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Optimal design of nonlinear diffraction gratings

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Abstract

The goal of the paper is to study the optimal design problem for nonlinear diffraction gratings. The problem arises in the study of surface enhanced nonlinear optical effects of second harmonic generation. In order to apply certain gradient based optimization methods, an explicit formula for the partial derivatives of the Rayleigh coefficients with respect to the parameters of the grating profile is derived. Using the formula, numerical results are presented on an optimal design problem of nonlinear binary gratings.

Keywords: Optimal design; Nonlinear material; Diffraction grating; Gradient formulae

1. Introduction

Consider a plane wave of frequency ω_1 incident on a grating or periodic structure ruled on 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 paper is concerned with important aspects for systematically design of surface (grating) enhanced nonlinear optical effects. Recently, in a sequence of papers [14–16], 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 [15] and [16] that SHG can be greatly enhanced by using diffraction gratings or periodic structures and the PDE model can predict the field propagation accurately.

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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 [1,2,4,10,12]. For linear grating structures, significant results have been obtained by Dobson [9] (weak convergence), Bao and Bonnetier [2] (homogenization), and Eschner and Schmidt [10,12] (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 [4] and [5]. 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 [3]. 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 [13] and Bao et al. [6]. For the underlying physics of nonlinear optics, we refer the reader to the classic books of Bloembergen [8] and Shen [17].

The outline of this paper is as follows. In Section 2, we present the nonlinear scattering problem. In Section 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 4.

2. Modeling of the 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:

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

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

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, and $\chi^{(2)}$ is the second order nonlinear susceptibility tensor of third rank, i.e., $\chi^{(2)} : \mathbf{E}\mathbf{E}$ is a vector whose jth 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 [15] and [16]. Under the approximation, Eq. (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 A 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

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

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

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

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

Because of Eq. (2.2),

$$\mathbf{E}(x,\omega_1) = \frac{c}{\mathrm{i}\omega_1\epsilon_1}\nabla \times \mathbf{H}(x,\omega_1) = \frac{c}{\mathrm{i}\omega_1\epsilon_1}(\partial_{x_2}H, -\partial_{x_1}H, 0). \tag{2.11}$$

Hence the second harmonic field satisfies

$$[\Delta + k_2^2]E = -\frac{4\pi\omega_2^2}{c^2}\sum_{j,l=1,2,3}\chi_{3jl}^{(2)}(x,\omega_2)(\mathbf{E}(x,\omega_1))_j(\mathbf{E}(x,\omega_1))_l, \tag{2.12}$$

$$= \sum_{j,l=1,2}\rho_{jl}\partial_{x_j}H\partial_{x_l}H, \tag{2.13}$$

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

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 Fig. 1.

Introduce the notation:

$$\begin{aligned}
&\Gamma_j = \{x_2 = (-1)^{j-1}b, 0 < x_1 < 2\pi\}, && S_j = \{0 < x_1 < 2\pi, x_2 = \phi_j(x_1)\},\\
&\Omega_1 = \{0 < x_1 < 2\pi, \phi_1(x_1) < x_2 < b\}, && \Omega_2 = \{0 < x_1 < 2\pi, -b < x_2 < \phi_2(x_1)\},\\
&\Omega_1^+ = \{0 < x_1 < 2\pi, x_2 \geqslant b\}, && \Omega_2^+ = \{0 < x_1 < 2\pi, x_2 \leqslant -b\},\\
&\Omega_0 = \{0 < x_1 < 2\pi, \phi_2(x_1) < x_2 < \phi_1(x_1)\}, && \Omega = \{0 < x_1 < 2\pi, -b < x_2 < b\}.
\end{aligned}$$

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

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

for $j = 1, 2$, where n_{j1} and n_{j2} are constants, n_{j1} are real and positive, and Re $n_{j2} > 0$, Im $n_{j2} \geqslant 0$. 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 $n_{j0} \geqslant 0$.

We wish to solve the system (2.10) and (2.12) when an incoming plane wave

$$u_I = u_i \, e^{i\alpha_1 x_1 - i\beta_1 x_2} \tag{2.14}$$

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

We are interested in "quasiperiodic" solutions (H, E), that is, solutions (H, E) such that

$$u = H\,e^{-i\alpha_1 x_1} \quad \text{and} \quad v = E\,e^{-i\alpha_2 x_1} \quad \left(\alpha_2 = k_{21}\sin\theta, k_{21} = \frac{\omega_2}{c} n_{21}\right)$$

are 2π-periodic in the x_1 direction.

It follows from the system (2.10) and (2.12) that

$$\nabla_{\alpha_1} \cdot \left(\frac{1}{k_1^2}\nabla_{\alpha_1} u\right) + u = 0, \tag{2.15}$$

$$\left(\Delta_{\alpha_2} + k_2^2\right)v = \sum_{j,l=1,2} \rho_{jl}^{\alpha}\partial_j^{\alpha_1} u \partial_l^{\alpha_1} u, \tag{2.16}$$

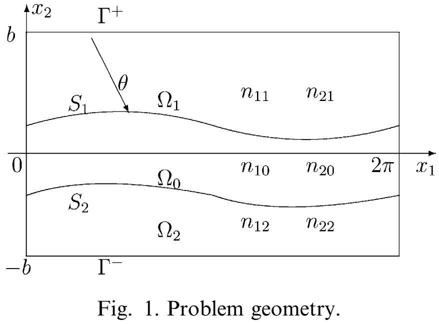

Fig. 1. Problem geometry.

where

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

and

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

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

$$\beta_{1j}^{(n)}(\alpha) = \mathrm{e}^{\mathrm{i}\gamma_{1j}/2}\left|k_{1j}^2 - (n+\alpha_1)^2\right|^{1/2}, \quad n \in Z,$$
$$\beta_{2j}^{(n)}(\alpha) = \mathrm{e}^{\mathrm{i}\gamma_{2j}/2}\left|k_{2j}^2 - (n+\alpha_2)^2\right|^{1/2}, \quad n \in Z,$$

where

$$\gamma_{1j} = \arg(k_{1j}^2 - (n+\alpha_1)^2), \quad 0 \leqslant \gamma_{1j} < 2\pi,$$
$$\gamma_{2j} = \arg(k_{2j}^2 - (n+\alpha_2)^2), \quad 0 \leqslant \gamma_{2j} < 2\pi.$$

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

$$(T_{sj}^{\alpha}f)(x_1) = \sum_{n\in Z} -\mathrm{i}\beta_{sj}^{(n)}(\alpha) f^{(n)}\,\mathrm{e}^{\mathrm{i}nx_1} \tag{2.17}$$

for $s, j = 1, 2$, where $f^{(n)} = (1/2\pi)\int_0^{2\pi} f(x_1)\,\mathrm{e}^{-\mathrm{i}nx_1}$ and the equality is taken in the sense of distributions.

From (2.17) and the definition of $\beta_{sj}^{(n)}(\alpha)$, it is clear that T_{sj}^{α} is a standard pseudodifferential operator (in fact, a convolution operator) of order one.

The scattering problem can be formulated as follows [3]:

$$\nabla_{\alpha_1}\cdot\left(\frac{1}{k_1^2}\nabla_{\alpha_1}u\right) + u = 0 \quad \text{in } \Omega, \tag{2.18}$$

$$\left(\Delta_{\alpha_2} + k_2^2\right)v = \sum_{j,l=1,2}\rho_{jl}^{\alpha}\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u \quad \text{in } \Omega, \tag{2.19}$$

$$\left(T_{11}^{\alpha} + \frac{\partial}{\partial v}\right)u = -2\mathrm{i}u_i\beta_1\,\mathrm{e}^{-\mathrm{i}\beta_1 b} \quad \text{on } \Gamma_1, \tag{2.20}$$

$$\left(T_{12}^{\alpha} + \frac{\partial}{\partial v}\right)u = 0 \quad \text{on } \Gamma_2, \tag{2.21}$$

$$\left(T_{21}^{\alpha} + \frac{\partial}{\partial v}\right)v = 0 \quad \text{on } \Gamma_1, \tag{2.22}$$

$$\left(T_{22}^{\alpha} + \frac{\partial}{\partial v}\right)v = 0 \quad \text{on } \Gamma_2. \tag{2.23}$$

Integration by parts results in the variational relation:

$$B_{\mathrm{TM}}(u,\varphi) = \int_\Omega \frac{1}{k_1^2}\nabla_{\alpha_1} u \cdot \overline{\nabla_{\alpha_1}\varphi} - \int_\Omega u\bar{\varphi} + \frac{1}{k_{11}^2}\int_{\Gamma_1}(T_{11}^\alpha u)\bar{\varphi} + \frac{1}{k_{12}^2}\int_{\Gamma_2}(T_{12}^\alpha u)\bar{\varphi}$$
$$= -\frac{2\mathrm{i}u_\mathrm{i}\beta_1\,\mathrm{e}^{-\mathrm{i}\beta_1 b}}{k_{11}^2}\int_{\Gamma_1}\bar{\varphi} \quad \forall\varphi\in H_p^1(\Omega), \tag{2.24}$$

$$B_{\mathrm{TE}}(v,\varphi) = \int_\Omega \nabla_{\alpha_2} v\cdot\overline{\nabla_{\alpha_2}\varphi} - \int_\Omega k_2^2 v\bar{\varphi} + \int_{\Gamma_1}(T_{21}^\alpha v)\bar{\varphi} + \int_{\Gamma_2}(T_{22}^\alpha v)\bar{\varphi}$$
$$= -\sum_{j,l=1,2}\rho_{jl}\int_{\Omega_0}\mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u\bar{\varphi} \quad \forall\varphi\in H_p^1(\Omega). \tag{2.25}$$

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 (2.24) and (2.25) with vanishing right-hand sides have only the trivial solution. Then it is well known [10] that the solution u of (2.24) belongs to the Sobolev space $H_p^{1+\delta}(\Omega)$ for some $\delta\in(0,1/2)$.

Furthermore, we have

$$\sum_{j,l=1,2}\rho_{jl}^\alpha\partial_j^{\alpha_1}u\,\partial_l^{\alpha_1}u \in H^{-1}(\Omega) \tag{2.26}$$

by a direct application of the following regularity result of Beals [7].

Proposition 2.1. *If $f\in H^{s_1}(\mathbb{R}^n)$, $g\in H^{s_2}(\mathbb{R}^n)$, $s_i\leqslant n/2$, $s_1+s_2\geqslant 0$, then the product $fg\in H^{s_1+s_2-n/2-\delta}(\mathbb{R}^n)$ for arbitrary $\delta>0$, and $\|fg\|_{s_1+s_2-n/2-\delta}\leqslant c(\delta)\|f\|_{s_1}\|g\|_{s_2}$.*

In view of (2.26), we obtain the following result.

Theorem 2.1. *Under the assumptions made above, the problems* (2.24) *and* (2.25) *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:

$$e_n^+ = \beta_{21}^{(n)}/\beta_2|E_n^+|^2 \quad\text{with}\quad E_n^+ = \frac{\mathrm{e}^{-2\mathrm{i}\beta_{21}^{(n)}b}}{2\pi}\int_{\Gamma_1} v\,\mathrm{e}^{-\mathrm{i}nx_1}\,\mathrm{d}x_1 \quad\text{for } \beta_{21}^{(n)} \text{ real},$$

$$e_n^- = \beta_{22}^{(n)}/\beta_2|E_n^-|^2 \quad\text{with}\quad E_n^- = \frac{\mathrm{e}^{-2\mathrm{i}\beta_{22}^{(n)}b}}{2\pi}\int_{\Gamma_2} v\,\mathrm{e}^{-\mathrm{i}nx_1}\,\mathrm{d}x_1 \quad\text{for } \beta_{22}^{(n)} \text{ real}.$$

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

$$\max_{\Lambda} e_n^+(\Lambda) = e_n^+(\Lambda^0). \tag{3.1}$$

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

$$\Lambda_h = \Phi_h(\Lambda), \quad \Phi_h(x) = x + h\chi(x), \tag{3.2}$$

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

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

Therefore, to compute De_n^+ with respect to the perturbation (3.2), it suffices to calculate the derivatives DE_n^+ defined by

$$DE_n^+(\chi) = \lim_{h\to 0} \frac{\mathrm{e}^{-2\mathrm{i}\beta_{21}^{(n)}b}}{2\pi h}\int_{\Gamma_1}(v_h - v)\,\mathrm{e}^{-\mathrm{i}nx_1}\,\mathrm{d}x_1,$$

where v solves (2.24), (2.25) and v_h is the solution of the perturbed problem

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

To compute (3.3), it is useful to employ the concept of the material derivative [18]. 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

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

Hence

$$DE_n^+(\chi) = \lim_{h\to 0}\frac{\mathrm{e}^{-2\mathrm{i}\beta_{21}^{(n)}b}}{2\pi h}\int_{\Gamma_1}\left(\Psi_h^{-1}v_h - v\right)\mathrm{e}^{-\mathrm{i}nx_1}\,\mathrm{d}x_1. \tag{3.4}$$

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^h_{TM} and B^h_{TE}. Note that $k_j^h = \Psi_h k_j$ and

$$\mathrm{d}y = J(x)\mathrm{d}x$$

with

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

and

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

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

Applying the change of variables to the domain integrals of B^h_{TM}, we obtain

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

where

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

and the remainder term satisfies

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

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

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

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

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

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

Theorem 3.1 [12]. *If the* TM *diffraction problem* (2.24) *has a unique solution and the perturbation of the grating geometry is given by the regular mapping* (3.2), *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*

$$\Psi_h^{-1} u_h = u + h u_1 + h^2 u_{2,h}, \tag{3.7}$$

where u is the solution of the original problem (2.24), $u_1 \in H_p^1(\Omega)$ *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 $\|u_{2,h}\|_1 \leqslant c$ *for* $|h| \leqslant h_0$.

Theorem 3.1 indicates that the material derivative of u

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

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^h_{TE}, we obtain

$$\int_\Omega \Big(-(k_2^h(y))^2 \Psi_h v \overline{\Psi_h \varphi} + \nabla_{\alpha_2} \Psi_h v \cdot \overline{\nabla_{\alpha_2} \Psi_h \varphi} \Big) \, \mathrm{d}y = \int_\Omega \left(-k_2^2 v \overline{\varphi} + \nabla_{\alpha_2} v \overline{\nabla_{\alpha_2} \varphi} \right) \mathrm{d}x + h B_{\mathrm{TE},1}(v, \varphi) + h^2 B_{\mathrm{TE},2,h}(v, \varphi)$$

with

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

The remainder term satisfies

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

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

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

Introduce the adjoint TE problem

$$B_{\mathrm{TE}}(\varphi, w) = \frac{\mathrm{e}^{-2\mathrm{i}\beta_{21}^{(n)} b}}{2\pi} \int_{\Gamma_1} \varphi \, \mathrm{e}^{-\mathrm{i} n x_1} \, \mathrm{d}x_1 \quad \forall \varphi \in H_p^1(\Omega), \tag{3.11}$$

which has a unique solution $w \in H_p^2(\Omega)$ [10].

From (3.4), it is obvious that

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

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

$$B^h_{\mathrm{TE}}(v_h, \Psi_h w) = B_{\mathrm{TE}}(\Psi_h^{-1} v_h, w) + h B_{\mathrm{TE},1}(\Psi_h^{-1} v_h, w) + h^2 B_{\mathrm{TE},2,h}(\Psi_h^{-1} v_h, w). \tag{3.13}$$

On the other hand,

$$B^h_{\mathrm{TE}}(v_h, \Psi_h w) = -\sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0^h} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)y_1} \partial_j^{\alpha_1} u_h \partial_l^{\alpha_1} u_h \overline{\Psi_h w}\, \mathrm{d}y. \tag{3.14}$$

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 $j = l = 1$

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

with

$$\begin{aligned}\mathscr{J}_{11}(u,\varphi) = &\int_{\Omega_0} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1} (\partial_1\chi_1 + \partial_2\chi_2 + \mathrm{i}(2\alpha_1-\alpha_2)\chi_1)(\partial_1^{\alpha_1} u)^2 \overline{\varphi} \\ &- 2\int_{\Omega_0} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1} \partial_1^{\alpha_1} u(\partial_1\chi_1\partial_1 u + \partial_1\chi_2\partial_2 u)\overline{\varphi}.\end{aligned}$$

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

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

with

$$\begin{aligned}\mathscr{J}_{12}(u,\varphi) = &-\int_{\Omega_0} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1} \Big(\partial_2\chi_1(\partial_1 u)^2 + \partial_1\chi_2(\partial_2 u)^2\Big)\overline{\varphi} + \mathrm{i}\alpha_1 \int_{\Omega_0} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1} u(\partial_1\chi_1\partial_2 u - \partial_2\chi_1\partial_1 u)\overline{\varphi} \\ &+ \mathrm{i}(2\alpha_1-\alpha_2)\int_{\Omega_0} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1} \chi_1 \partial_1^{\alpha_1} u \partial_2 u \overline{\varphi}.\end{aligned}$$

3. For $j = l = 2$

$$\int_{\Omega_0^h} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)y_1} \big(\partial_{y_2}\Psi_h u\big)^2 \overline{\Psi_h \varphi}\, \mathrm{d}y = \int_{\Omega_0} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1} (\partial_2 u)^2 \overline{\varphi} + h\mathscr{J}_{22}(u,\varphi) + h^2 \mathscr{L}_{22}(u,\varphi)$$

with

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

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

$$\begin{aligned}\sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0^h} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)y_1} \partial_{y_j}^{\alpha_1} u_h \partial_{y_l}^{\alpha_1} u_h \overline{\Psi_h w}\, \mathrm{d}y = &\sum_{j,l=1,2} \rho_{jl} \int_{\Omega_0} \mathrm{e}^{\mathrm{i}(2\alpha_1-\alpha_2)x_1} \partial_j^{\alpha_1} \Psi_h^{-1} u_h \partial_l^{\alpha_1} \Psi_h^{-1} u_h \overline{w}\, \mathrm{d}x \\ &+ h\sum_{j,l=1,2} \rho_{jl}\mathscr{J}_{jl}(\Psi_h^{-1}u_h, w) + h^2 \sum_{j,l=1,2} \rho_{jl}\mathscr{L}_{jl}(\Psi_h^{-1}u_h, w),\end{aligned}$$

where $\mathscr{I}_{21} = \mathscr{I}_{12}$. Note that due to (2.26) obviously

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

Using Theorem 3.1, we arrive at

$$\sum_{j,l=1,2}\rho_{jl}\int_{\Omega_0^h} e^{i(2\alpha_1-\alpha_2)y_1}\partial_{y_j}^{\alpha_1}u_h\partial_{y_l}^{\alpha_1}u_h\overline{\Psi_h w}\,dy = \sum_{j,l=1,2}\rho_{jl}\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\partial_l^{\alpha_1}u\overline{w}\,dx + 2h\sum_{j,l=1,2}\rho_{jl} \times \int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\partial_l^{\alpha_1}u_1\overline{w} + h\sum_{j,l=1,2}\rho_{ij}\mathscr{I}_{jl}(u,w) + O(h^2),$$

which implies

$$B_{\mathrm{TE}}^h(v_h, \Psi_h w) = B_{\mathrm{TE}}(v,w) + h\sum_{j,l=1,2}\rho_{ij}\left(\mathscr{I}_{jl}(u,w) + 2\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\partial_l^{\alpha_1}u_1\overline{w}\right) + O(h^2).$$

Thus from (3.13), we get

$$\begin{aligned} &B_{\mathrm{TE}}(\Psi_h^{-1}v_h, w) + hB_{\mathrm{TE},1}(\Psi_h^{-1}v_h, w) + h^2B_{\mathrm{TE},2,h}(\Psi_h^{-1}v_h, w)\\ &\quad = B_{\mathrm{TE}}(v,w) + h\sum_{j,l=1,2}\rho_{jl}\left(\mathscr{I}_{ij}(u,w) + 2\int_{\Omega_0} e^{i(2\alpha_1-\alpha_2)x_1}\partial_j^{\alpha_1}u\partial_l^{\alpha_1}u_1\overline{w}\right) + O(h^2), \end{aligned}$$

which together with (3.12) proves the following theorem.

Theorem 3.2. *The derivative of the reflection coefficients $E_n^{\pm}$ with respect to the variations* (3.2) *of the interface Λ is given by the formula*

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

where the bilinear form $B_{\mathrm{TE},1}$ is defined by (3.9), *u and v denote the solutions of the diffraction problems* (2.24), (2.25), *respectively*, u_1 *solves* (3.8) *and w is the solution of the adjoint TE problem* (3.11).

Following [12], the form $B_{\mathrm{TE},1}(v,w)$ given by (3.9) can be transformed to

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

where we have used Eq. (2.19) 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

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

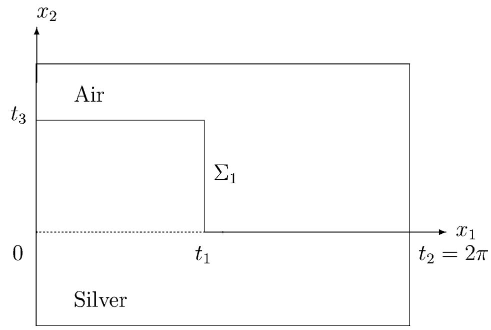

Fig. 2. Crosssection of a simple binary gratings.

Remark 3.1. To apply the above results to binary gratings by choosing different χ, we can compute the derivative $D_j E_n^{\pm}$ of the Rayleigh coefficients with respect to the transition points. For simplicity, consider a binary grating with two transition points t_1, $t_2 = 2\pi$ and the height t_3, as shown in Fig. 2. Denote $O_1 = (t_1, 0)$, $O_2 = (t_1, t_3)$, $O_3 = (0, t_3)$, and $\Sigma_1 = \overline{O_1 O_2}$, $\Sigma_2 = \overline{O_3 O_2}$, the fill factor $FF = t_1/2\pi$. To compute the derivative $D_1 E_n^{\pm}$ of the Rayleigh coefficients with respect to the variation of t_1, the mapping (3.2) 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).

4. Numerical examples

The described approach was numerically tested for different examples described in the literature. The numerical solution is based on GFEM discretizations of the sesquilinear forms B_{TM} and B_{TE}, described in [10]. This discretization avoids pollution effects, which are usually connected with domain–based methods for solving Helmholtz equations, but is restricted to piecewise rectangular subpartitioning of the integration domain. Therefore the numerical test were performed for binary gratings.

To obtain start values for the optimization we have first determined grating structures which provide minimal reflection in the TM case, i.e. which minimize the cost functional

$$\sum_{\beta_1^{(n)}(\alpha)>0} \beta_1^{(n)}/\beta_1 |H_n^+|^2 \quad \text{with} \quad H_n^+ = \frac{\mathrm{e}^{-2\mathrm{i}\beta_{21}^{(n)} b}}{2\pi} \int_{\Gamma_1} u\,\mathrm{e}^{-\mathrm{i}nx_1}\,\mathrm{d}x_1,$$

u being the solution of (2.24). This is done with the program DIPOG for the optimal design of linear diffractive gratings which uses conjugate gradient and inner point methods to minimize different cost functionals [11]. Since these functionals possess as a rule several local minima we use different start values to find a structure with minimal TM reflection. For this problem the gradients can be computed by certain line integrals which involve the solution of two variational problems, of the direct problem (2.24) and of a corresponding adjoint TM problem (see [12]). The program DIPOG offers efficient iterative solvers and well tested optimization parameters, such that for the physical parameters of our examples the determination of structures with minimal TM reflection can be performed within minutes.

After that this structure is used as start value for a simple gradient based line search algorithm to maximize the functional (3.1). For the same step size of the FE-discretization we determined numerically the derivatives with respect to grating depth and transition points as described in Remark 3.1. Note that the computation of the derivatives is inexpensive even though one has to solve four linear systems. In fact, the saving is largely due to the fact that the chosen starting value is close to a local maximum of (3.1). As the result, only few steps of line search and even less computation of derivatives are required to find an optimal solution for maximal efficiencies of the second harmonic field.

First we present numerical results on an example introduced in [16]. It is concerned with the grating enhancement of the second harmonic nonlinear optical effects for a silver layer. The enhancement is the ratio of the grating efficiency over the efficiency for the flat surface. Obviously, the TE efficiency (the nonlinear effect) for the flat layer is small which is confirmed by the calculated efficiency 1.2003160E-04.

The TE efficiency for the binary grating with period $d = 0.556$ μm, incidence angle 64.5°, and wavelength 1.06 μm is then computed. With fill-factor 0.5, similar enhancement results are obtained as those reported in [16] concerning the efficiency dependence on the groove depth. In particular, the maximal enhancement is about 45 which occurs when the groove depth is chosen close to 0.3 μm. Our calculation indicates in addition that by using the above algorithm, with the same data, a better enhancement for fill-factor 0.834 may be achieved. In fact, at groove depth 0.392 μm, the enhancement is more than 80. As it is shown in Fig. 3, around the optimal depth, the enhancement depends on the groove depth sharply. Fig. 3 presents the enhancement of the efficiency of the second harmonic field at various groove depths.

The calculations were performed in the rectangle (0.556, 0.6 μm) with a 138×150 grid. As start value for finding the optimal structure described above, we used a grating with the physical parameters fill factor 0.854 and groove depth of 0.392 μm, which reflects only 28.4% of the incident TM field.

The second example is concerned with the grating enhancement of the second harmonic nonlinear optical effects for ZnS overcoated binary silver gratings. The enhancement at 2ω is computed with respect to the associated flat structure. The period of the grating is $d = 0.4$ μm, the incidence angle being 28.92° with wavelength $\lambda = 1.06$ μm. The optimization parameters are the thickness of the ZnS coating, the fillfactor and the depth of the binary grating. Optimal results were obtained for a thickness of 0.33 μm of the coating layer, the fill factor 0.43 and the depth of 0.099 μm for the binary grating. For this grating we obtain the enhancement factor 686.6. Fig. 4 illustrates the enhancement dependence on the grating depth.

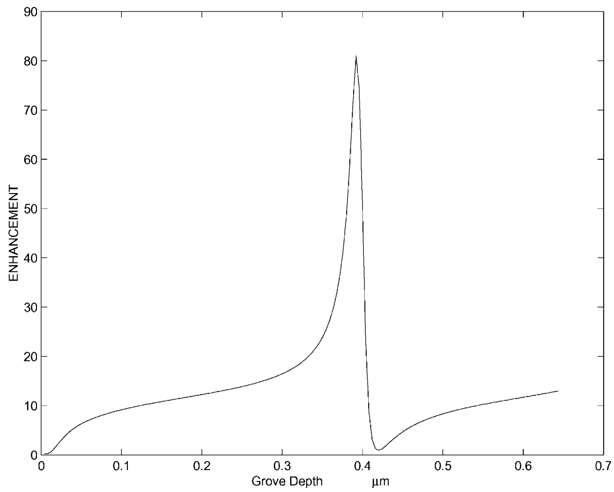

Fig. 3. Groove depth (μm) and enhancement.

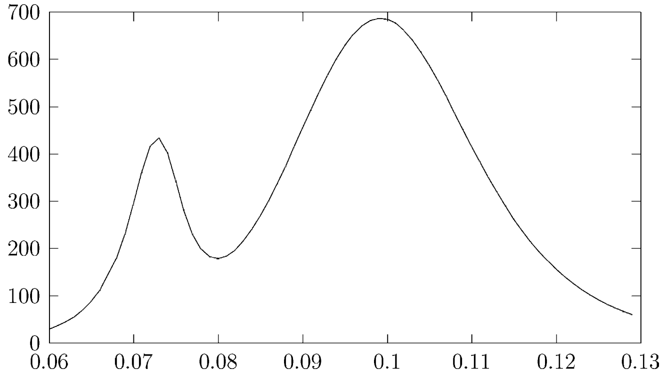

Fig. 4. Groove depth μm.

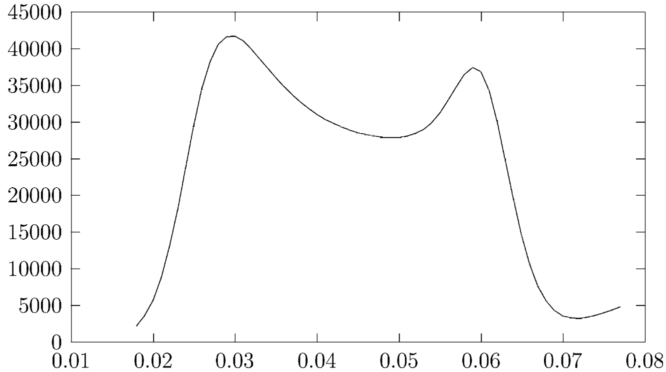

Fig. 5. Groove depth μm.

These calculations were performed in the rectangle (0.4, 0.5 μm) with a 200×250 grid. The start value for the optimization procedure was a grating with the thickness of 0.33 μm of the coating layer the fill factor 0.43 and groove depth of 0.092 μm, which reflects only 1.57 % of the incident TM field. In this case we had to determine only two search directions.

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 flat structures, Fig. 5 presents the corresponding enhancement factors for the thickness of 0.672 μm and a binary grating with fill factor 0.505. The maximum enhancement factor 41687.9 is obtained for the depth 0.03 μm. However the maximum value only amounts to 17% of the maximum for the thickness 0.33 μm.

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Appendix A

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

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

where

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

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 nonvanishing, 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 A.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 A.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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