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OPTIMAL DESIGN OF DIFFRACTIVE OPTICS

By

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ABSTRACT

OPTIMAL DESIGN OF DIFFRACTIVE OPTICS

By

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In this dissertation, we consider two problems. Both problems deal with diffractive optics and design of grating structures.

The first is known as the resonance design problem. In this case, we encounter one of the most interesting new developments in diffractive optics which is the integration of a zero-order grating and a planar waveguide to create a resonance. Such structures are able to yield ultra narrow bandwidth filters which potentially have many extraordinary applications. The main step in the design of such a grating structure is to find the resonant wavelength. For any fixed grating structure, calculation of the resonant wavelength is found by solving a nonlinear eigenvalue problem.

The second of the two design problems focuses on nonlinear diffraction gratings. Here, we will consider a plane wave of frequency ω_1 incident on a grating composed of some nonlinear optical material. The effects of the nonlinear material interacting with field give rise to diffracted waves with frequencies ω_1 and $\omega_2 = 2\omega_1$. The creation of waves with the doubled frequency is a phenomenon unique to nonlinear optics known as second harmonic generation (SHG). The design problem in this context is to create a grating structure which enhances the very weak nonlinear optical effects.

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Introduction

The field of diffractive optics has developed over the past few decades in concurrence with the semiconductor industry. The practical application of diffractive optics technology has driven the need for mathematical models and numerical codes which provide rigorous solutions of the electromagnetic vector-field equations for grating structures. Such models and codes allow scientists to predict performance of a given structure, and to carry out optimal design of new structures.

One of the most interesting new developments in diffractive optics involves the integration of a zero-order grating with a planar waveguide to create a resonance. Such structures take the form of a planar dielectric layer with the grating providing a periodic modulation of the dielectric constant in one or more of the layers. These grating structures can yield ultra narrow bandwidth filters for a selected wavelength. In practice, it is desirable to design the grating structures to focus the filtering properties around a predetermined frequency. The design requirements are specified in terms of the resonant wavelength λ_{res} at which maximum reflectance occurs, the spectral bandwidth of the resonance $\Delta\lambda$, the polarization and angle of the incident wave, and possibly the "out-of-band" reflectance away from resonance. A great deal of computation is necessary to draw the reflectance curve response to many different wavelengths. One of the problems is to find the resonant wavelength without drawing the reflectance curve. Instead of computing the entire reflectance curve, we will see that information about the location of the resonance frequency can be found by studying the scattering frequency which saves much in the way of computational cost.

In another grating problem, we consider a plane wave of frequency ω_1 incident on a grating or periodic structure consisting of some nonlinear optical material. The nonlinear material produces nonlinear optical interactions which give rise to diffracted waves at frequencies ω_1 and $\omega_2 = 2\omega_1$. The creation of waves with the doubled frequency represents the simplest situation which is unique to nonlinear optics – second harmonic generation (SHG). An exciting application of SHG is to obtain coherent radiation at a wavelength shorter than that of currently available lasers. Unfortunately, it is well known that nonlinear optical effects, including SHG, are generally so weak that they can only be observed in the presence of very strong coherent electromagnetic fields such as lasers. Effective enhancement of nonlinear optical effects presents one of the most challenging tasks in nonlinear optics.

The dissertation is organized as follows. In chapter 1, we describe the direct diffraction problem. Some basic results that will be used in the next two chapters are provided . The formulas for the partial derivatives of the reflection and transmission coefficients with respect to the parameters of a binary grating profile are introduced. The formulas will be used in determining the thickness of grating in resonant filter design. Chapter 2, presents the resonant filter design problem. First we consider how to find a good initial guess of grating thickness and period. Then, we try to find the resonant wavelength for a given grating structure. Finally, we consider the design problem. Also, numerical examples are presented . Chapter 3 discusses the nonlinear grating design problem. In section 3.2, we present the nonlinear scattering problem. Subsequently, in section 3.3, the perturbed diffraction problem with respect to smooth variations of the interfaces is studied and a gradient formula is derived. Numerical examples are given in section 3.4.

CHAPTER 1

The diffraction problem

1.1 Preliminaries

Suppose that the whole space is filled with non-magnetic material with a permittivity function ε, which in Cartesian coordinates (x_1, x_2, x_3) does not depend on x_3, is periodic in x_1, and homogeneous above and below certain interfaces. In practice, the period Λ of optical gratings under consideration is comparable with the wavelength $\lambda = 2\pi c/\omega$ of incoming plane optical waves, where c denotes the speed of light. Suppose also that the media are nonmagnetic; i.e., the magnetic permeability constant μ is a fixed constant everywhere. The upper interface is denoted by S^+, the lower interface is denoted by S^-. The medium between S^+ and S^- is inhomogeneous with $\varepsilon = \varepsilon_0(x_1, x_2)$, and we assume that the function ε_0 is periodic in x_1, $\varepsilon_0(x_1, x_2) = \varepsilon_0(x_1 + \Lambda, x_2)$ and piecewise constant. Above the surface S^+ and below the surface S^-, the media are assumed to be homogeneous with $\varepsilon = \varepsilon^\pm$.

Assume the grating is illuminated by a monochromatic plane wave

$$\mathbf{E}^{\mathrm{i}} = \mathbf{A} e^{i\alpha x_1 - i\beta x_2} e^{-i\omega t}, \quad \mathbf{H}^{\mathrm{i}} = \mathbf{B} e^{i\alpha x_1 - i\beta x_2} e^{-i\omega t}$$

with $\beta \neq 0$.

Here, the complex amplitude vector $\mathbf{A}$ is perpendicular to the wave vector $\mathbf{k} =$

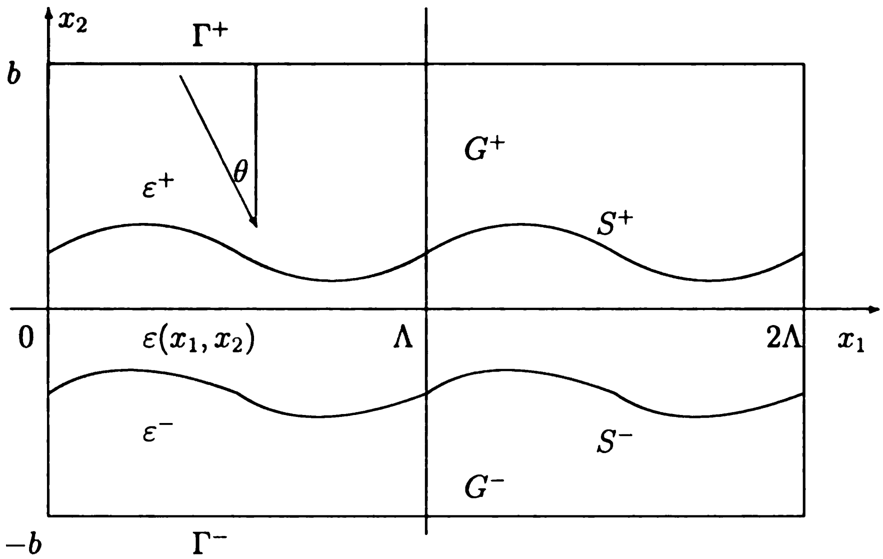

Figure 1.1. Geometry of Grating

$(\alpha, -\beta, 0)$ and $\mathbf{B} = (\omega\mu)\mathbf{k} \times \mathbf{A}$.

The incident wave $(\mathbf{E}^{\mathrm{i}}, \mathbf{H}^{\mathrm{i}})$ will be diffracted by the grating.

In region G^+ above the grating surface S^+, the total fields will be given by

$$\mathbf{E}^{\mathrm{up}} = \mathbf{E}^{\mathrm{i}} + \mathbf{E}^{\mathrm{refl}}, \quad \mathbf{H}^{\mathrm{up}} = \mathbf{H}^{\mathrm{i}} + \mathbf{H}^{\mathrm{refl}}.$$

In region G^- below the grating surface S^-, the total fields will be given by

$$\mathbf{E}^{\mathrm{down}} = \mathbf{E}^{\mathrm{refr}}, \quad \mathbf{H}^{\mathrm{down}} = \mathbf{H}^{\mathrm{refr}}.$$

Dropping the factor $\exp(-i\omega t)$, total fields satisfy the time-harmonic Maxwell equations

$$\nabla \times E = i\omega\mu H \tag{1.1}$$

$$\nabla \cdot \varepsilon E = 0 \tag{1.2}$$

$$\nabla \times H = -i\omega\varepsilon E \tag{1.3}$$

$$\nabla \cdot H = 0 \tag{1.4}$$

Additionally, the tangential components of the total fields are continuous when crossing an interface between two continuous media

$$\nu \times (\mathbf{E}^1 - \mathbf{E}^2) = 0, \quad \nu \times (\mathbf{H}^1 - \mathbf{H}^2) = 0 \quad \text{on} \quad S^+, S^- \tag{1.5}$$

where ν is the unit normal to the interface $S^{\pm}$.

E and **H** can be represented as the superposition of solutions corresponding to the **TE** case (field transverse electric), where

$$\begin{aligned} \mathbf{E}^{\mathrm{i}} &= (0, 0, A_3) \exp(i\alpha x_1 - i\beta x_2), \\ \mathbf{H}^{\mathrm{i}} &= -(\omega\mu)^{-1}(-\beta A_3, \alpha A_3, 0) \exp(i\alpha x_1 - i\beta x_2), \end{aligned}$$

and to the **TM** case (field transverse magnetic) with

$$\begin{aligned} \mathbf{E}^{\mathrm{i}} &= (A_1, A_2, 0) \exp(i\alpha x_1 - i\beta x_2), \\ \mathbf{H}^{\mathrm{i}} &= (0, 0, \beta A_1 + \alpha A_2) \exp(i\alpha x_1 - i\beta x_2). \end{aligned}$$

Denote by u^{i} the normed transverse component $\mathbf{E}^{\mathrm{i}} \cdot \mathbf{x}_3$ for **TE** or $\mathbf{H}^{\mathrm{i}} \cdot \mathbf{x}_3$ for **TM**, i.e.

$$u^{\mathrm{i}} = \exp(i\alpha x_1 - i\beta x_2) \ \text{ with } \quad \alpha = \omega\sqrt{\mu\varepsilon^+} \sin\theta, \beta = \omega\sqrt{\mu\varepsilon^+} \cos\theta.$$

The functions $u^{\pm}(x_1, x_2)$ and $u_0(x_1, x_2)$ equal to either the transverse component $\mathbf{E} \cdot \mathrm{x}_3$ for **TE** or $\mathbf{H} \cdot \mathrm{x}_3$ for **TM** in $G^{\pm}$ and G_0, resp.

The boundary conditions (1.5) are translated into transmission conditions for the unknowns $u^{\pm}$ and u_0 in the following way:

- **TE** mode:

$$\begin{aligned} u^+ + u^{\mathrm{i}} = u_0, \quad & \frac{\partial(u^+ + u^{\mathrm{i}})}{\partial\nu} = \frac{\partial u_0}{\partial\nu} \quad \text{on } S^+, \\ u^- = u_0, \quad & \frac{\partial u^-}{\partial\nu} = \frac{\partial u_0}{\partial\nu} \quad \text{on } S^-. \end{aligned}$$

- **TM** mode:

$$u^+ + u^{\mathrm{i}} = u_0, \quad \frac{1}{\varepsilon^+}\frac{\partial(u^+ + u^{\mathrm{i}})}{\partial\nu} = \frac{1}{\varepsilon_0}\frac{\partial u_0}{\partial\nu} \quad \text{on } S^+,$$
$$u^- = u_0, \quad \frac{1}{\varepsilon^-}\frac{\partial u^-}{\partial\nu} = \frac{1}{\varepsilon_0}\frac{\partial u_0}{\partial\nu} \quad \text{on } S^-,$$

We shall assume throughout that the optical index of the grating materials is such that the ε satisfies

$$\sqrt{\varepsilon^+} > 0, \tag{1.6}$$

$$\mathrm{Re}\,\sqrt{\varepsilon^-} > 0, \qquad \mathrm{Im}\,\sqrt{\varepsilon^-} \geq 0, \tag{1.7}$$

$$\mathrm{Re}\,\sqrt{\varepsilon_0(x_1,x_2)} > 0, \quad \mathrm{Im}\,\sqrt{\varepsilon_0(x_1,x_2)} \geq 0. \tag{1.8}$$

It is easily seen that the Maxwell's equations become Helmholtz equation.

TE case:

$$\Delta u + \omega^2\mu\varepsilon u = 0 \tag{1.9}$$

TM case :

$$\nabla\cdot(\frac{1}{\mu\varepsilon}\nabla u) + \omega^2 u = 0 \tag{1.10}$$

1.2 Radiation condition and Grating formula

It is obvious that the incident field u^{i} satisfies the following condition:

$$u^{\mathrm{i}}(x_1 + p\Lambda, x_2) = u^{\mathrm{i}}(x_1,x_2)e^{ip\Lambda\alpha} \tag{2.1}$$

Suppose now that u is a solution of (1.9) (resp. (1.10)). Then by the periodicity of the index ε, every field $u^{(p)}$ of the form

$$u^{(p)}(x) = u(x_1 + p\Lambda, x_2)e^{-ip\alpha\Lambda}$$

for $p \in \mathbf{Z}$ is a solution of the same problem. Of course, the associated diffracted field $u^{(p)}$ has the same behavior for $x_2 \to \infty$ as u, and there is no physical criterion to eliminate some of these solutions.

In order for the problem not to have infinitely many solutions, we will look only for α-periodic solutions, i.e. solutions u such that

$$u(x_1 + p\Lambda, x_2) = u(x_1, x_2)e^{ip\Lambda\alpha} \qquad \forall p \in \mathbf{Z}. \tag{2.2}$$

As usual, diffraction problems (1.9) and (1.10) are not well-posed and must be completed by a radiation condition. Since the grating is unbounded in the x_1-direction, the classical Sommerfeld condition is not appropriate.

Because the domain is unbounded in the x_2-direction, a radiation condition on the scattering problem must be imposed at infinity, namely the diffracted fields $u^{\pm}$ remain bounded and that they should be representable as superpositions of outgoing waves.

Define the coefficients

$$\alpha_p = \alpha + p\frac{2\pi}{\Lambda} \tag{2.3}$$

$$\beta_p^{\pm} = \beta_p^{\pm}(\alpha) = e^{\frac{i\nu_p}{2}}|\omega^2\mu\varepsilon^{\pm} - \alpha_p^2|^{\frac{1}{2}} \tag{2.4}$$

where $\nu_p = arg(\omega^2\mu\varepsilon - \alpha_p^2) \in (-\pi, \pi]$ is an argument of the complex number.

Define the finite sets of indices

$$P^{\pm} = \{p \in \mathbf{Z} : \beta_p^{\pm} \in \mathbf{R}\}. \tag{2.5}$$

The α-periodicity condition will allow us now to write a radiation condition in the x_2-direction. Indeed, if the diffracted field u is α-periodic, it means that the function

$$v(x_1, x_2) = u(x_1, x_2)e^{-i\alpha x_1} \tag{2.6}$$

is periodic.

Moreover, since $u^{\pm}$ are analytic above S^+ (resp. below S^-) by the classical regularity results for the Helmholtz equation, the Fourier decomposition of v leads us to the so-called α-periodic Fourier decomposition of u:

$$u^+(x_1,x_2) = \sum_{p\in\mathbf{Z}} A_p^+ e^{i\alpha_p x_1 + i\beta_p^+ x_2} + B_p^+ e^{i\alpha_p x_1 - i\beta_p^+ x_2} \qquad \text{for } x_2 > \max S^+$$

$$u^-(x_1,x_2) = \sum_{p\in\mathbf{Z}} A_p^- e^{i\alpha_p x_1 - i\beta_p^- x_2} + B_p^- e^{i\alpha_p x_1 + i\beta_p^- x_2} \qquad \text{for } x_2 < \min S^-$$

The physics of the problem imposes the obvious condition that the diffracted field remains bounded as $|x_2| \to \infty$. Thus, we will insist that $u^{\pm}$ satisfy the outgoing wave condition (OWC) $B_p^{\pm} = 0$, i.e. they are composed of bounded outgoing plane waves in $G^{\pm}$:

$$\begin{aligned} u^+(x_1,x_2) &= \sum_{p\in\mathbf{Z}} A_p^+ e^{i\alpha_p x_1 + i\beta_p^+ x_2} && \text{for } x_2 > \max S^+ \\ u^-(x_1,x_2) &= \sum_{p\in\mathbf{Z}} A_p^- e^{i\alpha_p x_1 - i\beta_p^- x_2} && \text{for } x_2 < \min S^- \end{aligned}$$

Since $\beta_p^{\pm}$ is real for at most finitely many p, there are only a finite number of propagating plane waves in the sums of (2.7). Note that physically the case $\beta_p^{\pm} = 0$ corresponds to a plane wave propagating parallel to the grating. We assume that $\beta_p^{\pm} \neq 0$. i.e.

$$(\omega^2 \mu \varepsilon^{\pm}) \neq (\alpha + \frac{2p\pi}{\Lambda})^2 \tag{2.7}$$

$$\begin{aligned} u^+(x_1,x_2) &= \sum_{p\in\mathbf{Z}} A_p^+ e^{i\alpha_p x_1 + i\beta_p^+ x_2} \\ &= \sum_{p\in P+} A_p^+ e^{i\alpha_p x_1 + i\beta_p^+ x_2} \quad \text{“ outgoing waves ”} \\ &\quad + \sum_{p\notin P+} A_p^+ e^{i\alpha_p x_1 + i\beta_p^+ x_2} \quad \text{“ evanescent waves ”} \end{aligned}$$

$$\begin{aligned} u^-(x_1,x_2) &= \sum_{p\in\mathbf{Z}} A_p^- e^{i\alpha_p x_1 - i\beta_p^- x_2} \\ &= \sum_{p\in P^-} A_p^- e^{i\alpha_p x_1 - i\beta_p^- x_2} \quad \text{" outgoing waves "} \\ &\quad + \sum_{p\notin P^-} A_p^- e^{i\alpha_p^- x_1 - i\beta_p^- x_2} \quad \text{" evanescent waves "} \end{aligned}$$

Each term of the outgoing waves in the above represents a propagating plane wave, which is called the **diffracted wave in the p-th order**.

Thus we have derived the following **grating formula**:

$$\alpha_p = \alpha + p\frac{2\pi}{\Lambda}$$

or

$$\sin\theta_p = \sin\theta + p\frac{\lambda}{\Lambda}$$

Let $H_p^s(\Omega)$ denote the restriction to Ω of all functions in the Sobolev space $H_{loc}^s(\mathbf{R}^2)$ which are Λ-periodic in x_1.

Since we look now for α-periodic fields, the problems can be written on a cell of the grating and we introduce $\tilde{\Omega} = \{(x_1,x_2) : x_1 \in (0,\Lambda)\}$.

Define $u_\alpha = ue^{-i\alpha x_1}$. It is easily seen that if u satisfies (1.9) then u_α satisfies

$$\Delta_\alpha u + \omega^2\mu\varepsilon u = 0 \quad \text{in } \mathbf{R}^2$$

where Δ_α is defined by $\Delta_\alpha = (\nabla_\alpha)^2 = (\partial_{x_1} + i\alpha)^2 + (\partial_{x_2})^2$.

Let us consider the following problems:

TE problem P_{TE}: find $u \in H_p^1(\tilde{\Omega})$

$$\Delta_\alpha u + \omega^2\mu\varepsilon u = 0 \quad \text{in } \tilde{\Omega} \tag{2.8}$$

$$u^{\text{dif}} = u - u^{\text{i}} \text{ has the form (2.7) for } |x_2| \text{ big enough} \tag{2.9}$$

TM problem P_{TM}: find $u \in H_p^1(\tilde{\Omega})$

$$\nabla_\alpha \cdot \left(\frac{1}{\mu\varepsilon}\nabla_\alpha u\right) + \omega^2 u = 0 \quad \text{in } \tilde{\Omega} \tag{2.10}$$

$$u^{\text{dif}} = u - u^{\text{i}} \text{ has the form (2.7) for } |x_2| \text{ big enough} \tag{2.11}$$

1.3 Truncating of the domain

We introduce the following notations:

Fix number $b > \max S^+$ and $-b < \min S^-$ and let $\Omega = (0, \Lambda) \times (-b, b), \Omega^\pm = \Omega \cap G^\pm, \Omega_0 = \Omega \cap G_0, \Gamma^+ = \{x_2 = b\} \cap \bar{\Omega}, \Gamma^- = \{x_2 = -b\} \cap \bar{\Omega}$.

We introduce the following space:

$$H^s(\Gamma^\pm) = \{v = \sum_{p \in Z} v_p e^{i(2p\pi/\Lambda)x_1}, \sum_{p \in Z}(1 + 4p^2\pi^2/\Lambda^2)^s |v_p|^2 < \infty\} \tag{3.1}$$

We define the operators $T^\pm$:

$$\begin{aligned} T^\pm : H^{\frac{1}{2}}(\Gamma^\pm) &\rightarrow H^{-\frac{1}{2}}(\Gamma^\pm) \\ T^\pm : v = \sum_{p \in Z} v_p e^{i(2p\pi/\Lambda)x_1} &\rightarrow T^\pm(v) = \sum_{p \in Z} i\beta_p^\pm v_p e^{i(2p\pi/\Lambda)x_1} \end{aligned} \tag{3.2}$$

which are periodic pseudo-differential operators of order 1.

It is easy to check that

$$\frac{\partial u}{\partial n} = T^- u \quad \text{on } \Gamma^- \tag{3.3}$$

$$\frac{\partial u}{\partial n} = T^+ u - 2\beta e^{-i\beta b} e^{i\alpha x_1} \quad \text{on } \Gamma^+ \tag{3.4}$$

Thus, the problem can be formulated as following:

TE problem P_{TE}^b: find $u \in H_p^1(\Omega)$

$$\Delta_\alpha u + \omega^2 \mu \varepsilon u = 0 \text{ in } \Omega \tag{3.5}$$

$$\partial_n u = T^+ u - 2i\beta_1 e^{-i\beta_1 b} \text{ on } \Gamma^+ \tag{3.6}$$

$$\partial_n u = T^- u \text{ on } \Gamma^- \tag{3.7}$$

Similarly, the **TM** problem can be formulated as following:

TM problem P_{TM}^b: find $u \in H_p^1(\Omega)$

$$\nabla_\alpha \cdot (\frac{1}{\mu\varepsilon} \nabla_\alpha u) + \omega^2 u = 0 \text{ in } \Omega \tag{3.8}$$

$$\partial_n u = T^+ u - 2i\beta_1 e^{-i\beta_1 b} \text{ on } \Gamma^+ \tag{3.9}$$

$$\partial_n u = T^- u \text{ on } \Gamma^- \tag{3.10}$$

Problems P_{TE} (resp. P_{TM}) and P^b_{TE} (resp. P^b_{TM} are clearly equivalent in the sense of the following proposition.

Proposition 1.3.1 *If u is a solution of P_{TE} (resp. P_{TM}) such that $\tilde{u} = u|_\Omega \in H^1_\alpha(\Omega)$, then $\tilde{u}$ is a solution of P_{TE} (resp. P_{TM}). Conversely, if $\tilde{u}$ is a solution of P^b_{TE}(resp.P^b_{TE}), it can be extended to a solution u of P_{TE} (resp. P_{TM}).*

1.4 Variational formulation

From the **TE** problem P^b_{TE}, integration by parts results in the variational relation

$$\int\limits_{\Omega} \nabla_\alpha \cdot \nabla \bar{v} - \omega^2 \mu\varepsilon u\bar{v} - \int\limits_{\Gamma^+} \frac{\partial u}{\partial n}\bar{v} - \int\limits_{\Gamma^-} \frac{\partial u}{\partial n}\bar{v} = 0$$

By (3.3) and (3.4), we have the variational formulation for the **TE** diffraction problem

$$B_{TE}(u,v) = L_{TE}v \tag{4.1}$$

$$B_{TE}(u,v) := \int\limits_{\Omega} (\nabla_\alpha u \cdot \nabla_\alpha \bar{v} - \omega^2 \mu\varepsilon u\bar{v}) - \int\limits_{\Gamma^+} T^+ u\bar{v} - \int\limits_{\Gamma^-} T^- u\bar{v} \tag{4.2}$$

$$L_{TE}v := -\int\limits_{\Gamma^+} 2i\beta e^{-i\beta b}\bar{v} \tag{4.3}$$

Similarly, the TM diffraction problem can be formulated as follows.

Find $u \in H^1_p(\Omega)$ that satisfies

$$B_{TM}(u,v) = L_{TM}v \tag{4.4}$$

$$B_{TM}(u,v) := \int\limits_{\Omega} (\frac{1}{\mu\varepsilon}\nabla_\alpha u \cdot \nabla_\alpha \bar{v} - \omega^2 u\bar{v}) - \frac{1}{\mu\varepsilon^+}\int\limits_{\Gamma^+} T^+ u\bar{v} - \frac{1}{\mu\varepsilon^-}\int\limits_{\Gamma^-} T^- u\bar{v} \tag{4.5}$$

$$L_{TM}v := -\frac{1}{\mu\varepsilon^+}\int\limits_{\Gamma^+} 2i\beta e^{-i\beta b}\bar{v} \tag{4.6}$$

We have the following theorem:

Theorem 1.4.1 *[2] The problem P^b_{TE} (P^b_{TM}) is well-posed for every value of k except maybe for a discrete set of values k.*

1.5 Efficiency

Let u be the solution of the **TE** or **TM** variational problem (4.1) or (4.4). The reflection and transmission coefficients are determined by traces of u on the artificial boundaries $\Gamma^{\pm}$:

$$
\begin{aligned}
A_n^+ &= (2\pi)^{-1} e^{-i\beta_n^+ b} \int_{\Gamma^+} u e^{-inx_1}, \\
A_0^+ &= -e^{-2i\beta b} + (2\pi)^{-1} e^{-i\beta b} \int_{\Gamma^+} u, \\
A_n^- &= (2\pi)^{-1} e^{-i\beta_n^- b} \int_{\Gamma^-} u e^{-inx_1}.
\end{aligned}
$$

Then the reflected an transmitted efficiencies in the **TE** case are defined by

$$
e_p^{\pm} = \frac{\beta_p^{\pm}}{\beta} |A_p^{\pm}|^2, \qquad p \in P^{\pm}, \tag{5.1}
$$

and in the **TM** case by

$$
e_p^+ = \frac{\beta_p^+}{\beta} |A_p^+|^2, \qquad p \in P^+, \tag{5.2}
$$

$$
e_p^- = \frac{\varepsilon^+}{\varepsilon^-} \frac{\beta_p^-}{\beta} |A_p^-|^2, \quad p \in P^-, \tag{5.3}
$$

For lossless gratings, i.e. all optical indices are real, the principle of conservation of energy then, in either case, yields the relation

$$
\sum_{p \in P^+} e_p^+ + \sum_{p \in P^-} e_p^- = 1. \tag{5.4}
$$

1.6 Optimization of grating efficiency

Consider a binary grating profile Γ which is composed of a finite number of horizontal and vertical segments and is determined by the height d and by , say $m+1$ transition

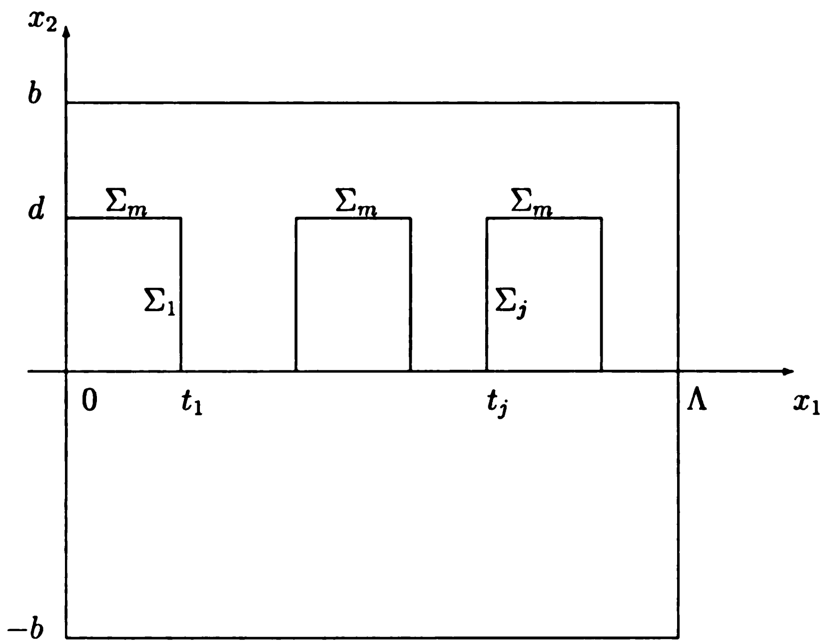

Figure 1.2. Binary Grating

points $0 = t_0 < t_1 < \cdots < t_{m-1} < t_m = \Lambda$. Since t_0 and t_m are assumed to be fixed, we write $\Gamma = \Gamma(t_1, \cdots, t_{m-1}, d)$

Assume that the number of transition points is fixed and, for given numbers $c_n^\pm \in \{-1, 0, 1\}$, define the functional

$$J(\Gamma) = J(t_1, \cdots, t_{m-1}, d) := \Sigma c_n^\pm e_n^\pm \tag{6.1}$$

We consider the following minimization problem.

Find a binary grating profile Γ^0 such that

$$\min_{(t_1, \cdots, t_{m-1}, d) \in K} J(\Gamma) = J(\Gamma^0) \tag{6.2}$$

where K is some compact set in the parameter space $\mathbf{R}^m$ reflecting some natural constraints on the design of the profile. Note that the choice $c_n^\pm = -1$ (resp. $c_n^\pm = 1$) in (6.1) amounts to maximizing (resp. minimizing) the efficiency of the corresponding reflected or transmitted propagating mode of order n.

To find local minimal of problem (6.1), gradient-based minimization methods can be applied. Thus, we must calculate the gradient of $J, \nabla J(\Gamma) = (D_j J(\Gamma))_1^m$, where e.g. for $j = 1$

$$D_1 J(\Gamma) = \lim_{h\to 0} h^{-1}(J(\Gamma_h) - J(\Gamma)) \tag{6.3}$$

$$= \lim_{h\to 0} h^{-1}(J(t_1 + h, \cdots, d) - J(t_1, \cdots, d)) \tag{6.4}$$

Here Γ_h denotes the binary profile with the height d and the transition points $t_1 + h, t_2, \cdots, d$.

We obviously have, for $j = 1, \cdots, m$

$$\begin{aligned} D_j J(\Gamma) &= \Sigma 2(\beta_n^+/\beta)\{c_n^{TE}\mathrm{Re}\,(\overline{A_n^+(\Gamma)})D_j A_n^+(\Gamma)\} \\ &\quad + \Sigma 2(\beta_n^-/\beta)\{c_n^+\mathrm{Re}\,(\overline{A_n^-(\Gamma)})D_j A_n^-(\Gamma)\} \end{aligned} \tag{6.5}$$

Therefore , we have to calculate the partial derivatives $D_j A_n^{\pm}(\Gamma)$ of the reflection and transmission coefficients.

We fix $n \in P^+$ and derive a formula for the partial derivative $D_1 A_n^+(\Gamma)$ of the Rayleigh coefficient of the n-th reflected mode in the TE case.

Let u be the solution of the TE transmission problem and let u_h denote the solution of the corresponding problem for the profile $\Gamma_h = \Gamma(t_1 + h, t_2, \cdots, d)$:

$$B^h(u_h, \varphi) := \int_\Omega \nabla_\alpha \cdot \overline{\nabla_\alpha \varphi} - \omega^2 \varepsilon_h \mu u_h \bar{\varphi} - \int_{\Gamma^+} (T_\alpha^+ u_h)\bar{\varphi} - \int_{\Gamma^-} (T_\alpha^- u_h)\varphi \tag{6.6}$$

$$= -\int_{\Gamma^+} 2i\beta exp(-i\beta b)\bar{\varphi} \quad \forall \varphi \in H_p^1(\Omega) \tag{6.7}$$

where

$$\varepsilon_h = \begin{cases} \varepsilon_0, & h > 0 \\ \varepsilon^+, & h < 0 \end{cases} \text{ in } \Pi_h,$$

$$\varepsilon_h = \varepsilon \text{ in } \Omega \backslash \Pi_h$$

By the reflection and transmission coefficients and the definition of $D_1 A_n^+(\Gamma)$, we have

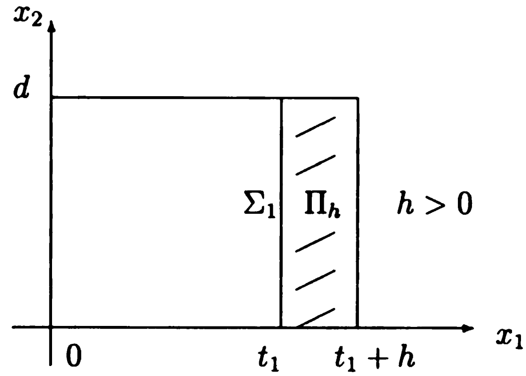

Figure 1.3. Geometry for the calculation of gradients

$$D_1 A_n^+(\Gamma) = \lim_{h\to} \frac{exp(-i\beta_n^+ b)}{2\pi h} \int_{\Gamma+} (u_h - u) exp(-inx_1) dx_1 \tag{6.8}$$

We define the adjoint TE problem, seeks $v \in H_p^1(\Omega)$ such that

$$B(\varphi, v) = (\varphi, f^+) + (\varphi, f^-) \text{ for all } \varphi \in H_p^1(\Omega) \tag{6.9}$$

where $f^\pm \in H_p^{-1/2}(\Gamma^\pm)$.

Let w be the solution of the adjoint transmission problem

$$B(\varphi, w) = \int_{\Gamma+} \varphi exp(-inx_1) dx_1 \forall \varphi \in H_p^1(\Omega). \tag{6.10}$$

Then obviously

$$h^{-1} \int_{\Gamma+} (u_h - u) exp(-inx_1) dx_1 = h^{-1} B(u_h - u, w) \tag{6.11}$$

$$= h^{-1}(B(u_h, w) - B^h(uh, w))) \tag{6.12}$$

$$= h^{-1} \int_{\Omega} \omega^2 \mu(\varepsilon_h - \varepsilon) u_h \bar{w} \tag{6.13}$$

$$= \omega^2 \mu(\varepsilon_0 - \varepsilon^+) |h|^{-1} \int_{\Pi_h} u_h \bar{w} \tag{6.14}$$

we can prove

$$\lim_{h\to 0} |h|^{-1} \int\limits_{\Pi_h} u_h \bar{w} = \int\limits_{\Sigma_1} u\bar{w} dx_2. \tag{6.15}$$

Together , we have the formulas ([17]):

$$D_j A_n^{\pm}(\Gamma) = \frac{(-1)^{j-1}}{2\pi} e^{-i\beta_n^{\pm} b} \omega^2 \mu(\varepsilon_0 - \varepsilon^+) \int\limits_{\Sigma_j} u\bar{w}_{\pm} dx_2, j = 1, \cdots, m-1 \tag{6.16}$$

$$D_m A_n^{\pm} = \frac{1}{2\pi} e^{-i\beta_n^{\pm}} \omega^2 \mu(\varepsilon_0 - \varepsilon^+) \int\limits_{\Sigma_m} u\bar{w}_{\pm} dx_1 \tag{6.17}$$

CHAPTER 2

Guided Mode Grating Resonance Filters (GMGRF)

2.1 Introduction

The anomalies of optical diffraction gratings have been of interest since they were discovered by Wood in 1902. They manifest themselves as rapid variation in the intensity of the various diffracted spectral orders in certain narrow frequency bands. They were termed anomalies because the effects could not be explained by ordinary grating theory. There are two principal types of anomalous effects; the Rayleigh type, which is the classical Wood's anomaly, and the less common resonant type.

The Rayleigh type is due to one of the spectral orders appearing (or disappearing) at the grazing angle (propagating along the surface). Note that for fixed $\varepsilon^{\pm}$ and incidence angle θ, condition (2.7) is violated for a discrete set of frequencies $\omega_j, \omega_j \to \infty$, referred to as Rayleigh frequencies and corresponding to physically anomalous behavior first observed by Wood. From the efficiency formula, it is natural to expect that efficiencies will be redistributed when the new propagating mode appears or disappears.

The resonant type anomaly is due to possible guided modes supportable by the waveguide grating.

One of the most interesting new developments in diffractive optics involves the integration of a zero-order grating with a planar waveguide to create a resonance. Taking the form of a planar dielectric layer with the grating providing a periodic modulation of the dielectric constant in one or more of the layers, such structures have been demonstrated to yield ultra narrow bandwidth filters for a selected center wavelength.

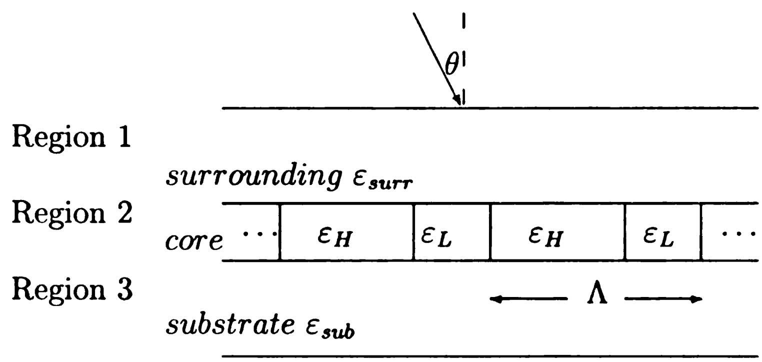

Figure 2.1. Waveguide (Single layer)

A conceptual structure representing a GMGRF is illustrated in Figure 2.1. Region 2 consisting of a planar thin film, separates two homogeneous half-space.

The upper half-space is the "surrounding" and designated region 1; The lower half-space is the "substrate", called region 3. Electromagnetic radiation ("light") in the form of a polarized plane wave can be incident on region from either half-space.

Region 2 is constrained to have two special properties:

1. it must satisfy the requirement of a planar waveguide and have an average refractive index greater than the refractive indices of both half-spaces.

2. it must have a periodically modulated dielectric function

Thus, in addition to being the core of a waveguide that supports guided modes, region 2 is also a grating.

For a given incident plane wave of wavelength λ, incident angle, and polarization, it is possible to find a grating period Λ such that a first diffractive order of the grating couples to a guided mode of the waveguide.

By arranging the grating to support only the zero propagating order, energy of the guided mode diffracted out of the core can only lie along the direction of the incident wave, and through this coupling a resonance is established which can lead in principle to 100% reflectance in a very narrow spectral bandwidth, as illustrated in Figure 2.2.

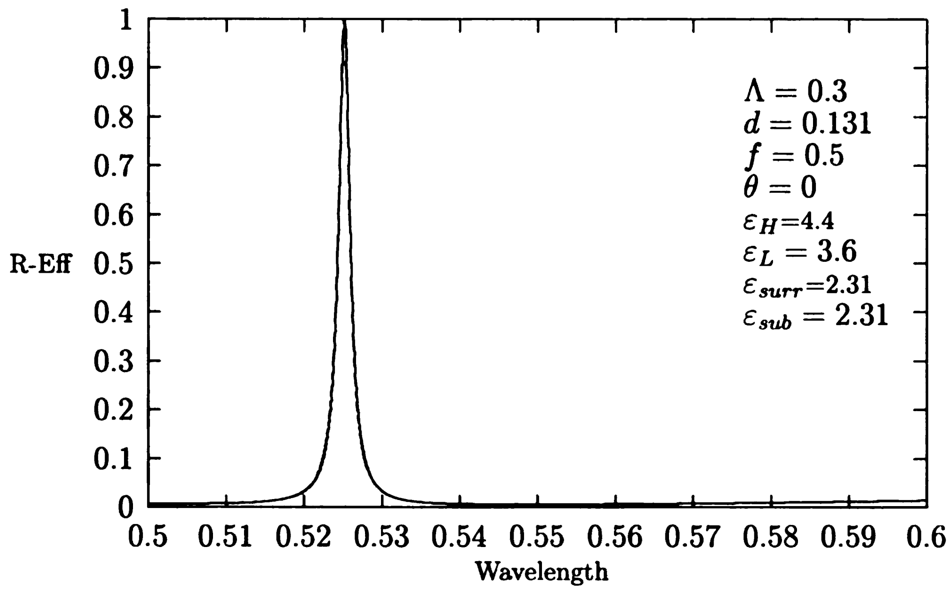

Figure 2.2. Resonance example

The resonant wavelength is determined primarily by the grating period, and the bandwidth primarily by the modulation of refractive index in the grating.

Furthermore, for wavelengths outside the resonance region, the structure appears "homogenized" in its dielectric properties. Thus it may be considered approximately as a simple thin film structure with reflectance properties described by well-known thin film expressions ([12], section 1.6). In particular, it is possible to achieve antireflection conditions in the thin film structure away from the resonant wavelength.

With such extraordinary potential performance, these "resonant reflectors" have attracted attention for many applications, such as lossless spectral filters with arbitrarily narrow, controllable line width, efficient and low-power optical switch elements, polarization control etc.

2.2 The reflectance in thin film

For wavelengths outside the resonance region, the structure appear " homogenized " in its dielectric properties, and thus it may be considered approximately as a simple thin film structure with reflectance properties described by well-known thin film expressions.

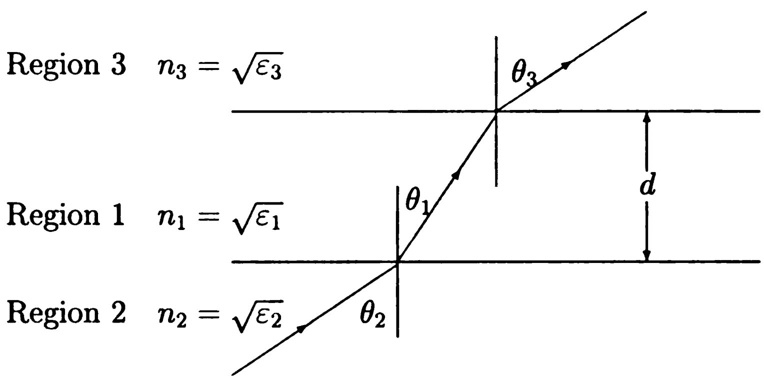

Figure 2.3. Propagation of an electromagnetic wave through a homogeneous film.

Define

$$\beta = \frac{2\pi}{\lambda_0} n_1 d \cos\theta_1 \tag{2.1}$$

$$p_j = n_j \cos\theta_j \quad (j = 1, 2, 3) \tag{2.2}$$

According to the Fresnel formulae, we have, for a TE wave,

$$r_{21} = \frac{n_2\cos\theta_2 - n_1\cos\theta_1}{n_1\cos\theta_1 + n_2\cos\theta_2} = \frac{p_2 - p_1}{p_1 + p_2} \tag{2.3}$$

$$t_{21} = \frac{2n_2\cos\theta_2}{n_1\cos\theta_1 + n_2\cos\theta_2} = \frac{2p_2}{p_1 + p_2} \tag{2.4}$$

$$r_{13} = \frac{n_1\cos\theta_1 - n_3\cos\theta_3}{n_1\cos\theta_1 + n_3\cos\theta_3} = \frac{p_1 - p_3}{p_1 + p_3} \tag{2.5}$$

$$t_{13} = \frac{2n_1\cos\theta_1}{n_1\cos\theta_1 + n_3\cos\theta_3} = \frac{2p_1}{p_1 + p_3} \tag{2.6}$$

$$\tag{2.7}$$

The formula for r and t become

$$r = \frac{r_{21} + r_{13}e^{2i\beta}}{1 + r_{21}r_{13}e^{2i\beta}} \tag{2.8}$$

$$t = \frac{t_{21}t_{13}e^{2i\beta}}{1 + r_{21}r_{13}e^{2i\beta}} \tag{2.9}$$

The reflectivity and transmissivity are therefore given by

$$R = |r|^2 = \frac{r_{21}^2 + r_{13}^2 + 2r_{21}r_{13}\cos 2\beta}{1 + r_{21}^2 r_{13}^2 + 2r_{21}r_{13}\cos 2\beta} \tag{2.10}$$

$$T = \frac{p_3}{p_2}|t|^2 \frac{n_3\cos\theta_3}{n_2\cos\theta_2} \frac{t_{21}^2 t_{13}^2}{1 + r_{21}^2 r_{13}^2 + 2r_{21}r_{13}\cos 2\beta} \tag{2.11}$$

We first note (2.10) and (2.11) remain unchanged when β is replaced by $\beta + \pi$, i.e., when d is replaced by $d + \Delta d$, where

$$\Delta d = \frac{\lambda_0}{2n_1\cos\theta_1}.$$

Hence the reflectivity and transmissivity of dielectric films which differ in thickness by an integral multiple of $\dfrac{\lambda_0}{2n_1\cos\theta_1}$ are the same.

If we set

$$d = \frac{m\lambda_0}{4\cos\theta_1}, \quad (m = 0, 1, 2, \cdots) \tag{2.12}$$

we find from (2.10) that

$$R' = 0 \tag{2.13}$$

We must distinguish two cases:

1. When m is odd,

$$d = \frac{\lambda_0}{4\cos\theta_1}, \frac{3\lambda_0}{4\cos\theta_1}, \frac{5\lambda_0}{4\cos\theta_1}, \cdots \tag{2.14}$$

   then $\cos 2\beta = -1$ and (2.10) reduces to

$$R = (\frac{r_{21} - r_{13}}{1 - r_{21}r_{13}})^2. \tag{2.15}$$

   In particular for normal incidence, one has

$$R = (\frac{n_2 n_3 - n_1^2}{n_2 n_3 + n_1^2})^2 \tag{2.16}$$

2. When m is even, i.e. when the optical thickness has any of the values

$$d = \frac{\lambda_0}{2\cos\theta_1}, \frac{2\lambda_0}{2\cos\theta_1}, \frac{3\lambda_0}{2\cos\theta_1}, \cdots$$

   then $\cos\beta = 1$ and (2.10) reduces to

$$R = (\frac{r_{21} + r_{13}}{1 + r_{21}r_{13}})^2 \tag{2.17}$$

   In particular, for normal incidence, this becomes

$$R = (\frac{n_2 - n_3}{n_2 + n_3})^2 \tag{2.18}$$

Next we must determine the nature of these extreme values.

After a straightforward calculation we have that

$$\text{maximum, if} \quad (-1)^m(n_2 - n_1)(n_1 - n_3) > 0. \tag{2.19}$$

$$\text{minimum, if} \quad (-1)^m(n_2 - n_1)(n_1 - n_3) < 0. \tag{2.20}$$

Example

In Figure 2.2, thickness $d = 0.131\mu m$ is the half-wavelength and since the waveguide is symmetric ($\varepsilon_{surr} = \varepsilon_{sub}$), the almost zero reflectance is obtained.

When the grating thickness is not close to a multiple of a half-wavelength determined by the resonance wavelength, a filter response with an asymmetrical line is obtained. For parameters $\varepsilon_H = 4.0, \varepsilon_L = 3.61, \varepsilon_{surr} = 1.0, \varepsilon_{sub} = 2.31$ and $\lambda_{res} = 0.609$, Figure 2.4 illustrates a calculated asymmetrical line shape corresponding to thickness $d = 0.2\mu m$ while the thickness determined by the resonance wavelength is $d = 0.16\mu m$.

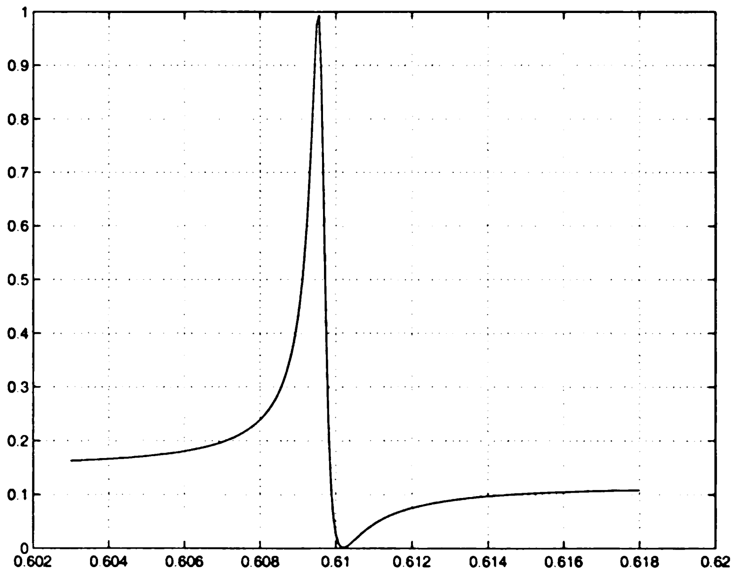

Figure 2.4. Asymmetric reflectance curve

2.3 Guided Modes for the Slab Waveguide

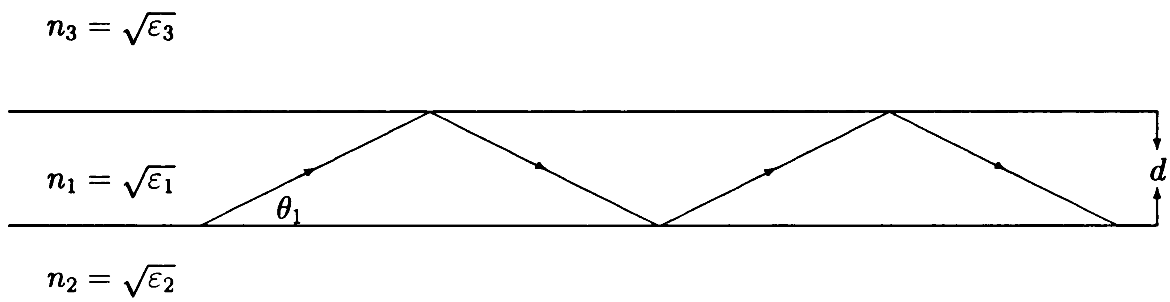

Figure 2.5. Guided wave in the slab waveguide.

We simplify the description of the slab waveguide by assuming that there is no variation in z direction, which we express symbolically by the equation

$$\frac{\partial}{\partial z} = 0 \tag{3.1}$$

Maxwell's equations can be written in the form

$$\nabla \times H = \varepsilon_0 n^2 \frac{\partial E}{\partial t} \tag{3.2}$$

and

$$\nabla \times E = -\mu_0 \frac{\partial H}{\partial t} \tag{3.3}$$

TE modes have only three field components : E_z, H_x and H_y.

Since we are interested in obtaining the normal modes of the slab waveguide, we assume that the x dependence of the mode fields is given by the function

$$e^{-i\beta x} \tag{3.4}$$

By combining the two factors, we obtain

$$e^{-i\omega t-\beta x} \tag{3.5}$$

With $E_x = 0, E_y = 0$ and $H_z = 0$, we obtain from Maxwell's equations:

$$\begin{aligned} -i\beta H_y - \frac{\partial H_x}{\partial y} &= i\omega\varepsilon_0 n^2 E_z && (3.6) \\ i\beta E_z &= -i\omega\mu_0 H_y && (3.7) \\ \frac{\partial E_z}{\partial y} &= -i\omega\mu_0 H_x && (3.8) \end{aligned}$$

We thus obtain the H components in terms of the E_z component

$$\begin{aligned} H_y &= -i\omega\mu_0 \frac{\partial E_z}{\partial x} && (3.9) \\ H_x &= \frac{i}{\omega\mu_0}\frac{\partial E_z}{\partial y} && (3.10) \end{aligned}$$

Substitution of these two equations into (3.6) yields the one-dimensional reduced wave equation for the E_z component:

$$\frac{\partial^2 E_z}{\partial x^2} + (n^2k^2 - \beta^2)E_z = 0 \tag{3.11}$$

with $k^2 = \omega^2\varepsilon_0\mu_0 = (\frac{2\pi}{\lambda})^2$.

Solve the ordinary differential equation, we must require that E_z are continuous at $y = 0$, $y = -d$ and vanish at $y = \pm\infty$.

$$\begin{aligned} E_z &= Ae^{-\delta y} && \text{for } y \geq 0 && (3.12) \\ &= A\cos\kappa y + B\sin\kappa y && \text{for } 0 \geq y \geq -d && (3.13) \\ &= (A\cos\kappa d - B\sin\kappa d)e^{\gamma(y+d)} && \text{for } y \leq -d && (3.14) \end{aligned}$$

The H_x component is obtained

$$\begin{aligned} H_x &= (-i\delta/\omega\mu_0)Ae^{-\delta y} && \text{for } x \geq 0 && (3.15) \\ &= (-i\kappa/\omega\mu_0)(A\sin\kappa y - B\cos\kappa y) && \text{for } 0 \geq y \geq -d && (3.16) \\ &= (i\gamma/\omega\mu_0)(A\cos\kappa d - B\sin\kappa d)e^{\gamma(y+d)} && \text{for } y \leq -d && (3.17) \end{aligned}$$

The H_x component does not immediately satisfy the boundary conditions. The requirement of continuity of H_x at $y = 0$ and $y = -d$ leads to the following system of equations:

$$\delta A + \kappa B = 0 \tag{3.18}$$

$$(\kappa \sin \kappa d - \gamma \cos \kappa d)A + (\kappa \cos \kappa d + \gamma \sin \kappa d)B = 0 \tag{3.19}$$

This homogeneous equation system has a solution only if the system determinant vanishes. We thus obtain the eigenvalue equation

$$\delta(\kappa \cos \kappa d + \gamma \sin \kappa d) - \kappa(\kappa \sin \kappa d - \gamma \cos \kappa d) = 0 \tag{3.20}$$

The eigenvalue equation can be written in a different form:

$$\tan \kappa d = \frac{\kappa(\gamma + \delta)}{\kappa^2 - \gamma\delta} \tag{3.21}$$

where

$$\kappa = (\varepsilon_0 k^2 - \beta^2)^{1/2},$$

$$\gamma = (\beta^2 - \varepsilon_1 k^2)^{1/2},$$

$$\delta = (\beta^2 - \varepsilon_3 k^2)^{1/2}.$$

2.4 Design Methodology

Design requirements are specified in terms of the resonant wavelength, λ_{res}, at which maximum reflectance occurs, the spectral bandwidth of the resonance $\Delta\lambda$, as well as the polarization and angle of the incident wave, and possibly the "out-of-band" reflectance away from resonance.

Given refractive indices for the surrounding (region 1) and the substrate (region 3), a thin film material must be chosen with refractive index greater than both. If AR (antireflection) properties are desired, then a multiple thin film structure is generally required for the waveguide. Since region 2 is also a grating, it must have a periodically modulated dielectric function.

With these modulated dielectric functions, we need to find the period Λ, thickness d of core, and fill factor f.

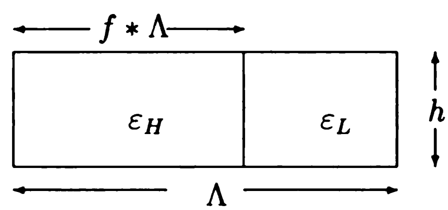

Figure 2.6. Design parameters

If f represents the fill-factor, the effective dielectric constant for the grating film is given by (for TE modes)

$$\varepsilon_{eff} = f * \varepsilon_H + (1 - f) * \varepsilon_L$$

This value of ε_{eff} is then used in ordinary thin film design expressions for the AR stack and in the calculation of the waveguide eigenvalues.

The calculation of the waveguide eigenvalues makes use of standard expressions for planar waveguide and can be found for a simple structure in section 2.3 and for a multilayer structure in [34].

Zero-order gratings are most effective in coupling incident radiation to a guided mode. Although it is possible to achieve a resonance with a higher order grating, the existence of more than one channel for light to propagate makes it difficult to get high reflectance, and in practice we constrain the design only to zero-order gratings.

Intuitively, the coupling between the grating and waveguide is realized by equation the first-order wave vector of the grating to a wave vector of a guided mode, viz.,

$$\beta = k(n_0 \sin\theta \pm i\frac{\lambda}{\Lambda}) \quad \text{mode matching condition,} \tag{4.1}$$

where

$\beta =$	guided mode eigenvalue = axial component of guided mode wavevector
$\lambda =$	wavelength of incident wave in vacuum
$k =$	incident wavenumber = $\frac{2\pi}{\lambda}$
$\theta =$	angle of incident plane wave in region 1
$n_0 =$	refractive index of region 1
$\Lambda =$	grating period

In the case that $\theta = 0$, zero-mode corresponding to $i = \pm 1$, and the mode matching condition becomes:

$$\Lambda = \frac{2\pi}{\beta} \tag{4.2}$$

For unmodulated ($\varepsilon(x) = \varepsilon_{eff}$) slab waveguide the eigenvalue equation for guided waves is

$$\tan(\kappa d) = \frac{\kappa(\gamma + \delta)}{\kappa^2 - \gamma\delta} \tag{4.3}$$

where d is the thickness of the slab waveguide,

$$\kappa = (\varepsilon_0 k^2 - \beta^2)^{1/2}$$

$$\gamma = (\beta^2 - \varepsilon_1 k^2)^{1/2}$$

$$\delta = (\beta^2 - \varepsilon_3 k^2)^{1/2}$$

The dielectric modulation is adjusted most easily by the fill factor of the grating.

Since the grating supports only zero order, the period is smaller than the wavelength, $\Lambda < \lambda_{res}$.

With the eigenvalues calculated for the effective structure, one can then estimate the required grating period using (4.1).

The design is not complete at this point because the expressions are only approximately true being rigorous in the limit $\varepsilon_H - \varepsilon_L \rightarrow 0$ [24, 33, 34].

To complete the design, one must calculate the performance of the structure using a rigorous Maxwell solver code to get accurate values for the resonant wavelength, spectral bandwidth and spectral reflectance. We will study the resonant wavelength in the following sections.

These values are then compared with the desired values, and if they exceed specified tolerance, the entire procedure is iterated until a satisfactory structure is found.

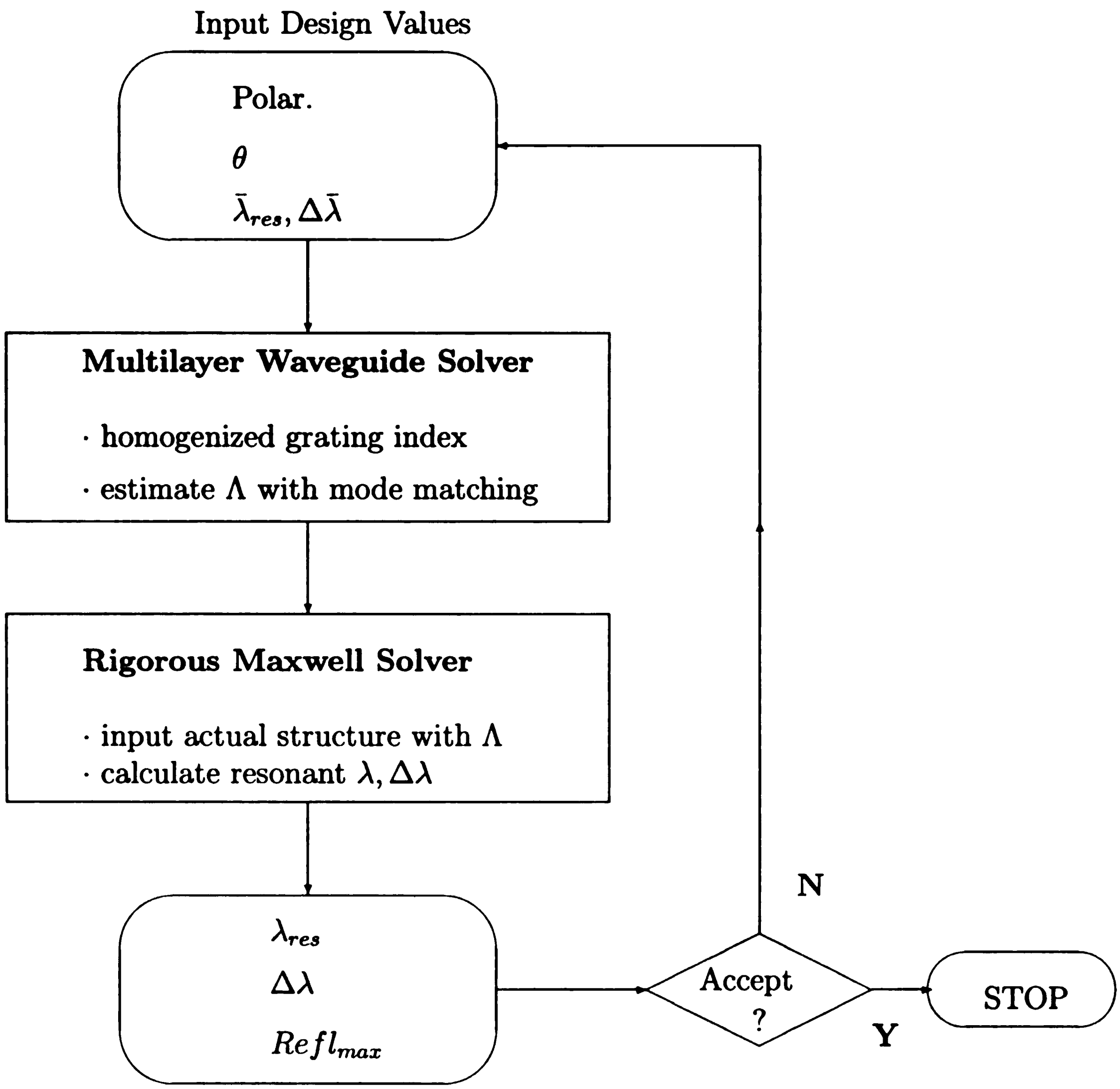

Figure 2.7. Design methodology for GMGRF

2.5 The dissipative diffraction problem

The direct determination of the resonant frequencies appears to be difficult. However, the study of the singularities of the scattering matrix is easier and provides valuable information about the resonant frequencies which stay along the real axis in the vicinity of these scattering frequencies (see Figure 2.8).

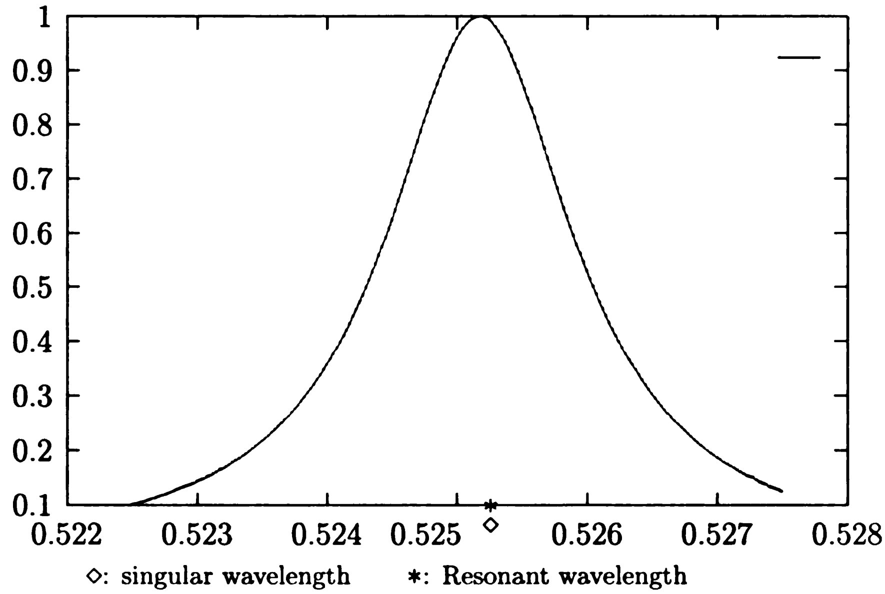

Figure 2.8. Resonance wavelength and singular wavelength

For sake of simplicity, we assume that only the zero order propagates, with amplitude A_0, which is dependent on ω, and the grating shape. If we assume the shape is fixed, A_0 is dependent on ω only, and we denote it by $A_0(\omega)$. We consider the extension of the problem to the complex plane. The research of poles for $A_0(\omega)$ implies that we try to see if it possible to find such solutions of Maxwell equations without any incident wave (homogeneous problem). If we find a value ω, for which the problem has a non trivial solution, it means that there exist finite coefficient A_0 without any incident wave, which has the consequence that, for a given incident wave with a complex frequency ω, A_0 is infinite. For ω_* lies not far from the real axis in the complex plane, when ω passes near the real part of ω_*, which is closed to the singular frequency ω_*, the coefficient A_0 takes very high values and gives rise to the resonance phenomenon.

For $\varepsilon(x) = n^2(x) \in \mathbf{R}$, consider the so-called **dissipative problem** obtained by extending the physical diffraction problem to complex values of $\omega \in \mathbf{C}$, let $\nu = \omega^2 \in \mathbf{C}$.

The variational formulation becomes:

$$a_\nu(u,v) = -\int_{\Gamma+} 2i\beta^{-i\beta b} v \quad \forall v \in H_p^1(\Omega) \tag{5.1}$$

We rewrite it as:

$$(I + T(\nu))u = L_f \quad \text{in} \quad H_p^1(\Omega) \tag{5.2}$$

where

$$\begin{aligned}
a_\nu(u,v) &= \int_\Omega (\nabla_\alpha u \cdot \nabla_{\bar\alpha} \bar v - \nu\varepsilon\mu u \bar v) - \int_{\Gamma+} T^+(\nu) u \bar v - \int_{\Gamma-} T^-(\nu) u \bar v \\
&= \int_\Omega [\nabla u \cdot \nabla \bar v + (|\alpha|^2 - \nu\varepsilon\mu) u \bar v - 2i\alpha\partial_1 u \bar v] - \int_{\Gamma+} T^+(\nu) u \bar v - \int_{\Gamma-} T^-(\nu) u \bar v \\
(T(\nu)u, v) &= \int_\Omega (\nabla_\alpha u \cdot \nabla_{\bar\alpha} \bar v - \nabla u \cdot \nabla \bar v - (\nu\varepsilon\mu + 1) u \bar v) - \int_{\Gamma+} T^+(\nu) u \bar v - \int_{\Gamma-} T^-(\nu) u \bar v \\
&= \int_\Omega [|\alpha|^2 - (\nu\varepsilon\mu + 1) u \bar v - 2i\alpha\partial_1 u \bar v] - \int_{\Gamma+} T^+(\nu) u \bar v - \int_{\Gamma-} T^-(\nu) u \bar v \qquad (5.3) \\
(L_f, v) &= -\int_{\Gamma+} 2i\beta^{-i\beta b} v
\end{aligned}$$

Let $A(\nu) : H_p^1(\Omega) \to H_p^1(\Omega)$ be the continuous operator associated to the sesqulinear form a_ν

$$(A(\nu)u, v) = a_\nu(u,v) \quad \text{for } u, v \in H_p^1(\Omega)$$

Proposition 2.5.1 *For any complex number ν, the operator $A(\nu)$ admits a Fredholm decomposition, i.e. we have $A(\nu) = B(\nu) + C(\nu)$, where $B(\nu)$ is an automorphism of $H_p^1(\Omega)$ and $C(\nu)$ is a compact operator on $H_p^1(\Omega)$.*

Proof:

Set $a_\nu = b_\nu + c_\nu$, where the sesqulinear forms b_ν and c_ν are defined on $H_p^1(\Omega) \times H_p^1(\Omega)$ by:

$$\begin{cases} b_\nu(u,v) &= \int\limits_\Omega (\nabla u \cdot \nabla \bar{v} + u \cdot \bar{v}) - \int\limits_{\Gamma+} T^+(\nu) u\bar{v} - \int\limits_{\Gamma-} T^-(\nu) u\bar{v} \\ c_\nu(u,v) &= -\int\limits_\Omega (\nu\varepsilon\mu + 1 - |\alpha|^2) u \cdot \bar{v} + i\alpha(u\partial_1\bar{v} - \partial_1 u\bar{v}) \end{cases}$$

Let $B(\nu)$ and $C(\nu)$ be the continuous operator of $H_p^1(\Omega)$ associated to the sesqulinear forms $b_\nu(\cdot,\cdot)$ and $c_\nu(\cdot,\cdot)$.

Then it is easy to check that $B(\nu)$ is an automorphism and $C(\nu)$ is compact operator. ∎

Proposition 2.5.2 *([9]) $T(\nu)$ is holomorphic in the domain* $\mathbf{C}\backslash\mathbf{R}^-$.

$A(\nu)$ is an analytic perturbation $T(\nu)$ of I. From now on we shall denote $(I + T(\nu))^{-1}$ by $R(\nu)$.

2.6 Scattering frequency

ν_* is scattering frequency, if there exists $u \neq 0$ such that

$$A(\nu_*)u = 0 \tag{6.1}$$

i.e.,

$$a_{\nu_*}(u,v) = \int\limits_\Omega \{\nabla_\alpha u \cdot \nabla_{\bar{\alpha}} \bar{v} - \nu_* \varepsilon\mu u\bar{v}\} - \int_{\Gamma+} T^+(\nu) u\bar{v} - \int\limits_{\Gamma-} T^-(\nu) u\bar{v} = 0 \quad \text{for } \forall v \in H^1(\Omega). \tag{6.2}$$

$$(I + T(\nu))u = 0 \quad \text{in } H_p^1(\Omega). \tag{6.3}$$

Proposition 2.6.1 *The scattering frequencies ν_* of the diffraction problem are the solutions of the nonlinear eigenvalue problem (6.3).*

Proposition 2.6.2 *If* Im $(\nu) > 0$, *the problem (5.1) has a unique solution.*

Proof: Suppose $A(\nu)u = 0$, then $a_\nu(u, v) = 0$ for $\forall v \in H^1(\Omega)$.

$$a_\nu(u,v) = \int_\Omega (\nabla_\alpha u \cdot \nabla_\alpha \bar{v} - \nu\varepsilon\mu u\bar{v}) - \int_{\Gamma+} T^+(\nu)u\bar{v} - \int_{\Gamma-} T^-(\nu)u\bar{v} = 0$$

$$\begin{aligned}
& \text{Im}\,(a_\nu(u,u)) \\
= \; & -\int_\Omega \text{Im}\,(\nu\mu\varepsilon)|u|^2 - \text{Im}\,(\int_{\Gamma+} T^+(\nu)u\bar{u}) - \text{Im}\,(\int_{\Gamma-} T^-(\nu)u\bar{u}) \\
= \; & -\int_\Omega \text{Im}\,(\nu\mu\varepsilon)|u|^2 - \int_{\Gamma+} \sum Re(\beta_n^+)u_n^+ e^{inx_1}\bar{u} - \int_{\Gamma-} \sum Re(\beta_n^-)u_n^- e^{inx_1}\bar{u} \\
= \; & -\int_\Omega \text{Im}\,(\nu\mu\varepsilon)|u|^2 - \text{Re}\,\sum \beta_n^+|u_n^+|^2 - \text{Re}\,\sum \beta_n^-|u_n^-|^2
\end{aligned}$$

Im $(\nu\mu\varepsilon) > 0$ and Re $\beta_p^\pm \geq 0$

All terms of this expression vanish since they are non-negative.

We have $u(x) = 0$ for $x \in \Omega$.

∎

Corollary 2.6.1 *The resolvent operator $R(\nu) = A^{-1}(\nu)$ is holomorphic in the half plane* Im $(\nu) > 0$. *i.e., The scattering frequency is the half plane* Im $(\nu) \leq 0$.

2.7 Numerical solution for scattering frequency

By V_h we denote a finite-dimensional subspace of $H_p^1(\Omega)$. We will find the scattering frequency ν approximation ν_h in V_h.

Let X denote a complex Banach space and $L(X)$ denote the set of bounded, linear operators on X. For pencil $[A, B]$ of operators in $L(X)$ let $\rho[A, B]$, $\sigma[A, B]$, and $P_{\sigma[A,B]}$ denote the resolvent set, the spectrum, and the point spectrum defined by

$$\begin{aligned}
\rho[A,B] &= \{\lambda \in \mathbf{C} : A - \lambda B \text{ is boundedly invertible }\} \\
\sigma[A,B] &= \mathbf{C} \backslash \rho[A,B] \\
P_\sigma[A,B] &= \{\lambda \in \mathbf{C} : A - \lambda B \text{ is not one-to-one }\} \\
Q_\sigma[A,B] &= \{\lambda \in P_\sigma[A,B] : \dim Ker[A - \lambda B] < +\infty\}
\end{aligned}$$

For each λ in some domain D in $\mathbf{C}$, let $F(\lambda)$ be a linear, compact operator on X and let F be holomorphic in λ. We call $\xi \in D$ a nonlinear eigenvalue if $A(\xi) = I - F(\xi)$ is not one-to-one.

Theorem 2.7.1 *([16, 25]) Define $\alpha(\lambda)$ to be the dimension of $Ker[I - F(\lambda)]$. Then $\alpha(\lambda)$ is constant on D except at a countable number of isolated points. If $\alpha(\lambda) = 0$ for at least one point of D, then $I - F(\lambda)$ is bounded invertible in D except at a countable number of isolated points.*

Let ξ be an isolated nonlinear eigenvalue of $I - F(\lambda)$. Let Π_h be a bounded projection from X onto X_n, a finite dimensional subspace of X, and assume that $\{\Pi_h\}$ converges pointwise to the identity I,

$$\Pi_h \to I. \quad \text{point wise} \quad \text{as } h \to 0 \tag{7.1}$$

It is obvious that ξ is an eigenvalue of $I - F(\xi)$ if and only if $0 \in Q_\sigma[I - F(\xi), I]$.

Theorem 2.7.2 *[16, 25] Let $\gamma > 0$ and Let $F(\lambda)$ be an $L(X)$ valued function which is holomorphic on $D = \{|\lambda| < \gamma\}$ in the complex plane $\mathbf{C}$. For $\xi \in D$ assume that $0 \in Q_\sigma[I - F(\xi), I]$ is an isolated point with algebraic multiplicity m. Let U be an open set which isolates 0 from the remainder of $\sigma[I - F(\xi), I]$. Then there is a positive δ, a positive integer p, and a positive integer $k \leq m$ so that for $|\lambda - \xi| \leq \delta$, the following hold:*

1. *$U \bigcap \sigma[I - F(\lambda), I]$ consists of m eigenvalues $\mu_1(\lambda), \cdots, \mu_m(\lambda)$ counted according to multiplicity, k of which are distinct; each function $\mu_i(\lambda)$ is a holomorphic function of the principal value of the p-th root of λ and satisfies $\mu_i(\xi) = 0$; the average $\bar{\mu}(\lambda) = \frac{\{\mu_1\lambda + \cdots + \mu_m(\lambda)\}}{m}$ is holomorphic in λ.*

2. *for h sufficiently small $U \bigcap \sigma[I - \Pi_h F(\lambda), I]$ consists of m eigenvalues $\mu_1(\lambda; h), \cdots, \mu_m(\lambda; h)$ counted according to multiplicity; the average $\bar{\mu}_h(\lambda)$ of these eigenvalues is holomorphic in λ;*

3. *$\mu_i(\lambda; h)$ converges uniformly to $\mu_i(\lambda)$ as $h \to 0$.*

With the above Theorem, we can find ξ_h such that $\bar{\mu}_h(\xi_h) = 0$.

To compute $\bar{\mu}_h$ the algebraic multiplicity m must be known. Given λ, we first compute the m eigenvalues $\mu_1(\lambda; h), \cdots, \mu_m(\lambda; n)$ of $I - \Pi_h F(\lambda)$ closest to 0, and then the arithmetic mean $a_h(\lambda) = \frac{\mu_1(\lambda;h) + \cdots + \mu_m(\lambda;h)}{m}$.

Let us consider the homogeneous dissipative problem:

$$[I + T(\nu)]u = 0$$

$$\begin{aligned}(T(\nu)u, v) &= \int_\Omega (\nabla_\alpha u \cdot \nabla_\alpha \bar{v} - \nabla u \cdot \nabla \bar{v} - (\nu\varepsilon\mu + 1)u\bar{v}) - \int_{\Gamma+} T^+(\nu)u\bar{v} - \int_{\Gamma-} T^-(\nu)u\bar{v} \\ &= \int_\Omega [|\alpha|^2 - (\nu\varepsilon\mu + 1)u\bar{v} - 2i\alpha\partial_1 u\bar{v}] - \int_{\Gamma+} T^+(\nu)u\bar{v} - \int_{\Gamma-} T^-(\nu)u\bar{v}\end{aligned}$$

$$(Ju, v) = \int_\Omega \nabla u \nabla v + uv \tag{7.2}$$

$$T(\nu_*)U(\nu_*) = \lambda(\nu_*)JU(\nu_*) \tag{7.3}$$

It is obvious that scattering frequency is the solution of

$$\lambda(\nu_*) = -1 \tag{7.4}$$

The solution of (*7.4*) by Newton's method requires the derivative $\lambda'(\nu)$ of $\lambda(\nu)$. We assume that $\lambda(\nu)$ is a simple eigenvalue of $A(\nu)$,

Proposition 2.7.1

$$\lambda'(\nu) = (T'(\nu)U(\nu), g(\nu))$$

where $g(\nu)$ is the associated eigenvector of the adjoint operator, i.e., satisfying

$$T^*(\nu)g(\nu) = \overline{\lambda(\nu)}Jg(\nu)$$

and

$$(JU(\nu), g(\nu)) = 1$$

proof:

$$\begin{aligned}
\lambda'(\nu) &= (T(\nu)U(\nu), g(\nu))' \\
&= (T'(\nu)U(\nu), g(\nu)) \\
&\quad +[(T(\nu)U'(\nu), g(\nu)) + (T(\nu)U(\nu), g'(\nu))]
\end{aligned}$$

$$\begin{aligned}
&(T(\nu)U'(\nu), g(\nu)) + (T(\nu)U(\nu), g'(\nu)) \\
= \; &(U'(\nu), T^*(\nu)g(\nu)) + (\lambda(\nu)JU(\nu), g'(\nu)) \\
= \; &(U'(\nu), \overline{\lambda(\nu)}Jg(\nu)) + (\lambda(\nu)JU(\nu), g'(\nu)) \\
= \; &\lambda(\nu)(JU'(\nu), g(\nu)) + \lambda(\nu)(JU(\nu), g'(\nu)) \\
= \; &\lambda(\nu)(1)' \\
= \; &0
\end{aligned}$$

∎

We can rewrite the eigenvalue problem as:

Find ν, such that there exists $u \neq 0$,

$$\int_{\Omega} \nabla u \cdot \nabla \bar{v} + |\alpha(\nu)|^2 u\bar{v} - 2i\alpha(\nu)\partial_1 u\bar{v} - \int_{\Gamma^+} T^+(\nu)u\bar{v} - \int_{\Gamma^-} T^-(\nu)u\bar{v} = \nu \int_{\Omega} \varepsilon\mu u\bar{v} \quad (7.5)$$

It is equivalent to

$$\int_{\Omega} \nabla u \cdot \nabla \bar{v} + |\alpha|^2 u\bar{v} - 2i\alpha\partial_1 u\bar{v} - \int_{\Gamma^+} T^+ u\bar{v} - \int_{\Gamma^-} T^- u\bar{v} = r(\nu) \int_{\Omega} \varepsilon\mu u\bar{v} \quad (7.6)$$

$$r(\nu) = \nu \quad (7.7)$$

It is a nonlinear eigenvalue problem

$$A(\lambda)x = \lambda Bx \quad (7.8)$$

where B $S.P.D.$

We can solve it by simple iteration, i.e., given ω_0, $r(\omega_n) = \omega_{n+1}$

The numerical experiment shows that the method converges, but we could not prove the convergence.

We can solve the nonlinear equation $r(\nu) - \nu = 0$ by secant method. It is faster than simple iteration, since the convergent rate 1.618.

Example

For parameters $\Lambda = 0.3\mu m$ (period), $d = 0.125\mu m$ (thickness of core), $f = 0.5$ (fill-factor), $\varepsilon_H = 4.4, \varepsilon_L = 3.6, \varepsilon_{surr} = 1, \varepsilon_{sub} = 2.31$ and $theta = 0$, we found 2 eigenvalues in $[0.5, 0.6]$, $\lambda_1 = 0.51152267, \lambda_2 = 0.51362098$.

At $\lambda_1 = 0.51152267$, the reflective efficiency is 0.99993363, it is a resonant wavelength, see Figure 2.7.

At $\lambda_2 = 0.51362098$, the reflective efficiency 0.1445, it is not a resonant wavelength, see 2.9. We notice that there is a small "bump" near this eigenvalue.

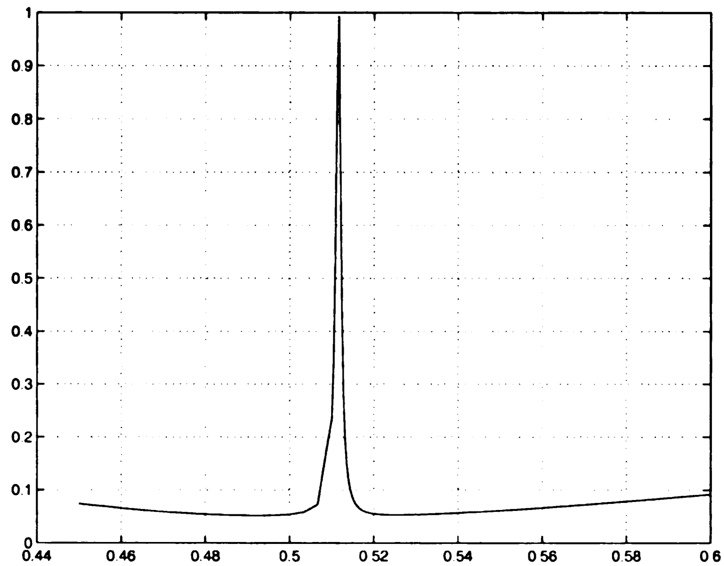

Figure 2.9. resonant wavelength

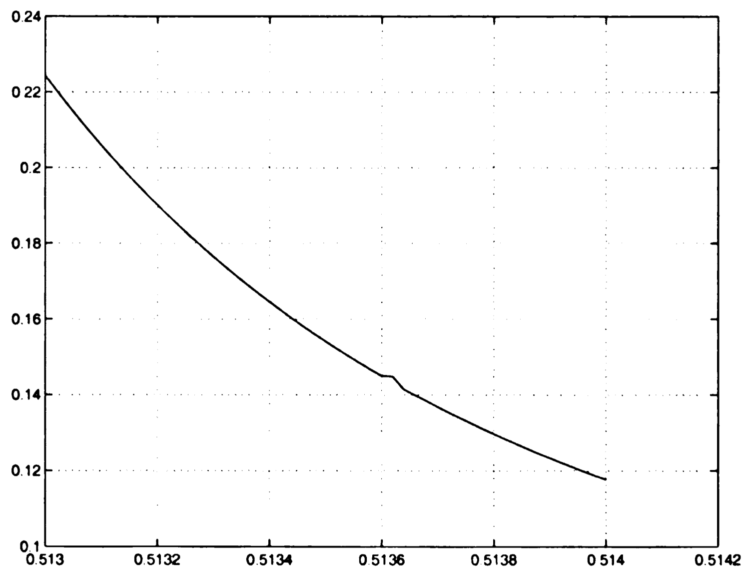

Figure 2.10. eigenvalue but not resonant wavelength

2.8 Design of GMGRF

With the function $r(f, d, \Lambda)$ which correspond the given grating structure to the resonance frequency (wavelength), we may consider the design problem.

Given permittivity constants $\varepsilon_H, \varepsilon_L, \varepsilon_{surr}$ and ε_{sub}, at first, we use fill-factor as 0.5. The grating film thickness is quarter-wavelength, or a multiple thereof. Solve the waveguide eigenvalue equation, we can decide the period of grating.

Next step, we need to compute the resonance wavelength and bandwidth. It is hard to get accurate values of the spectral bandwidth. But it is easy to know whether the bandwidth for the structure is greater or less than a given data.

These values are then compared with the desired values, and if necessary, the fill-factor will adjusted to get the the specified wavelength. This is to find zero of a nonlinear equation. After adjusted the fill-factor, we consider the reflectance out of resonance region. If necessary, we can change the thickness of the grating film. This is an optimization problem.

Given: $\varepsilon_{surr}, \varepsilon_{sub}, \varepsilon_H, \varepsilon_L, \theta$ (incident angle)

1. Waveguide solver

   Initial data :

   $f = 0.5$, fill-factor.

   $d = \dfrac{m\lambda}{4\sqrt{\varepsilon_{eff}}}$ thickness of core, $m = 1, 2, \cdots$

   Λ From mode-matching condition.

   (a) Waveguide eigenvalue

   Solve (3.21) for β (for single layer).

$$\tan \kappa d = \frac{\kappa(\gamma + \delta)}{\kappa^2 - \gamma\delta}$$

where

$$\kappa = (\varepsilon_0 k^2 - \beta^2)^{1/2}$$

$$\gamma = (\beta^2 - \varepsilon_1 k^2)^{1/2}$$

$$\delta = (\beta^2 - \varepsilon_3 k^2)^{1/2}$$

(b) mode-matching condition

Solve (4.1) for Λ.

$\theta = 0$, zero-mode $\rightarrow \Lambda = \frac{2\pi}{\beta}$

If Λ is not in the interval $(0, \lambda)$, we need to change the material.

2. Rigorous Maxwell Solver

   Input period Λ, calculate resonant wavelength λ

3. iteration

   modify fill-factor (first), thickness or period.

From initial start value f_0, d_0, Λ, we need solve the following two mathematical problems:

1. Solve nonlinear equation

$$r(f_{j+1}, d_j, \Lambda) = \lambda_{res}$$

This function is a real valued function, we use Van Wijingaarden-Dekker-Brent method. It combines the bisection and secant methods, providing a synthesis of the advantages of both.

2. Optimal problem:

   It is hard to get the accurate value of bandwidth. In fact, we don't need to know the accurate value of bandwidth.

   We can specified a desired bandwidth $\Delta\lambda$, compute the reflectance at wavelength $\lambda + \Delta\lambda$ and $\lambda - \Delta\lambda$, then we know whether the actual bandwidth is satisfied or not by comparing it with $\Delta\lambda$.

   At wavelengths $\lambda + \Delta\lambda$ (and/or $\lambda - \Delta\lambda$), we can compute the reflectance e_0 by solving the direct diffraction problem. If it is not satisfied, then at wavelength $\lambda = \lambda_c + \Delta\lambda$ ($\lambda = \lambda_c - \Delta\lambda$) solve the following optimal problem.

   Solve d_{j+1}

$$e_0(f_{j+1}, d_{j+1}, \Lambda) = \min_d e_0(f_{j+1}, d, \Lambda)$$

   For this optimization problem, we can use the gradient formula described in section 1.6.

The above procedures iterated until a satisfactory structure is found. In numerical experiment, this procedure is found to converge quite quickly.

2.9 Numerical example

Given $\varepsilon_H = 2.1^2 = 4.41, \varepsilon_L = 2.0^2 = 4.0, \varepsilon_{surr} = 1.0^2 = 1.0, \varepsilon_{sub} = 1.52^2 = 2.3104$ and $\theta = 0$.

The specified resonant center is $\lambda_{res} = 0.54$

1. First we need to estimate thickness, $d = \dfrac{0.54}{2 * (2.1 * 0.5 + 2.0 * 0.5)} \doteq 0.132$

   Solve (3.21) for β, we have $\beta \doteq 20.423$, then $\Lambda = \dfrac{2\pi}{\beta} \doteq 0.307$

2. For this structure ($\Lambda = 0.307, d = 0.132, f = 0.5$), we found that the eigenvalue is 0.5385

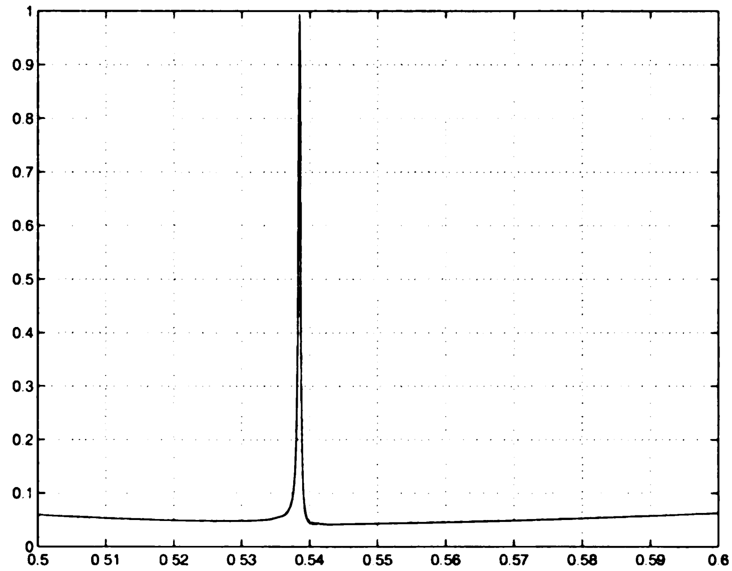

Figure 2.11. reflectance curve for initial data

Solve nonlinear equation (with $\Lambda = 0.307, d = 0.132$)

$$r(f) = 0.54$$

The solution is $f \doteq 0.714$.

With fill-factor $f = 0.714$, the reflectance curve is given by Figure 2.12:

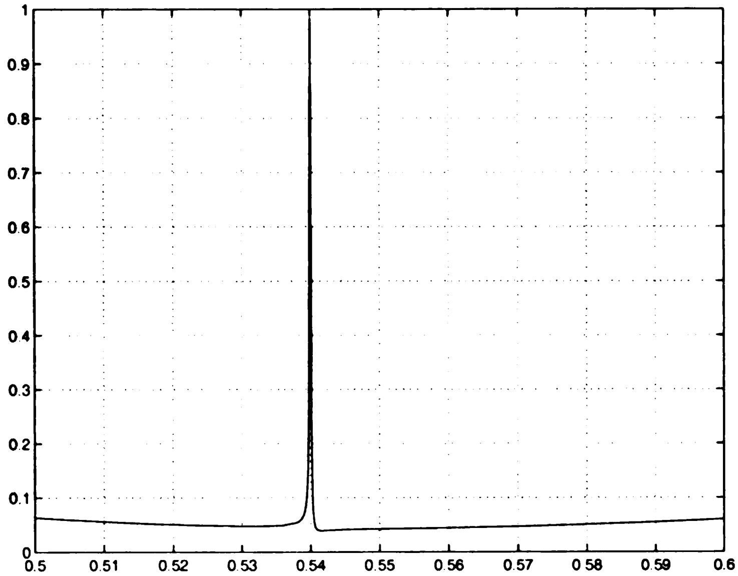

Figure 2.12. reflectance curve

3. Consider $\Delta\lambda = 0.015$,

   At $\lambda = \lambda_{res} + \Delta\lambda = 0.5415$, Reflectance is 0.0389.

   At $\lambda = \lambda_{res} - \Delta\lambda = 0.5385$, Reflectance is 0.0591.

   We need to solve the minimization problem at wavelength $\lambda = 0.5385$ (with $\Lambda = 0.307, f = 0.714$):

$$\min_{d} e_0(d)$$

   We got $d = 0.131$

   For this structure ($\Lambda = 0.307, d = 0.131$) , solve nonlinear equation $r(f) = 0.54$ again, the new fill-factor is $f = 0.741$.

At $\lambda = \lambda_{res} + \Delta\lambda = 0.5415$, Reflectance $= 0.041$

At $\lambda = \lambda_{res} - \Delta\lambda = 0.5385$, Reflectance $= 0.048$

We may stop with the parameters as $\Lambda = 0.307, d = 0.131, f = 0.741$.

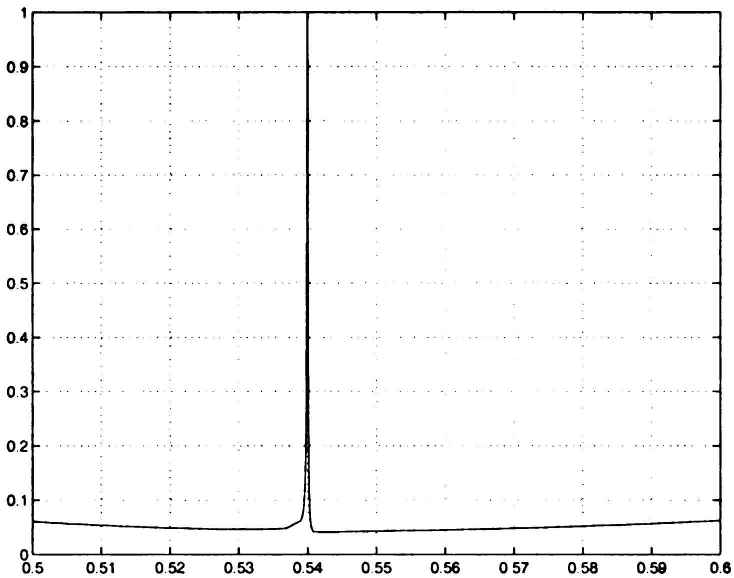

Figure 2.13. reflectance curve for the design example.

CHAPTER 3

Optimal design of nonlinear grating

3.1 Introduction

Consider a plane wave of frequency ω_1 incident on a grating or periodic structure consisting of some nonlinear optical material. Because of the presence of the nonlinear material, the nonlinear optical interaction gives rise to diffracted waves at frequencies ω_1 and $\omega_2 = 2\omega_1$. This process represents the simplest situation in nonlinear optics – second harmonic generation (SHG). An exciting application of SHG is to obtain coherent radiation at a wavelength shorter than that of the available lasers. Unfortunately, it is well known that nonlinear optical effects from SHG are generally so weak that their observation requires extremely high intensity of laser beams. Effective enhancement of nonlinear optical effects presents one of the most challenging tasks in nonlinear optics.

The present research is concerned with important aspects for systematically design of surface (grating) enhanced nonlinear optical effects. Recently, in a sequence of papers [29], [30], [27], a PDE model based on Maxwell's equations has been introduced to model nonlinear SHG in periodic structures. In particular, it has been announced in [29] and [30] that SHG can be greatly enhanced by using diffraction gratings or periodic structures and the PDE model can predict the field propagation accurately.

Our goal is to provide the mathematical foundation of optimization methods for solving the optimal design problem of nonlinear periodic gratings. By conducting a perturbation analysis of the grating problems that arise from smooth variations of the interfaces, we derive explicit formulas for the partial derivatives of the reflection and transmission coefficients. Such derivatives allow us to compute the gradients for a general class of functionals involving the Rayleigh coefficients.

Optimal design of periodic grating has recently received much attention [1], [3], [6], [17], [18]. For linear grating structures, significant results have been obtained by Dobson [15](weak convergence), Bao and Bonnetier [3](homogenization), and Eschner and Schmidt [17], [18] (optimization). To our best knowledge, the present work is the first attempt to solve the optimal design problem of nonlinear gratings. Little is known concerning the questions of existence and uniqueness for nonlinear Maxwell's equations in periodic structures. In two simple cases, where Maxwell's equations can be reduced to a system of nonlinear Helmholtz equations, existence and uniqueness results have been obtained recently in Bao and Dobson [6] and [7]. Computational results have also been obtained by using a combination of the method of finite elements and the fixed point iteration algorithm. More recently, a more general model has been studied by Bao and Chen [4]. Their model supports a general class of nonlinear optical materials with cubic symmetry structures. Our present work is devoted to study the optimal design problem for this model problem.

A good background on the linear theory of diffractive optics in grating structures may be found in Petit [28] and Bao, Cowsar and Masters [5]. For the underlying physics of nonlinear optics, we refer the reader to the classic books of Bloembergen [11] and Shen [31].

3.2 Modeling of the nonlinear scattering problem

Throughout, the media are assumed to be nonmagnetic with constant magnetic permeability. For convenience, the magnetic permeability constant is assumed to be equal to unity everywhere. Assume also that no external charge or current is present.

The time harmonic Maxwell equations that govern SHG then take the form:

$$\nabla \times \mathbf{E} = \frac{i\omega}{c}\mathbf{H}, \quad \nabla \cdot \mathbf{H} = 0\,, \tag{2.1}$$

$$\nabla \times \mathbf{H} = -\frac{i\omega}{c}\mathbf{D}, \quad \nabla \cdot \mathbf{D} = 0, \tag{2.2}$$

along with the constitutive equation:

$$\mathbf{D} = \epsilon\mathbf{E} + 4\pi\chi^{(2)}(x,\omega) : \mathbf{E}\mathbf{E}\,, \tag{2.3}$$

where $\mathbf{E}$ is electric field, $\mathbf{H}$ is magnetic field, $\mathbf{D}$ is electric displacement, ϵ is dielectric coefficient, c is speed of the light, ω is angular frequency, $\chi^{(2)}$ is the second order nonlinear susceptibility tensor of third rank, i.e., $\chi^{(2)} : \mathbf{E}\mathbf{E}$ is a vector whose j-th component is $\sum_{k,l=1}^{3} \chi^{(2)}_{jkl}\mathbf{E}_k\mathbf{E}_l, j = 1,2,3$.

Remark 2.1. The medium is said to be linear if $\mathbf{D} = \epsilon\mathbf{E}$ or $\chi^{(2)}$ vanishes. In principle, essentially all optical media are nonlinear, i.e., $\mathbf{D}$ is a nonlinear function of $\mathbf{E}$.

The physics of SHG may be described as follows: when a plane wave at frequency $\omega = \omega_1$ is incident on a nonlinear medium, because of the interaction of the incident wave and nonlinear medium, diffracted waves at frequencies $\omega = \omega_1$ and $\omega = 2\omega_1$ are generated. The fact that new frequency components are present is the most striking difference between nonlinear and linear optics. However, for most media, nonlinear optical effects are so weak that they may reasonably be ignored. In particular, the conversion of energy into the new frequency component is very small. The observation of nonlinear phenomena in the optical region normally can only be made by using high intensity beams, say by application of a high intensity laser.

Assume that the depletion of energy from the pump waves (at frequency $\omega = \omega_1$) may be neglected, which is the well known undepleted pump approximation in the literature, see [29] and [30]. Under the approximation, equation (2.3) at frequencies $\omega = \omega_1$ and $\omega = \omega_2 = 2\omega_1$, respectively, may be written as

$$\mathbf{D}(x,\omega_1) = \epsilon(x,\omega_1)\mathbf{E}(x,\omega_1) , \tag{2.4}$$

$$\mathbf{D}(x,\omega_2) = \epsilon(x,\omega_2)\mathbf{E}(x,\omega_2) + 4\pi\chi^{(2)}(x,\omega_2) : \mathbf{E}(x,\omega_1)\mathbf{E}(x,\omega_1) . \tag{2.5}$$

We then reduce the nonlinear coupled system (2.1) and (2.2). Throughout the paper, all fields are assumed to be invariant in the x_3 direction. Here, as in the linear case, in TE polarization the electric field is transversal to the (x_1, x_2)-plane, and in TM polarization the magnetic field is transversal to the (x_1, x_2)-plane. In the nonlinear case, however, the polarization is determined by group symmetry properties of $\chi^{(2)}$. In this work, motivated by applications, we assume that the electromagnetic fields are TM polarized at frequency ω_1 and TE polarized at frequency ω_2. This polarization assumption is known to support a large class of nonlinear optical materials, for example, crystals with cubic symmetry structures. See Appendix for additional discussion.

Therefore

$$\mathbf{H}(x,\omega_1) = H(x_1,x_2,\omega_1)\vec{x}_3 , \tag{2.6}$$

$$\mathbf{E}(x,\omega_2) = E(x_1,x_2,\omega_2)\vec{x}_3 . \tag{2.7}$$

Define for convenience

$$\epsilon_j = \epsilon(x_1,x_2,\omega_j),\ j = 1,2 , \tag{2.8}$$

$$k_j = \frac{\omega_j}{c}\sqrt{\epsilon_j} , \quad Im(k_j) \geq 0 , j = 1,2 . \tag{2.9}$$

The system (2.1), (2.2) at frequency ω_1 can be simplified to

$$\nabla \cdot (\frac{1}{k_1^2} \nabla H) + H = 0 \, . \tag{2.10}$$

Because of Equation (2.10),

$$\mathbf{E}(x, \omega_1) = \frac{c}{i\omega_1 \epsilon_1} \nabla \times \mathbf{H}(x, \omega_1) \tag{2.11}$$

$$= \frac{c}{i\omega_1 \epsilon_1} (\partial_{x_2} H, -\partial_{x_1} H, 0) \, . \tag{2.12}$$

Hence the second harmonic field satisfies

$$\left[\triangle + k_2^2\right] E = -\frac{4\pi\omega_2^2}{c^2} \sum_{j,l=1,2,3} \chi^{(2)}_{3jl}(x, \omega_2)(\mathbf{E}(x, \omega_1))_j (\mathbf{E}(x, \omega_1))_l \, , \tag{2.13}$$

$$= \sum_{j,l=1,2} \rho_{jl} \partial_{x_j} H \, \partial_{x_l} H \, , \tag{2.14}$$

where $\triangle$ is the usual Laplace operator and $\rho_{jl} = (-1)^{j+l} \frac{16\pi}{\epsilon_1^2} \chi^{(2)}_{3,j,l}(x, \omega_2)$.

Let us further specify the problem geometry. Assume that the medium and material are periodic in the x_1 variable of period 2π and are invariant in the x_3 variable. We may then restrict to a single period in x_1, as shown in Figure 3.1.

Introduce the notation:

$\Gamma_j = \{x_2 = (-1)^{j-1} b, \; 0 < x_1 < 2\pi\}$, $\quad S_j = \{0 < x_1 < 2\pi, \; x_2 = \phi_j(x_1)\}$,

$\Omega_1 = \{0 < x_1 < 2\pi, \; \phi_1(x_1) < x_2 < b\}$, $\quad \Omega_2 = \{0 < x_1 < 2\pi, \; -b < x_2 < \phi_2(x_1)\}$,

$\Omega_1^+ = \{0 < x_1 < 2\pi, \; x_2 \geq b\}$, $\quad \Omega_2^+ = \{0 < x_1 < 2\pi, \; x_2 \leq -b\}$,

$\Omega_0 = \{0 < x_1 < 2\pi, \; \phi_2(x_1) < x_2 < \phi_1(x_1)\}$, $\quad \Omega = \{0 < x_1 < 2\pi, \; -b < x_2 < b\}$.

Suppose that the whole space is filled with material in such a way that the "indexes of refraction" n_1 and n_2 satisfy

$$n_j(x) = \begin{cases} n_{j1} & \text{in } \Omega_1^+ \cup \bar{\Omega}_1 \, , \\ n_{j0} & \text{in } \Omega_0 \, , \\ n_{j2} & \text{in } \Omega_2^+ \cup \bar{\Omega}_2 \, , \end{cases}$$

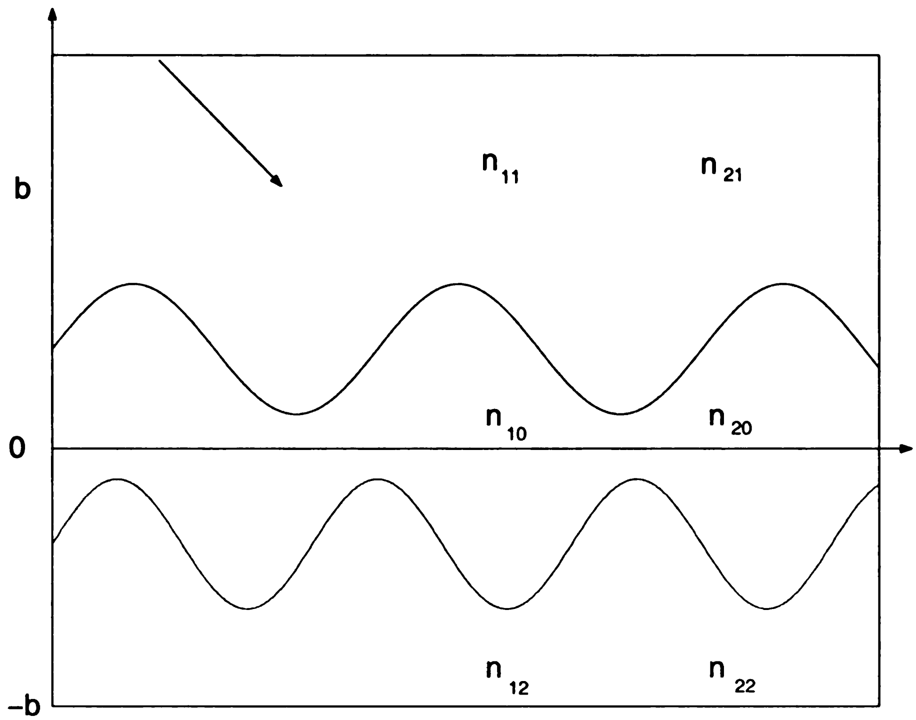

Figure 3.1. Problem geometry.

for $j = 1, 2$, where n_{j1} and n_{j2} are constants, n_{j1} are real and positive, and $Re\ n_{j2} > 0$, $Im\ n_{j2} \geq 0$. The case $Im\ n_{j2} > 0$ accounts for materials which absorb energy. We assume that $n_{j0}(x)$ are piecewise constant functions in Ω_0 satisfying $Re\ n_{j0} > 0$, $Im\ n_{j0} \geq 0$.

We wish to solve the system (3.8) and (2.13) when an incoming plane wave

$$u_I = u_i e^{i\alpha_1 x_1 - i\beta_1 x_2} \tag{2.15}$$

is incident on S_1 from Ω_1^+ where u_i is a real positive constant, $\alpha_1 = k_{11}\sin\theta$, $\beta_1 = k_{11}\cos\theta$, $k_{11} = \frac{\omega_1}{c}n_{11}$, and $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ is the angle of incidence.

We are interested in "quasi-periodic" solutions (H, E), that is, solutions (H, E) such that

$$u = He^{-i\alpha_1 x_1} \quad \text{and} \quad v = Ee^{-i\alpha_2 x_1} \quad (\alpha_2 = k_{21}\sin\theta, k_{21} = \frac{\omega_2}{c}n_{21})$$

are 2π-periodic in the x_1 direction.

It follows from the system (3.8) and (2.13) that

$$\nabla_{\alpha_1} \cdot \left(\frac{1}{k_1^2}\nabla_{\alpha_1} u\right) + u = 0\,, \tag{2.16}$$

$$\left(\Delta_{\alpha_2} + k_2^2\right) v = \sum_{j,l=1,2} \rho_{jl}^{\alpha} \partial_j^{\alpha_1} u \, \partial_l^{\alpha_1} u\,, \tag{2.17}$$

where

$$\Delta_{\alpha_2} = \Delta + 2i\alpha_2\partial_{x_1} - |\alpha_2|^2\,, \nabla_{\alpha_1} = \nabla + i(\alpha_1, 0) \tag{2.18}$$

and

$$\rho_{jl}^{\alpha} = \rho_{jl} e^{i(2\alpha_1 - \alpha_2)x_1}\,, \quad \partial_1^{\alpha_1} = \partial_{x_1} + i\alpha_1\,, \quad \partial_2^{\alpha_1} = \partial_{x_2}\,.$$

Define, for $j = 1, 2$, the coefficients

$$\beta_{1j}^{(n)}(\alpha) = e^{i\gamma_{1j}/2}\left|k_{1j}^2 - (n+\alpha_1)^2\right|^{1/2}, \quad n \in Z, \tag{2.19}$$

$$\beta_{2j}^{(n)}(\alpha) = e^{i\gamma_{2j}/2}\left|k_{2j}^2 - (n+\alpha_2)^2\right|^{1/2}, \quad n \in Z, \tag{2.20}$$

where

$$\gamma_{1j} = \arg(k_{1j}^2 - (n+\alpha_1)^2), \quad 0 \le \gamma_{1j} < 2\pi\,, \tag{2.21}$$

$$\gamma_{2j} = \arg(k_{2j}^2 - (n+\alpha_2)^2), \quad 0 \le \gamma_{2j} < 2\pi\,. \tag{2.22}$$

Throughout, assume that $k_{1j}^2 \neq (n+\alpha_1)^2$ and $k_{2j}^2 \neq (n+\alpha_2)^2$ for all $n \in Z$, $j = 1, 2$. This assumption excludes the "Rayleigh anomalous" cases where waves propagate along the x_1-axis.

For function $f \in H^{\frac{1}{2}}(\Gamma_j)$ (the Sobolev space of complex valued functions on the circle), define the operator T_{sj}^{α} by

$$(T_{sj}^{\alpha} f)(x_1) = \sum_{n\in Z} -i\beta_{sj}^{(n)}(\alpha) f^{(n)} e^{inx_1}, \tag{2.23}$$

for $s, j = 1, 2$, where $f^{(n)} = \frac{1}{2\pi}\int_0^{2\pi} f(x_1)e^{-inx_1}$ and the equality is taken in the sense of distributions.

From (2.23) and the definition of $\beta_{sj}^{(n)}(\alpha)$, it is clear that T_{sj}^{α} is a standard pseudo-differential operator (in fact, a convolution operator) of order one.

The scattering problem can be formulated as follows [4]:

$$\begin{aligned}
\nabla_{\alpha_1}\cdot(\frac{1}{k_1^2}\nabla_{\alpha_1}u)+u &= 0 \text{ in } \Omega, & (2.24)\\
(\Delta_{\alpha_2}+k_2^2)v &= \sum_{j,l=1,2}\rho_{jl}^{\alpha}\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u \text{ in } \Omega, & (2.25)\\
(T_{11}^{\alpha}+\frac{\partial}{\partial\nu})u &= -2iu_i\beta_1 e^{-i\beta_1 b} \text{ on } \Gamma_1, & (2.26)\\
(T_{12}^{\alpha}+\frac{\partial}{\partial\nu})u &= 0 \text{ on } \Gamma_2, & (2.27)\\
(T_{21}^{\alpha}+\frac{\partial}{\partial\nu})v &= 0 \text{ on } \Gamma_1, & (2.28)\\
(T_{22}^{\alpha}+\frac{\partial}{\partial\nu})v &= 0 \text{ on } \Gamma_2. & (2.29)
\end{aligned}$$

Integration by parts results in the variational relation:

$$\begin{aligned}
B_{TM}(u,\varphi) &= \int_{\Omega}\frac{1}{k_1^2}\nabla_{\alpha_1}u\cdot\overline{\nabla_{\alpha_1}\varphi}-\int_{\Omega}u\,\bar\varphi+\frac{1}{k_{11}^2}\int_{\Gamma_1}(T_{11}^{\alpha}u)\,\bar\varphi+\frac{1}{k_{12}^2}\int_{\Gamma_2}(T_{12}^{\alpha}u)\,\bar\varphi\\
&= -\frac{2iu_i\beta_1\,e^{-i\beta_1 b}}{k_{11}^2}\int_{\Gamma_1}\bar\varphi\,,\quad \forall\varphi\in H_p^1(\Omega)\,.
\end{aligned} \tag{2.30}$$

$$\begin{aligned}
B_{TE}(v,\varphi) &= \int_{\Omega}\nabla_{\alpha_2}v\cdot\overline{\nabla_{\alpha_2}\varphi}-\int_{\Omega}k_2^2\,v\,\bar\varphi+\int_{\Gamma_1}(T_{21}^{\alpha}v)\,\bar\varphi+\int_{\Gamma_2}(T_{22}^{\alpha}v)\,\bar\varphi\\
&= -\sum_{j,l=1,2}\rho_{jl}\int_{\Omega_0}e^{i(2\alpha_1-\alpha_2)x_1}\,\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u\,\bar\varphi\,,\quad \forall\varphi\in H_p^1(\Omega)\,.
\end{aligned} \tag{2.31}$$

Here $H_p^s(\Omega)$ contains the functions of $H^s(\Omega)$ that are 2π-periodic in the x_1 direction.

Note that usually the medium above the grating is air with optical index $n_{1j}=1$, which is independent of the wavelength. Thus $\alpha_2=2\alpha_1$ and $\rho_{jl}^{\alpha}=\rho_{jl}$ for all incidence angles, which simplify some of the formulas given below.

In the following, assume that the functions $n_{j0}(x)$ are constant on subdomains Ω_j with piecewise smooth boundaries $\partial\Omega_j$. The angles at the corners of Ω_j are strictly between 0 and 2π. Also, denote by

$$\Lambda=\bigcup_j\partial\Omega_j\setminus(\Gamma_1\cup\Gamma_2)$$

the set of interfaces between different materials. Assume further that the problems (2.30) and (2.31) with vanishing right–hand sides have only the trivial solution. Then it is well known [17] that the solution u of (2.30) belongs to the Sobolev space $H_p^{1+\delta}(\Omega)$ for some $\delta \in (0, 1/2)$.

Furthermore, we have

$$\sum_{j,l=1,2} \rho_{jl}^{\alpha} \partial_j^{\alpha_1} u \, \partial_l^{\alpha_1} u \in H^{-1}(\Omega) \tag{2.32}$$

by a direct application of the following regularity result of Beals [10].

Proposition 3.2.1 *If* $f \in H^{s_1}(\mathbf{R}^n)$, $g \in H^{s_2}(\mathbf{R}^n)$, $s_i \leq n/2$, $s_1 + s_2 \geq 0$, *then the product* $fg \in H^{s_1+s_2-n/2-\delta}(\mathbf{R}^n)$ *for arbitrary* $\delta > 0$, *and* $\|fg\|_{s_1+s_2-n/2-\delta} \leq c(\delta)\|f\|_{s_1}\|g\|_{s_2}$.

In view of (2.32), we obtain the following result.

Theorem 3.2.1 *Under the assumptions made above, the problem* (2.30), (2.31) *has a unique solution* $v \in H_p^1(\Omega)$.

Similar to the linear diffraction problem, the energy propagation of the diffracted fields is measured by the diffraction efficiencies. The efficiencies of the second harmonic fields are given by the formula:

$$e_n^+ = \beta_{21}^{(n)}/\beta_2 |E_n^+|^2 \quad \text{with} \quad E_n^+ = \frac{e^{-2i\beta_{21}^{(n)} b}}{2\pi} \int_{\Gamma_1} v \, e^{-inx_1} \, dx_1 \quad \text{for } \beta_{21}^{(n)} \text{ real.}$$

$$e_n^- = \beta_{22}^{(n)}/\beta_2 |E_n^-|^2 \quad \text{with} \quad E_n^- = \frac{e^{-2i\beta_{22}^{(n)} b}}{2\pi} \int_{\Gamma_2} v \, e^{-inx_1} \, dx_1 \quad \text{for } \beta_{22}^{(n)} \text{ real.}$$

3.3 Optimal design

Our goal is to determine (or design) grating geometries that ensure maximal efficiencies of the second harmonic fields. The optimal design problem may be stated as follows: Find a grating profile Λ^0 such that

$$\max_{\Lambda} e_n^+(\Lambda) = e_n^+(\Lambda^0) \,.$$

In order to apply certain gradient based optimization methods, it is essential to study the differentiability of the efficiencies with respect to perturbations of the interface Λ.

Consider a family of perturbed interfaces Λ_h given by

$$\Lambda_h = \Phi_h(\Lambda)\,, \quad \Phi_h(x) = x + h\,\chi(x)\,, \tag{3.1}$$

where $\chi = (\chi_1, \chi_2)$ is C^1 continuous, 2π–periodic in x_1 and has compact support in $[0, 2\pi] \times (-b, b)$. Clearly, for sufficiently small $|h|$ the mapping Φ_h is a C^1 diffeomorphism of Ω onto itself. Consequently, $\Phi_h(\Omega)$ corresponds to a perturbed grating geometry which yields new piecewise constant functions ε_j^h as well as the perturbed bilinear forms B_{TM}^h and B_{TE}^h. Moreover, the nonlinear material is contained in the subdomain $\Omega_0^h = \Phi_h(\Omega_0)$.

It follows that

$$De_n^+ = \lim_{h\to 0} h^{-1}(e_n^+(\Lambda_h) - e_n^+(\Lambda)) = 2\frac{\beta_{21}^{(n)}}{\beta_2} \operatorname{Re}(\overline{E_n^+} DE_n^+) \,.$$

Therefore, to compute De_n^+ with respect to the perturbation (3.1), it suffices to calculate the derivatives DE_n^+ defined by

$$DE_n^+(\chi) = \lim_{h\to 0} \frac{e^{-2i\beta_{21}^{(n)}b}}{2\pi h} \int_{\Gamma_1} (v_h - v)\, e^{-inx_1}\, dx_1\,, \tag{3.2}$$

where v solves (2.30), (2.31) and v_h is the solution of the perturbed problem

$$\begin{aligned} B_{TM}^h(u_h, \varphi) &= -\frac{2iu_i\beta_1\, e^{-i\beta_1 b}}{k_{11}^2} \int_{\Gamma_1} \bar{\varphi}\,, \\ B_{TE}^h(v_h, \varphi) &= -\sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)x_1}\, \partial_j^{\alpha_1} u_h\, \partial_l^{\alpha_1} u_h\, \bar{\varphi}\,, \quad \forall \varphi \in H_p^1(\Omega)\,. \end{aligned} \tag{3.3}$$

To compute (3.2), it is useful to employ the concept of the material derivative [32]. Using the mapping Φ_h, we introduce the isomorphism

$$\Psi_h : H_p^1(\Omega) \to H_p^1(\Omega)$$

which maps u to $u \circ \Phi_h^{-1}$.

Since χ is compactly supported in Ω, it is easily seen that

$$\Psi_h^{-1} u|_{\Gamma_j} = u|_{\Gamma_j} \; , \; j = 1, 2 \; , \; \forall u \in H_p^1(\Omega) \, .$$

Hence

$$DE_n^+(\chi) = \lim_{h \to 0} \frac{e^{-2i\beta_{21}^{(n)} b}}{2\pi h} \int_{\Gamma_1} (\Psi_h^{-1} v_h - v) \, e^{-inx_1} \, dx_1 \, . \tag{3.4}$$

Therefore, the derivative $DE_n^+(\chi)$ is a functional of the material derivative of v with respect to the diffeomorphisms Ψ_h, which is defined as

$$\lim_{h \to 0} h^{-1} (\Psi_h^{-1} v_h - v) \, .$$

The material derivative may be evaluated by introducing a change of the variables $y = \Phi_h(x)$ in the bilinear forms B_{TM}^h and B_{TE}^h. Note that $k_j^h = \Psi_h k_j$ and

$$dy = J(x) dx$$

with

$$J(x) = 1 + h\Big(\partial_{x_1} \chi_1 + \partial_{x_2} \chi_2\Big) + h^2 \Big(\partial_{x_1} \chi_1 \partial_{x_2} \chi_2 - \partial_{x_2} \chi_1 \partial_{x_1} \chi_2\Big)$$

and

$$\partial_{y_1} = J(x)^{-1} \Big((1 + h \, \partial_{x_2} \chi_2) \partial_{x_1} - h \, \partial_{x_1} \chi_2 \partial_{x_2} \Big) \, ,$$

$$\partial_{y_2} = J(x)^{-1} \Big(- h \, \partial_{x_2} \chi_1 \, \partial_{x_1} + (1 + h \, \partial_{x_1} \chi_1) \partial_{x_2} \Big) \, .$$

Applying the change of variables to the domain integrals of B_{TM}^h, we obtain

$$\begin{aligned}
&\int_\Omega \Big(- \Psi_h u \overline{\Psi_h \varphi} + \frac{1}{(k_1^h(y))^2} \, \nabla_{\alpha_1} \Psi_h u \cdot \overline{\nabla_{\alpha_1} \Psi_h \varphi} \Big) \, dy = - \int_\Omega u \overline{\varphi} \, J(x) \, dx \\
&+ \int_\Omega \frac{((1 + h\partial_2 \chi_2)\partial_1 + i\alpha_1 J(x) - h\partial_1 \chi_2 \partial_2) u \, ((1 + h\partial_2 \chi_2)\partial_1 - i\alpha_1 J(x) - h\partial_1 \chi_2 \partial_{x_2}) \overline{\varphi}}{J(x) k_1^2(x)} \\
&+ \int_\Omega \frac{(- h\partial_2 \chi_1 \partial_1 + (1 + h\partial_1 \chi_1)\partial_2) u \, (- h\partial_2 \chi_1 \partial_1 + (1 + h\partial_1 \chi_1)\partial_2) \overline{\varphi}}{J(x) k_1^2(x)} \\
&= \int_\Omega \Big(- u\overline{\varphi} + \frac{1}{k_1^2(x)} \nabla_{\alpha_1} u \overline{\nabla_{\alpha_1} \varphi} \Big) dx + h B_{TM,1}(u, \varphi) + h^2 B_{TM,2,h}(u, \varphi) \, ,
\end{aligned}$$

where

$$\begin{aligned}B_{TM,1}(u,\varphi) = & -\int_\Omega (\partial_1\chi_1+\partial_2\chi_2)u\overline{\varphi} + \int_\Omega \frac{\partial_1\chi_1}{k_1^2}(\partial_2 u\,\overline{\partial_2\varphi} - \partial_1 u\,\overline{\partial_1\varphi} + \alpha_1^2 u\overline{\varphi}) \\ & + \int_\Omega \frac{\partial_2\chi_2}{k_1^2}(\partial_1^{\alpha_1}u\,\overline{\partial_1^{\alpha_1}\varphi} - \partial_2 u\,\partial_2\overline{\varphi}) \\ & - \int_\Omega \Big(\frac{\partial_1\chi_2}{k_1^2}(\partial_1^{\alpha_1}u\,\overline{\partial_2\varphi} + \partial_2 u\,\overline{\partial_1^{\alpha_1}\varphi}) + \frac{\partial_2\chi_1}{k_1^2}(\partial_1 u\,\overline{\partial_2\varphi} + \partial_2 u\,\overline{\partial_1\varphi})\Big)\end{aligned} \tag{3.5}$$

and the remainder term satisfies

$$|B_{TM,2,h}(u,\varphi)| \le c\|u\|_1\|\varphi\|_1 \ , \ u,\varphi \in H_p^1(\Omega) \ , \ |h| \le h_0 \, .$$

Here we have used the notations $\partial_j = \partial_{x_j}$, $\partial_1^{\alpha_1} = \partial_{x_1} + i\alpha_1$ and the expression

$$J(x)^{-1} = 1 - h(\partial_1\chi_1 + \partial_2\chi_2) + O(h^2) \, , \ |h| \le h_0 \, ,$$

which holds uniformly in $x \in \Omega$.

Since the boundary terms in the TM bilinear form remain unchanged, we have thus obtained for $|h| \le h_0$

$$B_{TM}^h(\Psi_h u, \Psi_h\varphi) = B_{TM}(u,\varphi) + hB_{TM,1}(u,\varphi) + h^2 B_{TM,2,h}(u,\varphi) \, . \tag{3.6}$$

Theorem 3.3.1 ([18]) *If the TM diffraction problem* (2.30) *has a unique solution and the perturbation of the grating geometry is given by the regular mapping* (3.1), *then for all sufficiently small h the perturbed problem* (3.3) *is also uniquely solvable. Moreover, the solution of the perturbed problem takes the form*

$$\Psi_h^{-1}u_h = u + hu_1 + h^2 u_{2,h} \, , \tag{3.7}$$

where u is the solution of the original problem (2.30), *$u_1 \in H_p^1(\Omega)$ solves the equation*

$$B_{TM}(u_1,\varphi) = -B_{TM,1}(u,\varphi) \, , \quad \forall\,\varphi \in H_p^1(\Omega) \, , \tag{3.8}$$

and the remainder satisfies $\|u_{2,h}\|_1 \le c$ for $|h| \le h_0$.

Theorem 3.3.1 indicates that the material derivative of u

$$u_1 = \lim_{h\to 0} h^{-1}(\Psi_h^{-1} u_h - u)$$

exists in the sense of $H_p^1(\Omega)$ and satisfies the variational equation (3.8).

Next, we establish formulas to compute the derivative of the reflection coefficients with respect to the perturbation.

By applying the change of variables $y = \Phi_h(x)$ to the domain integrals of the form B_{TE}^h, we obtain

$$\begin{aligned}
&\int_\Omega \Big(- (k_2^h(y))^2 \Psi_h v \overline{\Psi_h \varphi} + \nabla_{\alpha_2} \Psi_h v \cdot \overline{\nabla_{\alpha_2} \Psi_h \varphi}\Big)\, dy \\
&= \int_\Omega \Big(- k_2^2 v\overline{\varphi} + \nabla_{\alpha_2} v \overline{\nabla_{\alpha_2}\varphi}\Big) dx + h B_{TE,1}(v,\varphi) + h^2 B_{TE,2,h}(v,\varphi)\,,
\end{aligned}$$

with

$$\begin{aligned}
B_{TE,1}(v,\varphi) = \; & -\int_\Omega k_2^2(\partial_1\chi_1 + \partial_2\chi_2) v\,\overline{\varphi} + \int_\Omega \partial_1\chi_1(\partial_2 v\,\overline{\partial_2\varphi} - \partial_1 v\,\overline{\partial_1\varphi} + \alpha_2^2 v\,\overline{\varphi}) \\
& + \int_\Omega \partial_2\chi_2(\partial_1^{\alpha_2} v\,\overline{\partial_1^{\alpha_2}\varphi} - \partial_2 v\,\overline{\partial_2\varphi}) \\
& - \int_\Omega \Big(\partial_1\chi_2(\partial_1^{\alpha_2} v\,\overline{\partial_2\varphi} + \partial_2 v\,\overline{\partial_1^{\alpha_2}\varphi}) + \partial_2\chi_1(\partial_1 v\,\overline{\partial_2\varphi} + \partial_2 v\,\overline{\partial_1\varphi})\Big).
\end{aligned} \tag{3.9}$$

The remainder term satisfies

$$|B_{TE,2,h}(v,\varphi)| \le c\|v\|_1\|\varphi\|_1\ ,\ v,\varphi \in H_p^1(\Omega)\,,\ |h| \le h_0\,.$$

Since again the boundary terms in B_{TE}^h remain unchanged, we have for $|h| \le h_0$

$$B_{TE}^h(\Psi_h v, \Psi_h\varphi) = B_{TE}(v,\varphi) + hB_{TE,1}(v,\varphi) + h^2 B_{TE,2,h}(v,\varphi)\,. \tag{3.10}$$

Introduce the adjoint TE problem

$$B_{TE}(\varphi, w) = \frac{e^{-2i\beta_{21}^{(n)} b}}{2\pi} \int_{\Gamma_1} \varphi\, e^{-inx_1}\, dx_1\,, \quad \forall\varphi \in H_p^1(\Omega)\,, \tag{3.11}$$

which has a unique solution $w \in H_p^2(\Omega)$ [17].

From (3.4), it is obvious that

$$DE_n^+(\chi) = \lim_{h\to 0} h^{-1} B_{TE}(\Psi_h^{-1} v_h - v, w)\,. \qquad (3.12)$$

Thus it suffices to consider the form $B_{TE}(\Psi_h^{-1}v_h, w)$. From (3.10), it follows that

$$B_{TE}^h(v_h, \Psi_h w) = B_{TE}(\Psi_h^{-1}v_h, w) + hB_{TE,1}(\Psi_h^{-1}v_h, w) + h^2 B_{TE,2,h}(\Psi_h^{-1}v_h, w) \quad (3.13)$$

On the other hand,

$$B_{TE}^h(v_h, \Psi_h w) = -\sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)y_1}\, \partial_j^{\alpha_1} u_h\, \partial_l^{\alpha_1} u_h\, \overline{\Psi_h w}\, dy\,. \qquad (3.14)$$

In the following, the right–hand side of (3.14) is expanded with respect to the powers of h. The terms are considered separately. In fact, the change of variables leads to the following formulas:

1. For $j = l = 1$:

$$\int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)y_1}((\partial_{y_1} + i\alpha_1)\Psi_h u)^2\, \overline{\Psi_h \varphi}\, dy$$
$$= \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}(\partial_1^{\alpha_1} u)^2\, \overline{\varphi} + h\, \mathcal{J}_{11}(u,\varphi) + h^2 \mathcal{L}_{11}(u,\varphi)$$

with

$$\mathcal{J}_{11}(u,\varphi) = \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}(\partial_1\chi_1 + \partial_2\chi_2 + i(2\alpha_1-\alpha_2)\chi_1)(\partial_1^{\alpha_1} u)^2 \overline{\varphi}$$
$$-2\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \partial_1^{\alpha_1} u\,(\partial_1\chi_1\partial_1 u + \partial_1\chi_2\partial_2 u)\,\overline{\varphi}$$

2. For $j = 1, l = 2$:

$$\int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)y_1}((\partial_{y_1} + i\alpha_1)\Psi_h u)\, \partial_{y_2}\Psi_h u\, \overline{\Psi_h \varphi}\, dy$$
$$= \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \partial_1^{\alpha_1} u\, \partial_2 u\, \overline{\varphi} + h\, \mathcal{J}_{12}(u,\varphi) + h^2 \mathcal{L}_{12}(u,\varphi)$$

with

$$\mathcal{J}_{12}(u,\varphi) = -\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}(\partial_2\chi_1(\partial_1 u)^2 + \partial_1\chi_2(\partial_2 u)^2)\,\overline{\varphi}$$
$$+\, i\alpha_1 \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} u(\partial_1\chi_1\, \partial_2 u - \partial_2\chi_1\, \partial_1 u)\,\overline{\varphi}$$
$$+\, i(2\alpha_1-\alpha_2)\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \chi_1 \partial_1^{\alpha_1} u\, \partial_2 u\, \overline{\varphi}$$

3. For $j = l = 2$:

$$\int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)y_1} (\partial_{y_2}\Psi_h u)^2\, \overline{\Psi_h \varphi}\, dy$$

$$= \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} (\partial_2 u)^2\, \overline{\varphi} + h\, \mathcal{J}_{22}(u,\varphi) + h^2 \mathcal{L}_{22}(u,\varphi)$$

with

$$\mathcal{J}_{22}(u,\varphi) = \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} ((\partial_1\chi_1 - \partial_2\chi_2 + i(2\alpha_1-\alpha_2)\chi_1)(\partial_2 u)^2 - 2\partial_2\chi_1\, \partial_1 u\, \partial_2 u)\, \overline{\varphi}\,.$$

Thus the right–hand side of (3.14) transforms to

$$\sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)y_1} \partial_{y_j}^{\alpha_1} u_h\, \partial_{y_l}^{\alpha_1} u_h\, \overline{\Psi_h w}\, dy$$

$$= \sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \partial_j^{\alpha_1} \Psi_h^{-1} u_h\, \partial_l^{\alpha_1} \Psi_h^{-1} u_h\, \overline{w}\, dx$$

$$+ h \sum_{j,l=1,2} \rho_{jl} \mathcal{J}_{jl}(\Psi_h^{-1} u_h, w) + h^2 \sum_{j,l=1,2} \rho_{jl} \mathcal{L}_{jl}(\Psi_h^{-1} u_h, w)\,.$$

where $\mathcal{J}_{21} = \mathcal{J}_{12}$. Note that due to (2.32) obviously

$$|\mathcal{L}_{ij}(\Psi_h^{-1} u_h, w)| \le c \|\Psi_h^{-1} u_h\|_1^2 \|w\|_2 \le c_1 \|u\|_1^2\,.$$

Using Theorem 3.3.1, we arrive at

$$\sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)y_1} \partial_{y_j}^{\alpha_1} u_h\, \partial_{y_l}^{\alpha_1} u_h\, \overline{\Psi_h w}\, dy = \sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \partial_j^{\alpha_1} u\, \partial_l^{\alpha_1} u\, \overline{w}\, dx$$

$$+ 2h \sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \partial_j^{\alpha_1} u\, \partial_l^{\alpha_1} u_1\, \overline{w} + h \sum_{j,l=1,2} \rho_{ij} \mathcal{J}_{jl}(u,w) + O(h^2)\,,$$

which implies

$$B_{TE}^h(v_h, \Psi_h w) = B_{TE}(v,w)$$

$$+ h \sum_{j,l=1,2} \rho_{ij} \Big(\mathcal{J}_{jl}(u,w) + 2 \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \partial_j^{\alpha_1} u\, \partial_l^{\alpha_1} u_1\, \overline{w} \Big) + O(h^2).$$

Thus from (3.13), we get

$$B_{TE}(\Psi_h^{-1} v_h, w) + h B_{TE,1}(\Psi_h^{-1} v_h, w) + h^2 B_{TE,2,h}(\Psi_h^{-1} v_h, w)$$

$$= B_{TE}(v,w) + h \sum_{j,l=1,2} \rho_{jl} \Big(\mathcal{J}_{ij}(u,w) + 2 \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1} \partial_j^{\alpha_1} u\, \partial_l^{\alpha_1} u_1\, \overline{w} \Big) + O(h^2)\,,$$

which together with (3.12) proves the following theorem.

Theorem 3.3.2 *The derivative of the reflection coefficients $E_n^{\pm}$ with respect to the variations* (3.1) *of the interface* Λ *is given by the formula*

$$DE_n^{\pm}(\chi) = -B_{TE,1}(v,w) + \sum_{j,l=1,2} \rho_{jl}\Big(\mathcal{J}_{jl}(u,w) + 2\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u_1\,\overline{w}\,dx\Big) \quad (3.15)$$

where the bilinear form $B_{TE,1}$ is defined by (3.9), *u and v denote the solutions of the diffraction problems* (2.30), (2.31), *respectively, u_1 solves* (3.8) *and w is the solution of the adjoint TE problem* (3.11).

Following [18], the form $B_{TE,1}(v,w)$ given by (3.9) can be transformed to

$$\begin{aligned} B_{TE,1}(v,w) = &- [k_2^2]_\Lambda \int_\Lambda (\chi,n)\,v\,\overline{w} \\ &+ \int_\Omega (\Delta_{\alpha_2}v + k_2^2 v)(\chi_1\,\overline{\partial_1 w} + \chi_2\,\overline{\partial_2 w}) + \int_\Omega (\chi_1\partial_1 v + \chi_2\,\partial_2 v)(\Delta_{\alpha_2}\overline{w} + k_2^2\overline{w}) \\ = &- [k_2^2]_\Lambda \int_\Lambda (\chi,n)\,v\,\overline{w} + \sum_{j,l=1,2}\rho_{jl}\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u\,(\chi_1\,\overline{\partial_1 w} + \chi_2\,\overline{\partial_2 w})\,, \end{aligned}$$

where we have used the equation (2.25) and

$$\Delta_\alpha w + \overline{k_2^2} w = 0 \quad \text{in } \Omega\,,$$

for the solution $w \in H^2(\Omega)$ of the adjoint problem (3.11). Here n denotes the normal to the interface Λ, and $[k_2^2]_\Lambda$ stands for the jump of the function k_2^2 when crossing Λ in the direction on n.

Thus (3.15) takes the form

$$\begin{aligned} DE_n^{\pm}(\chi) = &\; [k_2^2]_\Lambda \int_\Lambda (\chi,n)\,v\,\overline{w} + 2\sum_{j,l=1,2}\rho_{jl}\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u_1\,\overline{w}\,dx \\ &+ \sum_{j,l=1,2}\rho_{jl}\Big(\mathcal{J}_{jl}(u,w) - \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u\,(\chi_1\,\overline{\partial_1 w} + \chi_2\,\overline{\partial_2 w})\Big)\,. \end{aligned}$$

Remark 3.1. To apply the above results to binary gratings by choosing different χ, we can compute the derivative $D_jE_n^{\pm}$ of the Rayleigh coefficients with respect to the transition points. For simplicity, consider a binary grating with two transition points

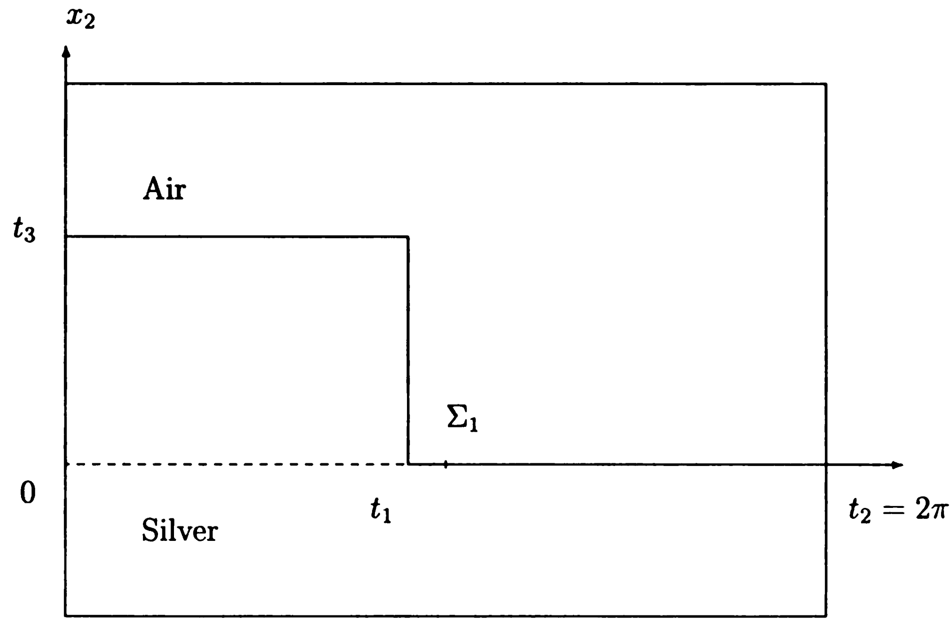

Figure 3.2. Cross section of a simple binary gratings

$t_1, t_2 = 2\pi$ and the height t_3, as shown in Figure 2. Denote $O_1 = (t_1, 0)$, $O_2 = (t_1, t_3)$, $O_3 = (0, t_3)$, and $\Sigma_1 = \overline{O_1O_2}, \Sigma_2 = \overline{O_3O_2}$, the fill factor $FF = \frac{t_1}{2\pi}$.

To compute the derivative $D_1E_n^{\pm}$ of the Rayleigh coefficients with respect to the variation of t_1, the mapping (3.1) takes the form

$$\Phi_h(x) = x + h\chi(x), \quad \chi(x) = (\chi_1(x), 0) \ ,$$

where $\chi_1 \equiv 1$ in a neighborhood of Σ_1 and $\chi \in C_0^\infty(U)$ for a bigger neighborhood U (not containing other corners of the profile curve Λ).

3.4 Numerical examples

The above described approach has been numerically tested on a number of examples in the literature. The numerical solution of the model equations is based on our generalized finite element (GFEM) discretizations of the bilinear forms B_{TM} and

B_{TE} [17]. This finite element method avoids the pollution effects associated with usual domain–based methods for solving Helmholtz equations. Since the method is restricted to piecewise rectangular sub-partitioning of the integration domain, the numerical tests have been performed for binary gratings. Also, to obtain the starting values for the optimization procedure, we have determined the grating structure which yields minimal reflection in the TM case. This is done by using gradient based minimization algorithms [17]. We then proceed to compute the derivatives with respect to the grating depth and transition points as described in Remark 3.1 by the line search algorithm.

In the following, we present results on specific examples.

First, we consider an example introduced in [30]. It is concerned with the grating enhancement of the second harmonic nonlinear optical effects for a silver layer. Obviously, the TE efficiency (the nonlinear effect) for the flat layer is small which is confirmed by our calculated the efficiency 1.2003160E-04.

The TE efficiency for the binary grating with the period $0.556\mu m$, the incidence angle $64.5°$, and the wavelength $1.06\mu m$ is then computed. With the fill-factor 0.5, similar enhancement results are obtained as those reported in [30] concerning the efficiency dependence on the groove depth. In particular, the maximal enhancement is about 45 which occurs when the groove depth is close to $0.3\mu m$.

Our computation indicates in addition that by using the above algorithm, with the same data, a better enhancement for the fill-factor 0.834 may be achieved. In fact, at the groove depth $0.392\mu m$, the enhancement is more than 80. Figure 3.4 presents the enhancement of the efficiency of the second harmonic field at various groove depths. It is shown that around the optimal depth, the enhancement depends on the groove depth sharply.

The second example is concerned with the grating enhancement of the second harmonic nonlinear optical effects for ZnS overcoated binary silver gratings. Once

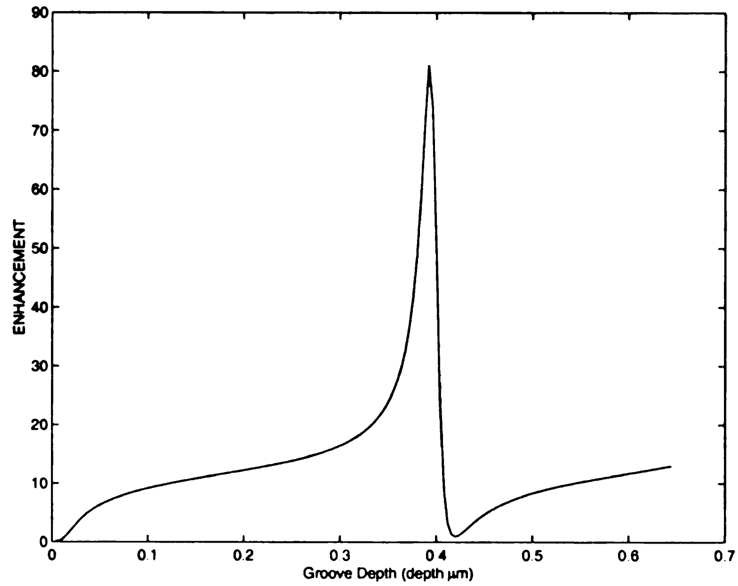

Figure 3.3. Numerical example 1.

again, the enhancement of the second harmonic fields is computed with respect to the associated flat structure. The period of the grating is $d = 0.4\mu m$, the incidence angle is 28.92° at the wavelength $\lambda = 1.06\mu m$. The optimization parameters are the thickness of the ZnS coating, the fill factor, and the depth of the binary grating. Our computation indicates that optimal results are obtained at the thickness of $0.33\mu m$ of the coating layer, the fill factor 0.43, and the depth of $0.099\mu m$ for the binary grating. Figure 3.4 illustrates the enhancement dependence on the grating depth.

It should be pointed out that other thicknesses of the ZnS coating provide even higher enhancements for the second harmonic nonlinear optical effects compared to the flat structure. Figure 3.5 presents the corresponding enhancement factors for the thickness of 0.672μm and a binary grating with the fill factor 0.505. Clearly, the maximum value is obtained at the depth 0.03μm. However this value only amounts to 17% of the maximum for the thickness 0.33μm.

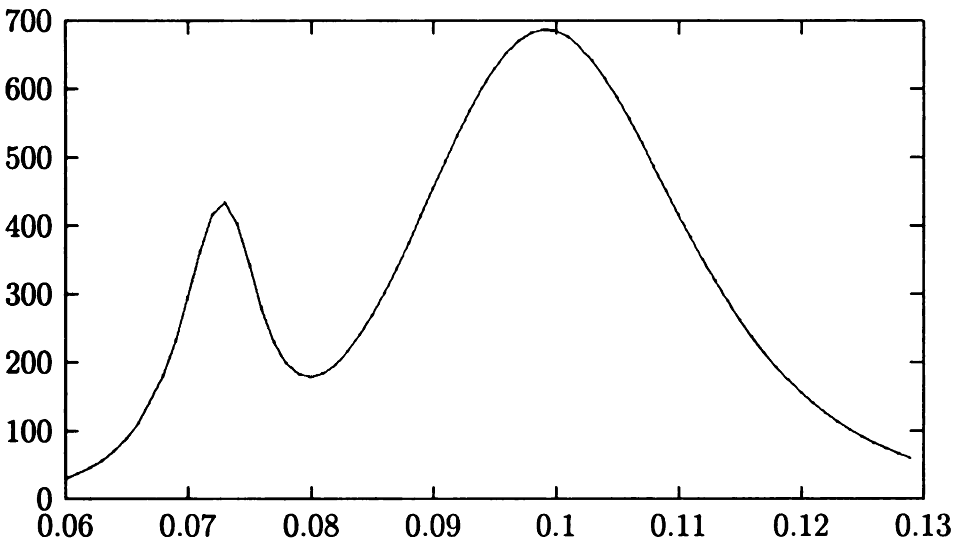

Figure 3.4. Numerical example 2.

Appendix

Recall that, for nonlinear material, the second order nonlinear susceptibility takes the form

$$\vec{P}^{(2)}(2\omega) = \chi^{(2)}(2\omega) : \vec{E}(\omega)\vec{E}(\omega) ,$$

i.e., for $j = 1, 2, 3$,

$$\vec{P}_j^{(2)}(2\omega) = \epsilon_0 \sum_{k,l} \chi_{j,k,l}^{(2)}(2\omega) E_k(\omega) E_l(\omega) .$$

According to the convention $\chi_{jkl}^{(2)} = 2d_{jkl}^{(2)}$ and by the permutation symmetry: $d_{jkl}^{(2)}(2\omega) = d_{jlk}^{(2)}(2\omega)$, define

$$d_{jm} = d_{jkl}^{(2)}, \quad m = 1, \cdots, 6 ,$$

where

$$m = \begin{cases} k, & \text{if } k = l, \\ 9 - (k + l), & \text{if } k \neq l. \end{cases}$$

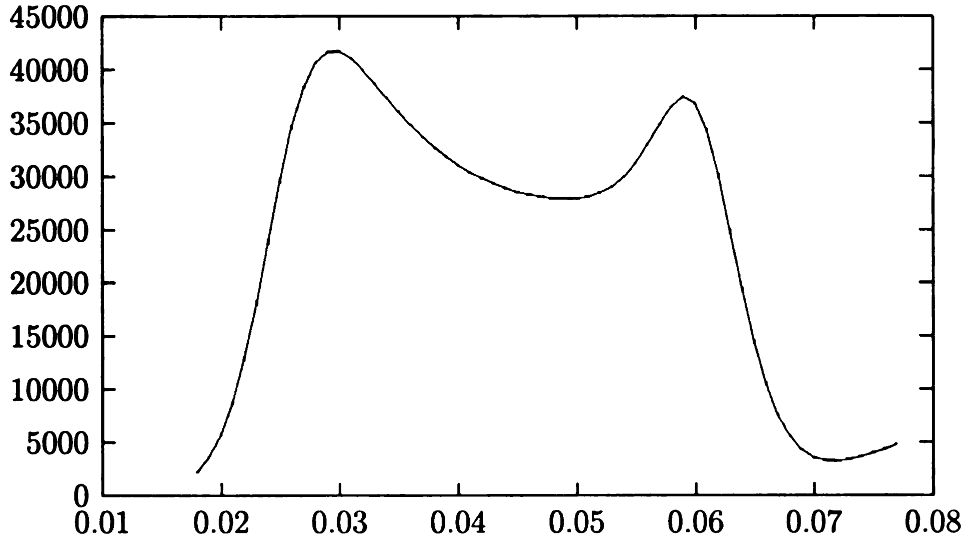

Figure 3.5. Numerical example 3.

Thus

$$\vec{P}^{(2)}(2\omega) = \epsilon_0 \begin{pmatrix} d_{11} & \cdots & d_{16} \\ d_{21} & \cdots & d_{26} \\ d_{31} & \cdots & d_{36} \end{pmatrix} \begin{pmatrix} E_x^2 \\ E_y^2 \\ E_z^2 \\ 2E_yE_z \\ 2E_xE_z \\ 2E_xE_y \end{pmatrix} (\omega) .$$

It is evident that the number of non-vanishing, independent elements of $\chi^{(2)}$ depends upon the group symmetry of the nonlinear medium. In particular, for crystals with cubic symmetry structures, such as Z_nS, the matrix d_{jm} is of the following form:

$$\begin{pmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{14} \end{pmatrix} .$$

For this class of nonlinear optical material, we have the following remarks:

Remark 5.1. In order to generate a nonlinear polarization at 2ω, the pump field may not be TE polarized.

In fact, it is easily seen that if the field is TE polarized, $\vec{E}(\omega) = (0, 0, E_z)$, then $\vec{P}^{(2)}(2\omega) = 0$.

Remark 5.2. If the pump field is TM, $\vec{H} = (0, 0, H_z)$, $\vec{E}(\omega) = (E_x, E_y, 0)$, then $\vec{P}^{(2)}(2\omega) = (0, 0, 2d_{14}\epsilon_0 E_x E_y)$, which induces nonlinear effects in TE polarization.

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