the books [17]–[19]. Finally, a preliminary description of some of the results was presented in [20].

2 The direct problem

Given the incident field and grating geometry, solving the direct problem predicts the behavior of the outgoing fields. Our goal is to solve Maxwell's equations rigorously.

2.1 The model

Figure 1 summarizes the geometry for the grating problem. The media are assumed to be nonmagnetic, and we assume a constant magnetic permeability μ to exist everywhere. We also assume that no currents are present and the fields are source free. Then the electromagnetic fields in the whole space are governed by the following time-harmonic (time dependence $e^{-i\omega t}$) Maxwell equations:

$$\nabla \times E - i\omega\mu H = 0 , \tag{2.1}$$

$$\nabla \times H + i\omega\epsilon E = 0 , \tag{2.2}$$

where E and H are the electric and magnetic field vectors, respectively.

The problem geometry and material properties are characterized completely by the dielectric coefficient $\epsilon(x)$ ($x = (x_1, x_2, x_3)$) and can be quite general. By this, we mean the following:

- The approach applies to both 1-D gratings and crossed gratings (biperiodic structures). In the 1-D grating case, the approach applies to both of the fundamental polarizations: TE and TM;
- The function $\epsilon(x)$ needs only to be bounded and homogeneous away from some finite region containing the gratings. Inside that region, however, ϵ can be a spatially varying periodic function.

For simplicity in presentation, we restrict ourselves to the two dimensional setting, the medium and grating surface are assumed to be constant in the x_2 direction. The basic variational approach presented here works equally well for biperiodic diffraction (3-D) problems with some necessary modifications described in Section 2.3.

By assuming the medium and grating surface are invariant along the x_2 axis, we may denote $\epsilon(x)$ by $\epsilon(x_1, x_3)$. Further the periodicity implies that

$$\epsilon(x_1 + n\Lambda, x_3) = \epsilon(x_1, x_3), \quad \text{for all } x_1,\ x_3 \tag{2.3}$$

where Λ is the period, n is any integer.

It is natural to assume that ϵ is constant away from a finite region $\{(x_1, x_3) : \ |x_3| < b\}$ for some $b > 0$, *i.e.*, there exist constants ϵ_1 and ϵ_2, such that

$$\epsilon(x_1, x_3) = \epsilon_1 , \quad \text{for } x_3 \geq b , \tag{2.4}$$

$$\epsilon(x_1, x_3) = \epsilon_2 , \quad \text{for } x_3 \leq -b . \tag{2.5}$$

In order to solve the problem, we also need to impose appropriate boundary conditions. The standard jump conditions for E and H still hold and are implicitly enforced by our variational formulation. But under our formulation, it is not necessary to break the domain into subdomains and study them separately. Rather, we treat the diffraction problem as a whole. Since the domain is unbounded in the x_3 direction, the radiation condition must be enforced at the infinity. An important step for the variational approach is to reduce the diffraction problem into a bounded domain, and for this we need a technique to derive the boundary conditions from the radiation condition. This topic is discussed in the next section.

2.2 Variational formulation

We want to demonstrate the variational approach by solving the diffraction problem with TE polarization in the 1-D grating case, where the electric field vector E is parallel to the grooves $E||\vec{x}_2$. Let $E = u\vec{x}_2$ where $u = u(x_1, x_3)$ is a scalar function. Maxwell's equations then become a Helmholtz equation:

$$(\triangle + k^2)u = 0 \,, \quad \text{in } \mathbf{R}^2 \,, \tag{2.6}$$

where k is the magnitude of the wave vector, $k^2 = \omega^2\epsilon\mu$, and $\triangle = \partial^2_{x_1} + \partial^2_{x_3}$ is the Laplacian. Correspondingly, let $k_1^2 = \omega^2\epsilon_1\mu$ and $k_2^2 = \omega^2\epsilon_2\mu$. Also, we assume that $Im\ k_j \geq 0$ $(j = 1, 2)$.

Suppose an incoming plane wave $u_I = e^{i\alpha x_1 - i\beta_1 x_3}$ is incident on the grating from the top, where $\alpha = k_1 \sin\theta$, $\beta_1 = k_1\cos\theta$, and $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ is the angle of incidence. We are interested in "quasiperiodic" solutions u, that is, solutions u such that $ue^{-i\alpha x_1}$ are Λ-periodic.

Define $u_\alpha = ue^{-i\alpha x_1}$. Then u_α satisfies

$$(\triangle_\alpha + k^2)u_\alpha = 0 \,, \quad \text{in } \mathbf{R}^2, \tag{2.7}$$

where the operator $\triangle_\alpha$ is defined by $\triangle_\alpha = \triangle + 2i\alpha\partial_{x_1} - |\alpha|^2$.

Let $\Omega_1 = \{x \in \mathbf{R}^2 : x_3 > b\}$, $\Omega_2 = \{x \in \mathbf{R}^2 : x_3 < -b\}$. Denote the plane $x_3 = b$ by Γ_1, and the plane $x_3 = -b$ by Γ_2. We wish to reduce the problem to the bounded domain $\Omega = \{(x_1, x_3) \in \mathbf{R}^2 : \ -b < x_3 < b\}$. This may be done by introducing a pair of "transparent" boundary conditions on Γ_1 and Γ_2. Let us first impose a radiation condition for the diffraction problem. We insist that u_α is composed of bounded outgoing plane waves in Ω_1 and Ω_2, plus the incident wave u_I in Ω_1.

For each n, let $\alpha_n = \dfrac{2\pi n}{\Lambda}$. Since u_α is periodic in the x_1 direction, it has a Fourier series expansion:

$$u_\alpha(x_1, x_3) = \sum_{n\in Z} u_\alpha^{(n)}(x_3)e^{i\alpha_n x_1}, \tag{2.8}$$

where

$$u_\alpha^{(n)}(x_3) = \frac{1}{\Lambda}\int_0^\Lambda u_\alpha(x_1, x_3)e^{-i\alpha_n x_1}dx_1.$$

Define for $j = 1, 2$ the coefficients

$$\beta_j^n(\alpha) = e^{i\gamma_j^n/2}|k_j^2 - (\alpha_n + \alpha)^2|^{1/2}, \quad n \in Z, \tag{2.9}$$

where

$$\gamma_j^n = arg(k_j^2 - (\alpha_n + \alpha)^2), \quad 0 \le \gamma_j^n < 2\pi. \tag{2.10}$$

In particular, for real k_j,

$$\beta_j^n(\alpha) = \begin{cases} \sqrt{k_j^2 - (\alpha_n + \alpha)^2}, & k_j^2 > (\alpha_n + \alpha)^2 \ , \\ i\sqrt{(\alpha_n + \alpha)^2 - k_j^2}, & k_j^2 < (\alpha_n + \alpha)^2 \ . \end{cases}$$

We assume that $k_j^2 \neq (\alpha_n + \alpha)^2$ for all $n \in Z$, $j = 1, 2$. This condition excludes "resonance" and ensures that the Green functions for (2.7) exist inside Ω_1 and Ω_2. It then follows from knowledge of the Green functions (see e. g. [21] and [22]) that inside Ω_1 and Ω_2, u_α can be expressed as a sum of plane waves:

$$u_\alpha|_{\Omega_j} = \sum_{n \in Z} a_j^n e^{\pm i\beta_j^n(\alpha)x_3 + inx_1}, \quad j = 1, 2, \tag{2.11}$$

where the a_j^n are complex scalars.

From (2.8) and (2.11) we then have the condition that

$$u_\alpha^{(n)}(x_3) = \begin{cases} u_\alpha^{(n)}(b)e^{i\beta_1^n(\alpha)(x_3-b)}, & n \neq 0, \text{ in } \Omega_1, \\ u_\alpha^{(0)}(b)e^{i\beta_1(x_3-b)} + e^{-i\beta_1 x_3} - e^{i\beta_1(x_3-2b)}, & n = 0, \text{ in } \Omega_1, \\ u_\alpha^{(n)}(-b)e^{-i\beta_2^n(\alpha)(x_3+b)}, & \text{in } \Omega_2. \end{cases} \tag{2.12}$$

From (2.12) we can then calculate the derivative of $u_\alpha^n(x_3)$ with respect to ν, the unit normal, on Ω:

$$\left.\frac{\partial u_\alpha^{(n)}}{\partial \nu}\right|_{\Gamma_j} = \begin{cases} i\beta_1^n(\alpha)u_\alpha^{(n)}(b), & n \neq 0, \text{ on } \Gamma_1, \\ i\beta_1 u_\alpha^{(0)}(b) - 2i\beta_1 e^{-i\beta_1 b}, & n = 0, \text{ on } \Gamma_1, \\ i\beta_2^n(\alpha)u_\alpha^{(n)}(-b) \ , & \text{on } \Gamma_2. \end{cases} \tag{2.13}$$

Thus from (2.11), (2.13), one can derive the following boundary conditions:

$$\left.\frac{\partial u_\alpha}{\partial \nu}\right|_{\Gamma_1} = \sum_{n \in Z} i\beta_1^n(\alpha)u_\alpha^{(n)}(b)e^{inx_1} - 2i\beta_1 e^{-i\beta_1 b} = T_1(u_\alpha|_{\Gamma_1}) - 2i\beta_1 e^{-i\beta_1 b} \ , \tag{2.14}$$

$$\left.\frac{\partial u_\alpha}{\partial \nu}\right|_{\Gamma_2} = \sum_{n \in Z} i\beta_2^n(\alpha)u_\alpha^{(n)}(-b)e^{inx_1} = T_2(u_\alpha|_{\Gamma_2}) \ , \tag{2.15}$$

where the operator T_j is defined by

$$(T_j f)(x_1) = \sum_{n \in Z} i\beta_j^n(\alpha)f^{(n)}e^{i\alpha_n x_1}, \tag{2.16}$$

where $f^{(n)} = \frac{1}{\Lambda}\int_0^\Lambda f(x_1)e^{-i\alpha_n x_1}$. Note that T_j is nonlocal.

The diffraction problem can be formulated as follows: find $u_\alpha \in H^1(\Omega)$ that satisfies

$$(\triangle_\alpha + k^2)u_\alpha = 0 \ , \quad \text{in } \Omega, \tag{2.17}$$

and (2.14-2.15). The function space $H^1(\Omega)$ is a standard Sobolev space that contains complex valued functions g that satisfy $g \in L^2(\Omega)$ and $\partial_{x_1}g$, $\partial_{x_3}g \in L^2(\Omega)$ in the distribution sense.

The space $L^2(\Omega)$ contains all of the functions that are square integrable in Ω. Similarly, $H^2(\Omega)$ contains square integrable functions, whose first order and second order derivatives are also square integrable in Ω. It is obvious to see that $H^2(\Omega) \subset H^1(\Omega) \subset L^2(\Omega)$. Note that the space H^l with superscript l should not be confused with the magnetic field vector H.

Finally, we can now derive the variational, or weak, formulation of the problem (2.17). Let ϕ be a smooth function, often referred to as a "test" function, which is periodic in the x_1 direction of the same period Λ as u_α.

Multiplying both sides of (2.17) by $\overline{\phi}$ (the complex conjugate of ϕ) gives

$$\int (\Delta_\alpha + k^2) u_\alpha \cdot \overline{\phi} = 0 \ .$$

Applying Green's formula reveals that

$$\begin{aligned} &- \int_\Omega \nabla u_\alpha \cdot \nabla \overline{\phi} + \int_\Omega (k^2 - \alpha^2) u_\alpha \overline{\phi} + 2i\alpha \int_\Omega (\partial_{x_1} u_\alpha) \overline{\phi} \\ &+ \int_{\Gamma_1} (T_1 u_\alpha) \overline{\phi} + \int_{\Gamma_2} (T_2 u_\alpha) \overline{\phi} - \int_{\Gamma_1} 2i\beta_1 e^{-i\beta_1 b} \overline{\phi} = 0 \ , \end{aligned} \tag{2.18}$$

which is the weak form of the problem (2.17) and the boundary conditions (2.14) and (2.15). We emphasize the usefulness of the weak formulation. It is easy to see that if $u_\alpha \in C^2$, *i.e.*, with continuously differentiable second derivatives, the weak form (2.18) will be equivalent to the boundary value problem (2.17), (2.14), and (2.15). Since it only involves the first order derivatives of u_α, the weak form allows us to seek the solutions in a broader functional space. In addition, the fact that the boundary conditions are enforced implicitly by the weak formulation has a definite advantage for the computation and analysis of the solutions.

2.3 Other models

We mention briefly how the idea can be further generalized to study more complicated situations.

The case of TM polarization for 1-D gratings can be modeled similarly. Once again, assume that the fields and geometry are invariant in the x_2 direction. TM polarization implies that the magnetic field vector H is directed along the x_2 axis, *i.e.*, $H = u\vec{x}_2$, where $u(x_1, x_3)$ is a scalar function. In this case, the Maxwell equations (2.1), (2.2) can be reduced to

$$\nabla_\alpha \cdot (\frac{1}{k^2} \nabla_\alpha u_\alpha) + u_\alpha = 0, \tag{2.19}$$

where the operator ∇_α is defined to be $\nabla + i(\alpha, 0)$. Since k is a fixed constant in Ω_j $(j = 1, 2)$, one may derive the boundary conditions of u_α on Γ_j in a similar fashion. Actually, the following weak form of the problem may be derived similarly as for the TE case:

$$\begin{aligned} &- \int_\Omega \frac{1}{k^2} \nabla u_\alpha \cdot \nabla \overline{\phi} + \int_\Omega (\omega^2 - \frac{\alpha^2}{k^2}) u_\alpha \overline{\phi} + i\alpha \int_\Omega \frac{1}{k^2} (\partial_{x_1} u_\alpha) \overline{\phi} - i\alpha \int_\Omega \frac{1}{k^2} u_\alpha \overline{\partial_{x_1} \phi} \\ &+ \int_{\Gamma_1} \frac{1}{k_1^2} (T_1 u_\alpha) \overline{\phi} + \int_{\Gamma_2} \frac{1}{k_2^2} (T_2 u_\alpha) \overline{\phi} - \int_{\Gamma_1} 2i\beta_1 \frac{1}{k_1^2} e^{-i\beta_1 b} \overline{\phi} = 0 \ , \end{aligned} \tag{2.20}$$

where T_j is defined in (2.16). Details on the formulation in TM polarization may be found in [23].

We next consider the biperiodic structure and conical diffraction. By biperiodic, we mean that there are two constants Λ_1 and Λ_2, such that

$$\epsilon(x_1 + n_1\Lambda_1, x_2 + n_2\Lambda_2, x_3) = \epsilon(x_1, x_2, x_3) \ . \tag{2.21}$$

Similar to (2.4), (2.5), we assume that

$$\epsilon(x_1, x_2, x_3) = \epsilon_1 \ , \ \text{for } x_3 \geq b \ , \tag{2.22}$$

$$\epsilon(x_1, x_2, x_3) = \epsilon_2 \ , \ \text{for } x_3 \leq -b \ . \tag{2.23}$$

Consider a plane wave in Ω_1

$$E_I = s e^{iq\cdot r} \ , \ H_I = p e^{iq\cdot r} \ , \tag{2.24}$$

incident on the grating structure. Here $q = (\alpha_1, \alpha_2, -\beta)$ is the incident wave vector, s and p are vectors in $\mathbf{R}^3$ satisfying

$$s = \frac{1}{\epsilon_1}(p \times q) \ , \ q \cdot q = k_1^2 \ , \ p \cdot q = 0 \ . \tag{2.25}$$

The incident wave vector is no longer constrained to lie in a plane orthogonal to one of the linear grating structures, thus corresponding to the more general conical diffraction problem.

We are interested in quasiperiodic solutions E and H, such that the fields E_α, H_α defined by

$$E_\alpha = e^{-i(\alpha_1 x_1 + \alpha_2 x_2)} E(x_1, x_2, x_3),$$

$$H_\alpha = e^{-i(\alpha_1 x_1 + \alpha_2 x_2)} H(x_1, x_2, x_3).$$

are periodic in the x_1 direction of period Λ_1 and in the x_2 direction of period Λ_2.

Denote

$$\nabla_\alpha = \nabla + i(\alpha_1, \alpha_2, 0) \ .$$

It is easy to see from (2.1) and (2.2) that E_α and H_α satisfy

$$\nabla_\alpha \times E_\alpha - i\omega\mu H_\alpha = 0 \ , \tag{2.26}$$

$$\nabla_\alpha \times H_\alpha + i\omega\epsilon E_\alpha = 0 \ . \tag{2.27}$$

It follows that for differentiable E_α and H_α, the system (2.26) and (2.27) are equivalent to:

$$\nabla_\alpha \times (\frac{1}{\epsilon\mu}\nabla_\alpha \times H_\alpha) - \omega^2 H_\alpha = 0 \ , \tag{2.28}$$

$$\nabla_\alpha \times H_\alpha + i\omega\epsilon E_\alpha = 0 \ . \tag{2.29}$$

Due to a consideration for coercivity, it turns out to be natural to solve

$$\nabla_\alpha \times (\frac{1}{\epsilon\mu}\nabla_\alpha \times H_\alpha) - \nabla_\alpha(\frac{1}{\epsilon\mu}\nabla_\alpha \cdot H_\alpha) - \omega^2 H_\alpha = 0 \ , \tag{2.30}$$

in stead of (2.28). Obviously, if H_α is a solution to (2.28), it must be a solution to (2.30). Conversely, if H_α satisfies (2.30) along with $\nabla_\alpha \cdot H_\alpha = 0$, then H_α satisfies (2.28).

In order to solve the system of differential equations, we need boundary conditions in the x_3 direction. These conditions may be derived by the radiation condition and the Green functions fashioning after the derivation in Section 2.2. A detailed account of the method and numerical examples may be found in [9].

Recently in [24] and [25], the variational method has also been generalized to model second harmonic generation of nonlinear optical media in a 1-D periodic structure.

2.4 Existence and uniqueness

Since 1990, considerable progress has been made in understanding the well-posedness of the diffraction problem. By well-posedness of a model, we mean that the following three conditions are satisfied: the model has a solution (existence); the solution is unique; the solution depends on the data continuously – a small perturbation of the data implies a small change of the solution. Obviously, well-posedness issues are of great importance in modeling any physical process. In 1980, Petit acknowledged, on Page 8 of [1], "To my knowledge, the existence of solution – which seems obvious to physicists – has never been established by mathematicians". At the time, there were also few uniqueness results, see [11]. Little was known on questions regarding continuous dependence arising from the error analysis in design and manufacturing of optical devices.

Here we give a brief summary of recent results and approaches dealing with issues of well-posedness of the rigorous grating problem. For Maxwell's equations in a biperiodic structure that separates two homogeneous materials and is piecewise C^2, the existence and uniqueness of the solutions were established in [22] by an integral equation approach. By using the jump conditions, the authors were able to reduce the problem to an equivalent system of integral equations and then applied the standard Fredholm theory. In particular, it was shown that there exists a unique solution at all but a countable set of frequencies. The result generalized the earlier work [21] for 1-D gratings, see also [26]. The integral equation approach was also implemented numerically [27].

Another approach is based on the variational method. It has the advantage for dealing with extremely general diffraction structures as well as materials. The basic idea is to establish coercivity for the bilinear form of the variational formulation then apply the Lax-Milgram lemma and the Fredholm alternative. Existence and uniqueness results were proved in TE polarization [28], in the TM case [23], and for biperiodic structures [9]. The general result may be stated as:

$$\begin{array}{l}\text{For all but a sequence of countable frequencies } \omega_j,\ |\omega_j| \to +\infty,\\ \text{the diffraction problem has a unique solution.}\end{array} \tag{2.31}$$

Abboud and Nédélec [29] independently developed the variational formulation for Maxwell's equations in a bounded inhomogeneous medium. They were interested in the more general problem where the magnetic permeability is also allowed to be a variable function. Their approach was further extended by Abboud to the periodic case in [10] and [30].

In general, the result (2.31) is the best possible. There are examples which indeed exhibit the existence of singular frequencies (the sequence) in (2.31). We refer to [31] where the authors constructed explicit examples and showed nonuniqueness at the singular frequencies in the TM case. It was also shown that in general the sequence in (2.31) is unbounded. It is interesting to note that, in additional to (2.31), Abboud [10] showed that

$$\text{If } Im\ \epsilon_1 > 0 \text{ or } Im\ \epsilon_2 > 0, \text{ then the diffraction problem has a unique solution.} \tag{2.32}$$

Thus, for media that are absorbing either in Ω_1 or Ω_2, the diffraction problem always has a unique solution.

Continuous dependence was studied [32] in a simple TE case with 1-D gratings that separate a dielectric medium from a perfectly reflecting medium (conductor). According to Section 2.2, the model equation has the form

$$(\Delta + k^2)u = 0\,, \tag{2.33}$$

$$u|_S = 0 \tag{2.34}$$

together with the boundary condition (2.14), where S is the grating profile. It was shown that the solution depends on k and θ analytically, provided that $(\alpha_n + k cos\theta)^2 \neq k^2$ for every integer n, where k^2 is real and θ is the angle of incidence. However, the dependence of solutions on the grating profile turns out to be a bit more complicated. In fact, using the variational formulation of Section 2.2, it was shown [32] that

$$||u_f - u_g||_{H^1} \leq C||f - g||_{C^1} \tag{2.35}$$

where the constant C is independent of u_f, u_g and f, g. Here u_f and u_g are the solutions generated by grating profiles f and g (2.33-2.34), respectively, for a given (fixed) incident wave.

3 Convergence of the variational approach

Having described the variational formulation and some basic mathematical properties, we now consider its numerical implementation by means of the finite element method. In this section we first describe basic ideas of the finite element method and present some recent convergence results for the finite element method in solving the diffraction problem in different polarization conditions, highlighting the fundamental differences between TE and TM polarizations with regard to convergence.

3.1 Finite element method

The method of finite elements offers effective means for solving differential equations numerically. Its mathematical foundation combines the variational approach and the approximation theory. The reader is referred to the classic book [33] for the basic theory and additional references.

To demonstrate the idea, let us once again concentrate on 1-D gratings – the 2-D diffraction problem. In fact, the method has been applied to solve biperiodic diffraction problems in [9] and [10], and scattering problems in general (nonperiodic) structures. As discussed in Sections 2.1 and 2.2, the diffraction problem has an equivalent variational form: find $u_\alpha \in H^1(\Omega)$ such that

$$a(u_\alpha, \phi) = (f, \phi)\,, \quad \forall \phi \in H^1(\Omega), \tag{3.1}$$

where a is a bilinear form, which is linear with respect to each of the components. In the TE case, according to (2.18), the bilinear form a is defined by

$$\begin{aligned} a(u_\alpha, \phi) &= \int_\Omega \nabla u_\alpha \cdot \nabla \overline{\phi} - \int_\Omega (k^2 - \alpha^2) u_\alpha \overline{\phi} - 2i\alpha \int_\Omega (\partial_{x_1} u_\alpha) \overline{\phi} \\ &\quad - \int_{\Gamma_1} (T_1 u_\alpha) \overline{\phi} - \int_{\Gamma_2} (T_2 u_\alpha) \overline{\phi}\,, \end{aligned} \tag{3.2}$$

and

$$(f, \phi) = -\int_{\Gamma_1} 2i\beta_1 e^{-i\beta_1 b} \overline{\phi}. \tag{3.3}$$

In the TM case, one only needs to replace (3.2) with

$$\begin{aligned} a(u_\alpha, \phi) &= -\int_\Omega \frac{1}{k^2} \nabla u_\alpha \cdot \nabla \overline{\phi} + \int_\Omega (\omega^2 - \frac{\alpha^2}{k^2}) u_\alpha \overline{\phi} + i\alpha \int_\Omega \frac{1}{k^2} (\partial_{x_1} u_\alpha) \overline{\phi} - i\alpha \int_\Omega \frac{1}{k^2} u_\alpha \overline{\partial_{x_1} \phi} \\ &\quad + \int_{\Gamma_1} \frac{1}{k_1^2} (T_1 u_\alpha) \overline{\phi} + \int_{\Gamma_2} \frac{1}{k_2^2} (T_2 u_\alpha) \overline{\phi} - \int_{\Gamma_1} 2i\beta_1 \frac{1}{k_1^2} e^{-i\beta_1 b} \overline{\phi} \end{aligned} \tag{3.4}$$

and (3.3) with

$$(f, \phi) = -\int_{\Gamma_1} 2i\beta_1 \frac{1}{k_1^2} e^{-i\beta_1 b} \overline{\phi} \tag{3.5}$$

because of (2.20).

Let $\{S^h : h \in (0,1]\}$ denote a family of finite dimensional subspaces of H^1, usually a space of piecewise polynomials, where h stands for the maximum mesh size after partitioning Ω into simple subdomains. Assume also that S^h satisfies some standard approximation assumptions. We define the finite element approximation u^h of the solution u_α of (3.1) by the following equation, for each $v^h \in S^h$,

$$a(u^h, v^h) = (f, v^h)\,. \tag{3.6}$$

In fact, this provides the basic idea for solving our model equation: One first chooses a basis of S^h, $\{\phi_1, \phi_2, ..., \phi_k\}$, which is a finite set according to the definition of S^h. Substituting the expression of

$$u^h = c_1\phi_1 + c_2\phi_2 + \cdots + c_k\phi_k \tag{3.7}$$

into the equation (3.6), by choosing $v^h = \phi_i$, $i = 1, \cdots, k$, one gets a system of linear equations. Solving this system for $\{c_j\}$ then leads to an approximation of u_α in S^h.

In practice, there are two general strategies to increase the accuracy of a finite element method. One can either increase the order of polynomials in S^h or reduce the grid size h. Due to the lack of regularity of the solutions, we shall adopt the latter. Also, the basis of

S^h can often be chosen so that the sequence ϕ_j satisfies some orthogonality condition. The advantage is the sparsity of the resulting system of linear equations. Having introduced the method of finite elements, the first question one should ask is: under what conditions is u^h of (3.7) a reasonable approximation of u_α ? Alternatively, in what sense does u^h converge to u_α ? In the next two sections, we shall answer these questions for the TE and TM cases. Without loss of generality, we shall assume in Sections 3.2-3.4 that the continuous problem (3.1) has a unique solution.

3.2 The TE case

In order to establish convergence, we analyze two sources of errors in the finite element approximation. First, we consider the discretization of the continuous problem. The goal is to show that u_h, the solution to (3.6), is a good approximation to u_α. Second, we analyze truncations of nonlocal boundary operators T_j ($j = 1,2$) (2.16). The fact T_j is nonlocal follows immediately from the infinite series expansion. In reality, it is essential to obtain error estimates when truncations of these operators take place. Of course, we also want to establish existence and uniqueness for the discretized problem. The following well-posedness results and error estimates were established in [34].

Concerning the discretization error, the following result holds.

> There exists a constant $0 < h_0 \leq 1$, such that for any h, $0 < h < h_0$, the discretized problem (3.6) attains a unique solution u^h, and
> $$||u_\alpha - u^h||_{L^2(\Omega)} \leq Ch^2 , \tag{3.8}$$
> $$||u_\alpha - u^h||_{H^1(\Omega)} \leq Ch^1 , \tag{3.9}$$
> where the constant C is independent of h.

Further, the error estimates are optimal.

Define u_N^h, the truncated finite element approximation to the solution u by the equation

$$a^N(u_N^h, v^h) = (f, v^h) , \quad \forall v^h \in S^h , \tag{3.10}$$

where a^N is given by replacing T_j in (3.2) with

$$(T_j^N f)(x_1) = \sum_{|n|<N} i\beta_j^n(\alpha) f^{(n)} e^{i\alpha_n x_1}. \tag{3.11}$$

Our next result indicates that the problem (3.10) is well-posed and estimates similar to (3.8), (3.9) hold, provided that sufficiently many (but finite) terms are taken in the expressions of T_j and h is sufficiently small.

> There exist $h_0 \in (0,1]$ and an integer N_0 independent of h_0, such that for $h \in (0, h_0)$ and $N \geq N_0$, the problem (3.10) attains a unique solution u_N^h. Moreover, the following estimates hold

$$||u_\alpha - u_N^h||_{L^2} \leq Ch(h + N^{-1/2}) \ . \tag{3.12}$$

$$||u_\alpha - u_N^h||_{H^1} \leq Ch \tag{3.13}$$

where C is independent of h and N.

Thus the estimates (3.19) and (3.20) remain valid for the truncated problem so long as the number of terms N is on the order of h^{-2}.

3.3 The TM case

For TM polarization, Maxwell's equations can be reduced to (see (2.19) of Section 2.3),

$$\nabla_\alpha \cdot (\frac{1}{k^2}\nabla_\alpha u_\alpha) + u_\alpha = 0 \ , \quad \text{in } \mathbf{R}^2, \tag{3.14}$$

where k^2 may vary in different parts of the medium. It follows from the standard theory in partial differential equations that in general the solution u_α is only in H^1 and may not be in $H^{1+\delta}$ for any $\delta > 0$. It is essentially due to the lack of smoothness that one can not expect explicit convergence rates in this case. Nevertheless, the following uniform convergence results together with well-posedness results for both the continuous and discretized problems were established in [23].

Suppose that (3.1) has a unique solution $u_\alpha \in H^1(\Omega)$. The first result concerns the finite element approximation (3.6).

For any given $\delta > 0$, there exists $h_0 = h_0(\delta)$, such that for $0 < h < h_0$,

$$||u_\alpha - u^h||_{L^2(\Omega)} \leq \delta ||u_\alpha - u^h||_{H^1(\Omega)} \ . \tag{3.15}$$

Moreover, if $f \in L^2(\Omega)$ in (3.1), there exists an $h_1 = h_1(\delta)$ such that for all $0 < h < h_1$,

$$||u_\alpha - u^h||_{H^1(\Omega)} \leq \delta ||f||_{L^2(\Omega)} \ . \tag{3.16}$$

The estimates establish the existence and uniqueness for the finite element approximation (3.6). Actually, because of the finite dimensionality of S^h, the uniqueness implies the existence. Moreover, since h_0, h_1 are independent of u_α, the estimates are uniform with respect to u_α.

Next, we consider the approximation of the boundary operators by T_j^N defined as, for $j = 1, 2$,

$$T_j^N f(x_1) = \sum_{|n|<N} i\beta_j^n f^{(n)} e^{inx_1} \ . \tag{3.17}$$

Denote u_N^h, the finite element approximation to the solution u_α by the equation

$$a^N(u_N^h, v^h) = (f, v^h) \ , \ \ \forall v^h \in S^h \ , \tag{3.18}$$

where a^N is defined by replacing T_j with T_j^N in (3.4). Then the following well-posedness and convergence result holds for (3.18).

> For any given $\delta > 0$, there exist $h_0(\delta) \in (0,1)$ and an integer N_0, such that for $0 < h < h_0$ and $N \geq N_0$, the problem (3.18) attains a unique solution u_N^h. Moreover,
>
> $$||u_\alpha - u_N^h||_{L^2(\Omega)} \leq e^{-\gamma N}||u_\alpha||_{H^1(\Omega')} + \delta||u_\alpha - u_N^h||_{H^1(\Omega)} \,. \qquad (3.19)$$
>
> In addition, if $f \in L^2(\Omega)$, there exists an $h_1 = h_1(\delta)$, such that for $0 < h < h_1$
>
> $$||u_\alpha - u_N^h||_{H^1(\Omega)} \leq \delta||f||_{L^2(\Omega)} + e^{-\frac{1}{2}\gamma N}||u_\alpha||_{H^1(\Omega')} \,. \qquad (3.20)$$
>
> Here $0 < \gamma \leq 1$ and $\Omega \subset\subset \Omega'$.

Once again, since h_0, h_1 are independent of u, the estimates are uniform with respect to u_α.

In applications, the material parameter function ϵ can often be assumed to be piecewise constant in the x_3 direction. In other words, the problem may be viewed as an interface problem with a finite number of interfaces. It then follows from the classical theory of partial differential equations that when the interfaces are of C^2, the solution (3.14) has improved regularity, *e.g.* H^2, up to both sides of an interface. In that case, optimal convergence rates will be possible when the problem is discretized in both sides as well. Therefore, by taking the specific problem geometry into account, one may obtain better convergence rates for the finite element method than the above estimates. However, since many useful grating structures are only piecewise smooth, the convergence results (3.15), (3.16), (3.19), and (3.20) in general may not be improved.

3.4 Discussions on convergence

Although the finite element method does converge in the TM case, the algorithm converges more slowly than the TE case. In general it is very difficult to obtain any explicit convergence rate without making use of the special grating structures. The difficulties are largely due to the discontinuous coefficient present in the second-order operator of the model equation. This presents a clear contrast to the TE case, where discontinuous coefficients only occur in the lower order terms. Thus in the TM case, the singularities caused by the discontinuous coefficients can spread more destructively. As a result, the solution is only in H^1, and is generally not any more regular, while the solution in the TE case is in H^2 in general.

Our variational approach has been discretized in finite element form and implemented in a FORTRAN computer code (MAXFELM). As part of the process of validating and testing the code for accuracy and convergence, we have examined numerous gratings having both dielectric and metallic substrates in both polarizations (TE and TM). We can draw on a simple numerical example from this work to illustrate the conclusions about convergence cited above.

We consider the simple linear grating in a silver substrate shown in Figure 2. The grating has a period 1.7μ illuminated by near infrared light (wavelength 0.78μ) incident at forty-five degrees in TE or TM polarization, and we wish to calculate the total reflectivity in all propagating orders for grating heights of 0.2μ and 0.3μ. This device was studied originally at Honeywell as a polarization beamsplitter for an optical disk readhead. We expect the execution time of the variational method to vary approximately as the number of grid points. This is corroborated by the data presented in Figure 3 showing the observed execution times needed to achieve numerical convergence of 0.0005 for TM polarization. Moreover, because this is a 2-D problem, the discretization parameter h is proportional to the square root of the number of grid points. Figure 4 shows the actual rates of convergence obtained using the MAXFELM code in both polarizations and for both grating heights. In both cases the variational method converges smoothly, but we find significantly faster convergence in TE polarization, in agreement with the conclusions of the previous two sections.

Because of the mathematical nature of the model equations, for general structures the convergence difficulties will appear, perhaps in a different manner, in all other known methods for solving the grating problem.

Although the above error analysis is absolutely essential for any robust finite element algorithm, it should be pointed out that additional errors or approximations may also take place. For example, the system of linear equations resulting from the finite element approximation usually can not be solved exactly. There are also numerical discretization and truncation errors. In computation, these additional errors could cause convergence difficulties as well.

Finally, we believe that the approach in [23] may be generalized to study convergence properties of the finite element method for the biperiodic case.

4 The inverse problem

Given the incident field and the desired out-going fields, the inverse problem concerns the determination of the grating profile.

4.1 Problem description

We describe some recent progress in the mathematical studies of inverse diffraction problems and optimal design problems. From now on, we assume that the structure is a 1-D grating and the fields are TE polarized. Note that even for 1-D gratings, very little is known in the TM case, see [35] for a stability result in the TM case.

Consider a plane wave incident on a periodic structure from above, see the problem geometry in Figure 5. The structure separates two regions. In one region, above the periodic structure, the dielectric coefficient ϵ is a fixed constant, so is the index of refraction k. The other region contains a perfectly reflecting material (or conductor). Given the incident field, an inverse diffraction problem is then to determine the periodic structure from the scattered field. Let the incident wave be of the form

$$u_I = e^{i\alpha x_1 - i\beta_1 x_3} \tag{4.1}$$

where $\alpha = k\sin\theta$, $\beta_1 = k\cos\theta$, and $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ is the angle of incidence.

As discussed in Sections 2.2 and 2.4, the direct model equation has a simple form

$$(\Delta + k^2)u = 0, \tag{4.2}$$
$$u|_S = 0, \tag{4.3}$$

where S is the grating profile. We again seek quasiperiodic solutions to this problem, *i.e.*, solutions u such that $ue^{i\alpha x_1}$ are Λ-periodic for every x_3, here Λ is the period of the grating. Using the quasiperiodicity of the solution and the radiation condition that requires the boundedness of u as x_3 tends to infinity, we arrive at the boundary condition as in Section 2.2

$$\frac{\partial u}{\partial \nu}|_{x_3=b} = B(u|_{x_3=b}) - 2i\beta e^{-i\beta b + i\alpha x_1}, \tag{4.4}$$

where

$$B(f) = \sum_{n\in Z} i\beta_j^n f^{(n)} e^{i(\alpha_n+\alpha)x_1}, \tag{4.5}$$

and α_n and β_n are defined in Section 2.2. Therefore, the inverse problem is to determine S from the information $u|_{x_3=b}$.

A closely related problem is to determine the grating structure on some nonconductive optimal material. In that case, one places optical detectors both above and below the material. Consequently, the measurements consist of information on the reflected wave and transmitted wave. Note that the boundary condition (4.3) should be replaced with a nonlocal boundary condition that is to (4.4). This inverse problem was proposed and studied in [35].

The optimal design problem concerns designing grating profiles that give rise to some specified diffraction patterns. A particular problem is the phase reconstruction problem, where the Fraunhofer approximation is employed and the direct problem is described approximately by the Fourier transform rather than the more complicated Maxwell equations. An optimization approach and convergence results were proposed in [36].

For the optimal design problem, the Maxwell equation approach would provide a more accurate model. In [37] and [28], the variational formulation was employed to model the direct problem, and the inverse (design) problem was solved by a relaxation approach. The variational approach was also used previously in [38] and [39] for solving optimal photocell design problems; while the relaxation optimization method for general design problems was first proposed in [40].

4.2 Uniqueness and stability

By counting the dimensions of the unknowns and data, it is easy to see that the inverse problem is underdetermined. Thus, in general, properties on uniqueness and stability are very hard, if not impossible, to establish. But because of the important impact of these properties on real applications, characterizations of uniqueness and stability are required.

Here, we present a uniqueness result for the inverse problem. Let us assume that for the given incident field u_I, u_1 and u_2 solve the direct problem (4.2-4.4) with respect to $S_1 = \{x_3 = f_1(x_1)\}$ and $S_2 = \{x_3 = f_2(x_1)\}$, respectively. The functions f_1 and f_2 are assumed to be sufficiently smooth, say C^2, and Λ-periodic. Let $b > max\{f_1(x_1), f_2(x_1)\}$ be a fixed constant. Denote $T = max\{f_1(x_1), f_2(x_1)\} - min\{f_1(x_1), f_2(x_1)\}$.

> Assume that $u_1(x_1, b) = u_2(x_1, b)$. Assume further that one of the following conditions is satisfied:
>
> (i) k has a nonzero imaginary part; (4.6)
>
> (ii) k is real and T satisfies $k^2 < 2[T^{-2} + \Lambda^{-2}]$. (4.7)
>
> Then $f_1(x_1) = f_2(x_1)$.

Thus in the case when k has nonzero imaginary part corresponding to a lossy medium, a global uniqueness result is available [41]. In the case with real k corresponding to a dielectric medium, one can only prove a local uniqueness result, *i.e.*, any two surface profiles are identical if they generate the same diffraction patterns and the area in between the two profiles are sufficiently small, see [42] or [43] for a proof. Moreover, the smallness of the area is characterized explicitly in terms of a condition which relates the index of refraction k, the period, and the maximum of the difference in height allowed for the two profiles, see [43] for details.

Uniqueness for the inverse diffraction problem in periodic structure was also studied in [44] for a dielectric medium, where a uniqueness theorem was proved by a approach for the general inverse scattering problem. The main idea was to prove by using many incident waves the denseness of a set of special solutions. For the optical applications we are interested in, one is only allowed to use single or a small number of incident plane waves.

In applications, it is impossible to make exact measurements. Stability is crucial in the real reconstruction of profiles since it contains necessary information to determine to what extent the data can be trusted.

Before stating the stability result, let us first introduce some notations. For any two domains D_1 and D_2 in $\mathbf{R}^2$, define $d(D_1, D_2)$ the Hausdorff distance between them by

$$d(D_1, D_2) = max\{\rho(D_1, D_2),\ \rho(D_2, D_1)\} \tag{4.8}$$

where

$$\rho(D_1, D_2) = sup_{x\in D_1}\ inf_{y\in D_2}|x - y|\ . \tag{4.9}$$

The Hausdorff distance provides a natural measure of the distance between two sets.

Denote $D = \{x;\ f(x_1) < x_3 < b\}$, and a sequence of domains $D_h = \{x;\ f(x_1) + h\sigma_h(x_1)\mu(x_1) < x_3 < b\}$ for any $0 < h < h_0$, where $\mu(x_1)$ is the normal to $S = \{x_3 = f(x_1)\}$. Assume also that the boundary $S_h = \{x_3 = f(x_1) + h\sigma_h(x_1)\mu(x_1)\}$ is periodic of the same period Λ. Further, the function σ_h satisfies $|\sigma_h(x_1)| \leq C$. Furthermore, for h_0 is sufficiently small, the sequence of domains is assumed to satisfied that

$$C_1 h \leq d(D, D_h) \leq C_2 h, \tag{4.10}$$

where C_1 and C_2 are positive constants.

For the fixed incident plane wave u_I, assume that u and u_h solve the scattering problem with respect to periodic structures S and S_h, respectively. Then we have the following stability result

$$d(D_h, D) \leq C||u_h|_{x_3=b} - u|_{x_3=b}||_{H^{1/2}}, \tag{4.11}$$

where the constant C may depend on the family $\{\sigma_h\}$. The result indicates that for small h if D_h is a family of domains which are $O(h)$ close to D in the Hausdorff distance, then the corresponding measurements are also $O(h)$ close to the true scattering fields in the $H^{\frac{1}{2}}$ norm. This result as well as stability results for other models were proved in [35].

4.3 Optimal design

The optimal design problem is easiest to approach in the simplest geometry: 1-D (linear) gratings in TE polarization. See Figure 6. We seek a periodic curve S which defines the grating profile.

Assume that the EM wave has a wave number k_1 in the material above S and wave number k_2 below S. Let $b > \max|S(t)|$, and consider the strip

$$\Omega = \{(x_1, x_3) : -b < x_3 < b\}.$$

As is well known, Maxwell's equations simplify to the scalar Helmholtz equation in this geometry. As discussed previously, a natural variational formulation exists for this problem. Suppose the incident wave vector makes the angle θ with the x_3-axis. Set $\alpha = k_1 \sin\theta$. We have the problem

$$(\Delta_\alpha + a_S)u = 0 \quad \text{in } \Omega, \tag{4.12}$$

$$(T_1 - \frac{\partial}{\partial x_3})u = 2i\beta e^{-i\beta b} \quad \text{on } \{x_3 = b\}, \tag{4.13}$$

$$(T_2 - \frac{\partial}{\partial x_3})u = 0 \quad \text{on } \{x_3 = -b\}, \tag{4.14}$$

where $\Delta_\alpha = \Delta + 2i\alpha\partial_{x_1} - \alpha^2$, and periodic boundary conditions are assumed in x_1. The operators T_j, $j = 1, 2$ are derived as in Section 2.2, with

$$(T_j f)(x_1) = \sum_{n \in Z} i\beta_j^n(\alpha) f^{(n)} e^{inx_1}. \tag{4.15}$$

The function a_S in (4.12) is defined by

$$a_S(x) = \begin{cases} k_1^2 & \text{if } x \text{ is above } S, \\ k_2^2 & \text{if } x \text{ is below } S. \end{cases}$$

As discussed previously, this problem has a unique weak solution $u_\alpha \in H^1(\Omega)$, except possibly for a discrete set of parameters.

Suppose that the materials, the period of the structure, and the frequency of the incoming waves are fixed. There are then a fixed number of propagating modes, each of which corresponds to an index n for which the propagation constant β_j^n is real-valued. Let us define the set of indices of the reflected propagating modes

$$P_r = \{n \text{ integer} : \beta_1^n(\alpha) \text{ is real}\},$$

and indices of transmitted modes

$$P_t = \{m \text{ integer} : \beta_2^m(\alpha) \text{ is real}\}.$$

The coefficients of each propagating reflected mode are determined by the trace of the solution u on the artificial boundary $\{x_3 = b\}$:

$$\begin{aligned} r_n &= u_n(b)e^{-i\beta_1 b} && \text{for } n \neq 0, \quad n \text{ in } P_r, \\ r_0 &= u_0(b)e^{-i\beta_1 b} - const. && \text{for } n = 0, \end{aligned}$$

where $u_n(x_2) = \frac{1}{2\pi}\int_0^{2\pi} u(x_1, x_2)e^{-inx_1}\,dx_1$. Similarly, the coefficients of the propagating transmitted modes are

$$t_m = u_m(-b)e^{-i\beta_2 b} \quad \text{for } m \text{ in } P_t.$$

Writing the reflection and transmission coefficients as vectors

$$r = (r_n)_{n\in P_r}, \quad t = (t_m)_{m\in P_t},$$

denote the pair $(r, t) = F$. The coefficients r_n and t_m, and hence F, are functions of the interface profile S. Denote this dependence by $F(S)$. A general optimal design problem is to find a profile S such that $F(S)$ is as close as possible to some specified diffraction pattern g. Asking that $F(S)$ is close to g in a least-square sense, one obtains the problem

$$\min_{S\in\mathcal{S}} J(S) = \|F(S) - g\|_2^2, \tag{4.16}$$

where $\mathcal{S}$ is some admissible class of profiles. One could of course generalize further and specify a range of incidence angles or a range of frequencies (or both). Such problems fit well within the present framework; one case was studied in [28].

The choice of the admissible set of profiles S is important. To achieve a well-posed optimization problem, there are two general routes. The first is to choose a relatively small admissible set, compact with respect to the topology induced by the map $J(S)$, thus ensuring that the minimization problem has a solution. This has the *possible* side-effect of introducing "artificial constraints", which could result in sub-optimal designs.

The other route is to begin with a large class of admissible curves, and "relax" the problem, enlarging the admissible set to include appropriate "mixtures" of materials (see [40] for a general framework for relaxed design). In the TE case, this relaxed set of admissible designs turns out to be

$$\mathcal{A} = \{a = k_2^2\gamma + k_1^2(1-\gamma) : \gamma \text{ is bounded and measurable}, \ 0 \le \gamma \le 1\}.$$

In this definition, γ represents the volume fraction of optical substrate at any given point in the domain. The weak form of problem (4.12)–(4.14) is well-posed for any mixture $a \in \mathcal{A}$.

The theoretical justification for the admissible set $\mathcal{A}$ is given in [28], where it is also proved that the problem

$$\min_{a\in\mathcal{A}} J(a) = \|F(a) - g\|_2^2, \tag{4.17}$$

is well-posed in the low-frequency case. This formulation of the optimal design problem is described in further detail in [45] and the references therein. Several examples where the minimization (4.17) is done numerically are presented in the same articles.

We mention here that straightforward approaches to the minimization problem, such as the gradient descent method, can be very computationally intensive. We have developed strategies combining preconditioned iterative solvers for the finite element discretization of the direct problem with "adjoint state" calculation of derivatives, and infeasible point techniques from constrained optimization to create reasonably efficient optimization codes.

A practical difficulty with the straightforward relaxed optimal design approach is that it can generate designs which are prohibitively expensive or difficult to fabricate. One remedy we have taken is the use of constraints and penalties in the relaxed design problem in an effort to generate "simple" designs [46]. This approach often yields structures composed of fairly homogeneous "blocks" of material mixtures, which may be achieved in practice by incorporating different materials into the structure. Still, this may not be the most satisfactory solution in many cases.

Another alternative is the following. Recall that the relaxed formulation was obtained by taking a very large class $\mathcal{S}$ of admissible interface profiles in problem (4.16), with the hope of not "artificially constraining" the problem. One can certainly take the opposite approach, and choose a smaller admissible class of interfaces. A natural choice is to restrict the admissible class $\mathcal{S}$ to interfaces given by the graph of a bounded function f of the x_1 variable. This can be done within the general framework of the variational approach.

To implement this approach numerically, we discretized the interface profile as the graph of a sum of step functions

$$f(x_1) = \sum_{j=1}^{N} f_j \chi_j$$

where χ_j is the indicator function in the interval $[(j-1)h, jh)$ and h is the cell width in the x_1 direction. Aligning the finite element grid with the jumps in f, the direct diffraction problem can then be solved using the same finite element codes used in the relaxed formulation. One can calculate the gradient of the least squares cost functional (4.16) with respect to the interface profile using a similar adjoint derivation as in the relaxed case, and solve the minimization problem using a modified version of the optimization code from the relaxed formulation.

This approach is promising, as the following example indicates. Consider the design of an "ideal array generator", a diffractive structure which splits a single normally incident plane wave into several equal intensity transmitted modes with 100% efficiency. We choose the substrate index $k_2 = 1.5$ and take the incoming wave with wavelength 0.63μ. The period of the grating is 1μ; this supports five transmitted orders and three reflected orders. We specify that all transmitted orders have equal energy and all reflected orders have zero energy. Figure 7a shows an example of a relaxed design for the array generator that we had obtained previously. Applying our interface optimization code, we obtained the profile in Figure 7b. The two designs in Figure 7 are equivalent, in the sense that they each generate the same diffraction pattern with near 100% efficiency (up to numerical modeling error). Both designs used a flat substrate as the initial guess for the minimization algorithm. A "binary optics" approximation to the interface profile in Figure 7b would probably be feasible, and simpler to fabricate than the design 7a.

On the other hand, this approach does have difficulties. The essential problem is that without further constraining the class of admissible interfaces, highly oscillatory minimizing sequences can occur. These sequences tend to oscillate more and more as the cost function is decreased, and never converge except in the sense of averages. This is precisely the situation we avoided with the relaxed design approach. As an illustration, consider the problem of maximizing the energy in the +1 transmitted order, given a normally incident wave on a transparent grating which supports nine transmitted orders. The optimal "ramp" profile one could obtain for example using a Fourier optics approximation is shown in Figure 8, along with a gray-scale plot of the real part of the field. This structure is roughly 70% efficient. Running our optimization code on this problem, beginning with a flat initial profile, we obtained a sequence of consecutively "rougher", more oscillatory interface profiles, and eventually stopped the code. An intuitive explanation of this behavior is that the interface profiles are trying to achieve localized "mixtures" by creating areas with finer and finer alternating regions of air and substrate. The design is trying to relax.

There are various ways to avoid this behavior. The simplest is to merely stop the algorithm before the interface gets too oscillatory, and accept the sub-optimal design. Combined with judicious choices of starting profiles, this can give reasonable results. A 98% efficient design for the +1-order maximization problem obtained in this way is shown in Figure 9 (compare with Figure 8).

A more satisfying (and more technically sound) approach is to apply constraints or penalties to the minimization problem (4.16). We are currently pursuing such an approach, using a total variation penalty formulation similar to the approach we took earlier for the relaxed problem. We are optimistic that this approach will result not only in a well-posed mathematical problem, but in an algorithm which generates optimal interface profiles that are easy to fabricate. This work will be described in a future article.

5 Summary

We have described a general variational approach for solving the electromagnetic diffraction and scattering problems in grating structures. Aspects of the well-posedness of this mathematical approach have been examined. In particular, we have presented convergence results for the finite element methods in both TE and TM polarizations. The variational approach and the finite element method exhibit good convergence properties and numerical stability. The approach treats complicated grating structures and general materials.

With regard to the inverse and optimal design problems, recent progress on the mathematical properties of uniqueness and stability has been discussed. We believe that the progress in this area is an important first step in understanding the degree to which it is possible to predict a grating profile from measurement of the efficiencies in the propagating orders. These properties should also be useful in solving optimal design problems. We have also presented some results on the optimal design problems.

There are many interesting research directions in diffractive optics. Here, we want to identify two important problems: nonlinear optics and finite gratings. Recently, we have made some preliminary progress in the study of nonlinear diffractive optics in grating structures, see [24], [47], and [25]. The fundamental problem is to solve the nonlinear Maxwell's equations rigorously and to design grating structures that enhance the nonlinear effects. By far, most of the research in the area of diffractive optics with periodic structure has assumed infinite gratings which allows one to model the problems in one "cell" or one period. In reality, however, one has to deal with gratings of finite extent. Thus a natural question arises: how to simplify the computation in the modeling of diffractive optics in finite structures ? The real challenge is how to take advantage of the finite periodic structures computationally. A closely related problem was first approached by Kriegsman, et al., see for example [48]. We anticipate that the finite grating problem may be solved by a combination of Kriegsman's approach and the variational method of this work.

In conclusion, the field of diffractive optics has presented the applied mathematicians with rich, fresh, and challenging mathematical problems. We hope we have demonstrated that by working together, real differences can be made by the engineering and applied mathematics communities.

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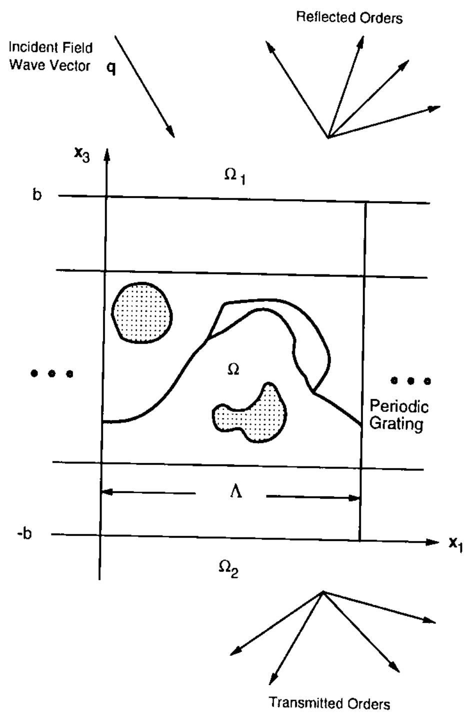

Figure 1: Problem geometry.

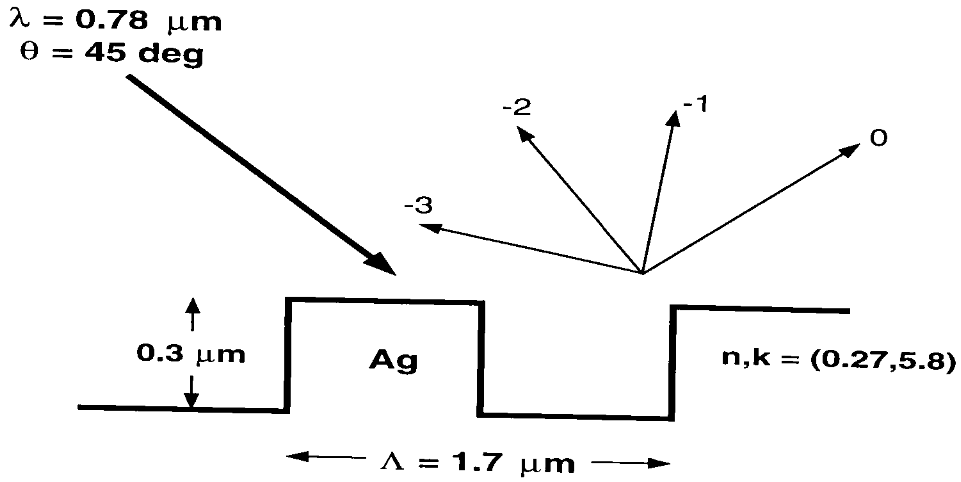

Figure 2: A linear grating in a silver substrate.

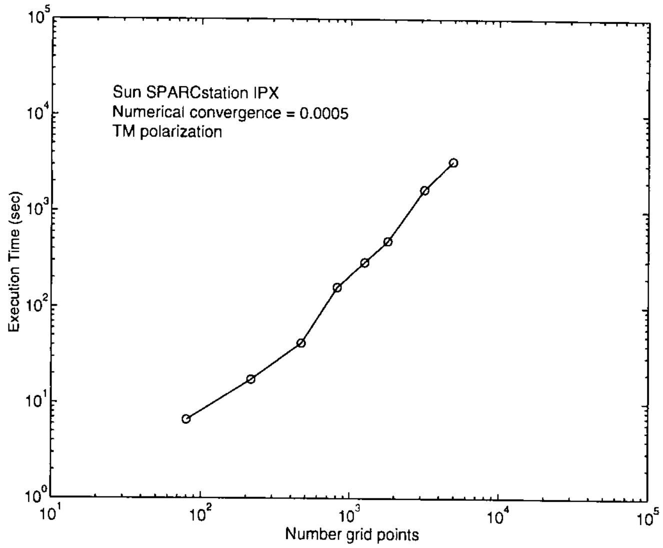

Figure 3: Convergence: the TM case.

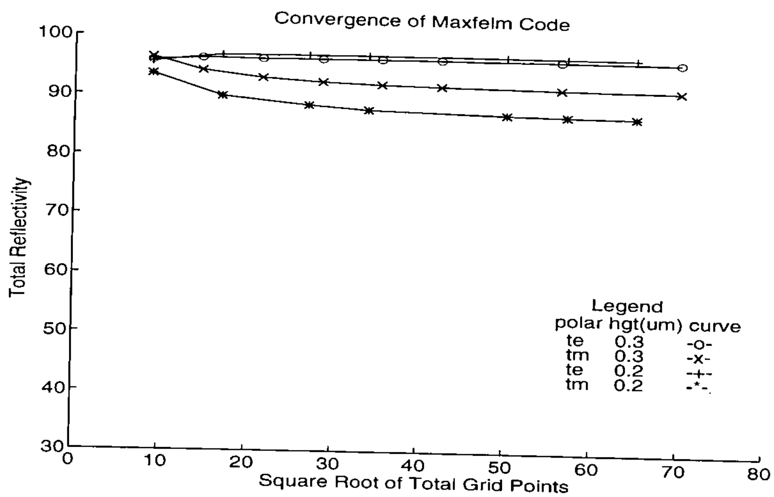

Figure 4: Convergence of the MAXFELM code in TE and TM polarizations.

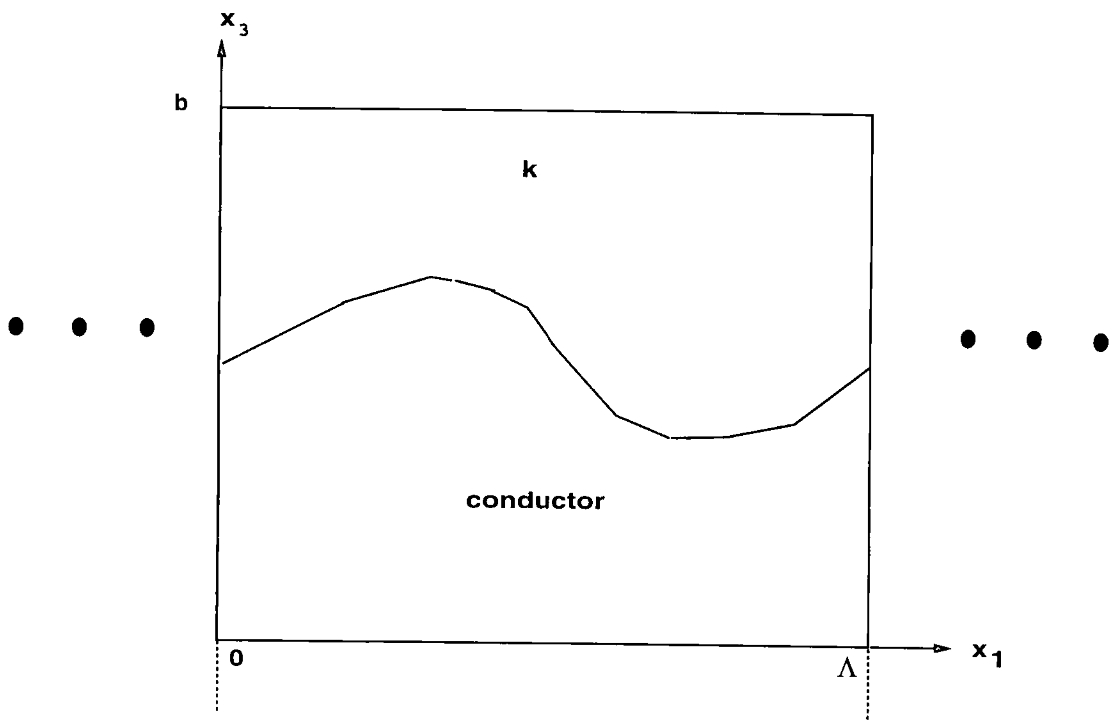

Figure 5: The condoctor problem geometry.

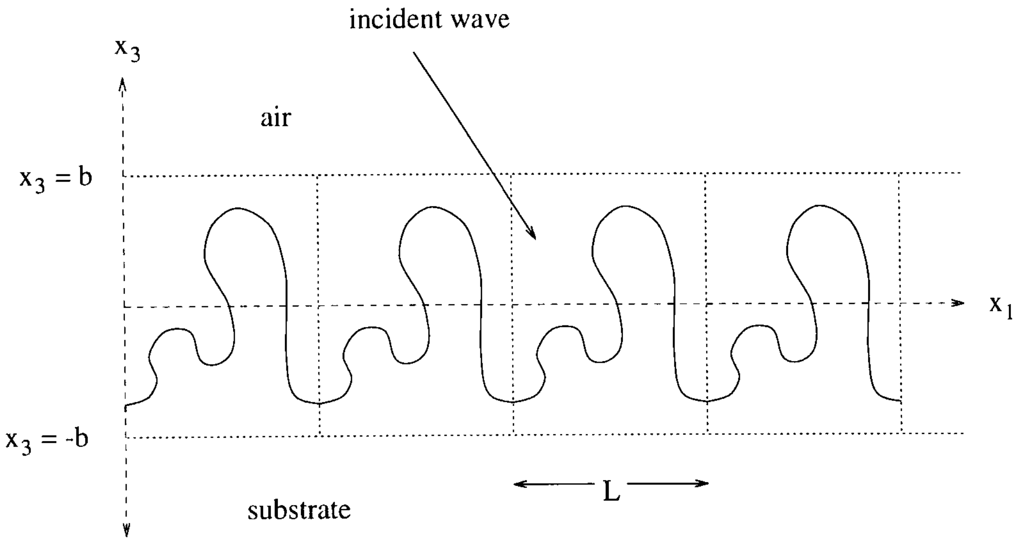

Figure 6: Geometrical configuration for TE design. For convenience, the problem is scaled so that the grating period $\Lambda = 2\pi$.

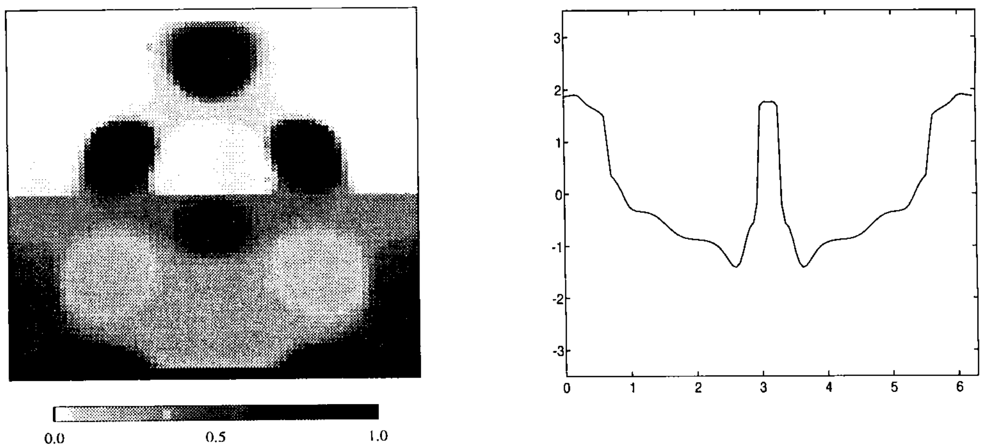

Figure 7: Ideal array generator designs. (a.) "Relaxed" mixture design; black indicates substrate, white indicates air. (b.) Equivalent interface profile; the line indicates a boundary between air and substrate.

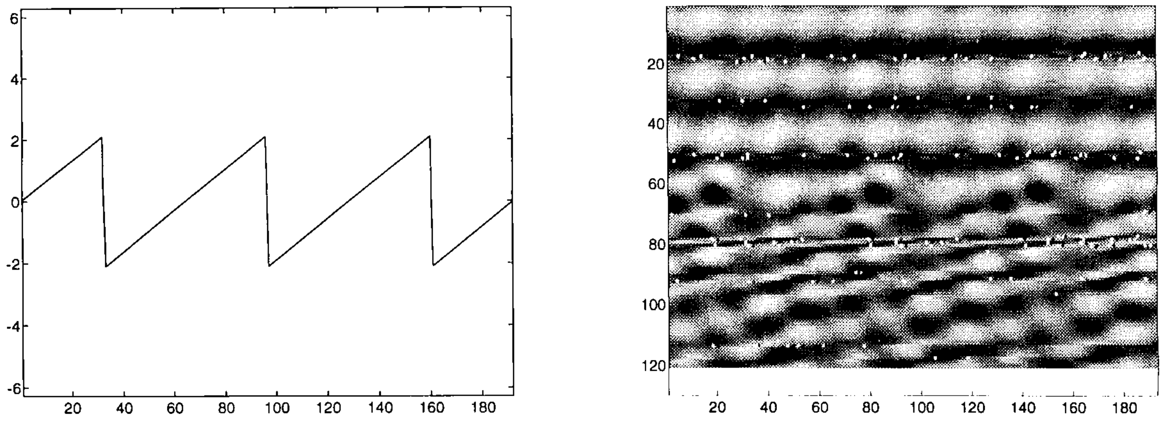

Figure 8: Optimal ramp profile and gray-scale plot of the real part of the resulting diffracted field.

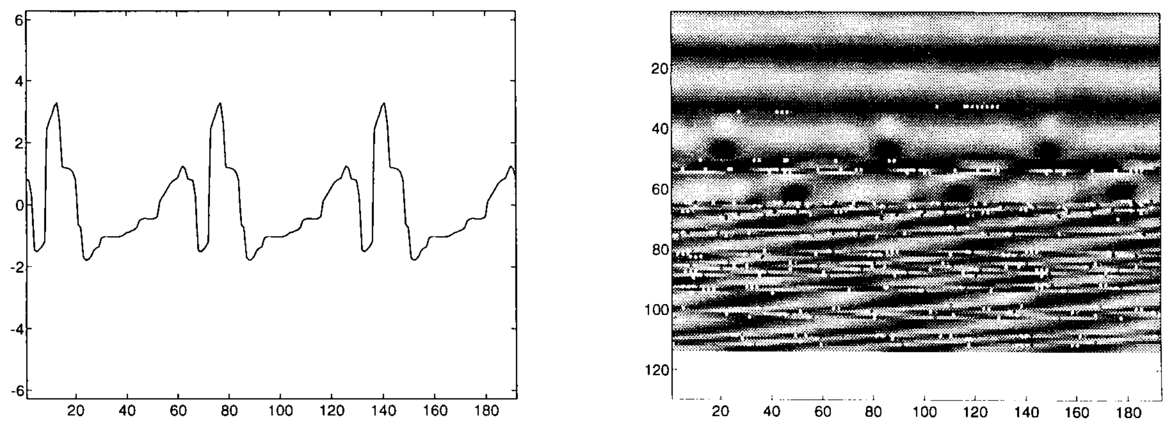

Figure 9: A particular near-optimal profile and gray-scale plot of the real part of the resulting diffracted field.

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