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Coupled-mode formalism and linear theory of diffraction for a simplified analysis of second harmonic generation at grating couplers

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Abstract

We present a new approach to study second harmonic generation at grating couplers where we take full advantage of the fact that, in this type of second harmonic generation, there is a resonant excitation of normal modes of the grating coupler (guided wave or surface plasmon). Therefore the analysis reported here is developed in the framework of the coupled-mode formalism. This allows us to show that the associated diffraction phenomenon, which occurs in *nonlinear* optics, can be handled using the *linear* theory of diffraction. The resulting simplicity, which arises from the simultaneous use of the coupled-mode and linear diffraction theories, allows an easy physical insight in the process of second harmonic generation at grating couplers. Proceeding along these lines, we derive not only the guided wave amplitude but also that of the *radiated* diffracted orders at the second harmonic frequency.

1. Introduction

Second harmonic generation at grating couplers usually makes use of the resonant excitation of normal modes of the structure which are guided waves in χ^2 nonlinear waveguides or surface plasmons along an interface between a metal and a χ^2 medium. The associated electromagnetic resonance gives rise to an enhancement of several orders of magnitude of the second harmonic intensity as compared to the off-resonance situation. Here is the interest of this type of geometry for second harmonic generation (SHG).

The grating coupler behaves as an optical resonator and the normal modes may be excited at the pump and/or the SH frequency.

SHG at grating couplers has been studied rigorously, i.e. in a non perturbative way with respect to the groove depth of the grating, in Refs. [1-3]. In this theory [1-3] (referred to as method 1), no hypothesis is made regarding the *y*-dependence of the field map (the *y*-axis is perpendicular to the mean plane of the grating). The differential equations, deduced from Maxwell equations, which describe the electromagnetic fields at the existing frequencies are integrated along *y*. Thus method 1 applies regardless to the fact that the resonant conditions are fulfilled or not. As a result, this kind of theory is general. But

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this method has the two following disadvantages: (i) it is computation time consuming and (ii) it only works easily for plane waves. Point (ii) is a serious drawback when dealing with second harmonic generation in the presence of sharp resonances.

We propose here another way to study SHG at grating couplers which takes into account the fact these grating couplers in guided wave nonlinear optics are used under the following conditions:

- it is possible to isolate a single resonance,
- the angle of incidence, θ_i , is chosen in such a way to excite an evanescent diffracted order resonantly,
- the angle of incidence, θ_i , remains close to its resonant value (θ_{res}): i.e. the difference $\theta_i - \theta_{res}$ is of the order of a few times the half-width at half-maximum of the resonance curve.

Under these conditions, the coupled-mode formalism [4,5] is particularly well suited for this kind of study since it shows that the transverse field map, at the second harmonic frequency, corresponds to the one of the *linear* regime. Thus in the *nonlinear* case, the transverse field map is *known* and it is no longer necessary to integrate along y , as required in method 1. Hence an important simplification in the study of SHG at gratings.

It is the aim of this paper to consider this new point of view where one takes full advantage of the fact that these grating couplers are used close to an isolated resonance.

The paper is organized as follows: Sect. 2 is devoted to the theoretical analysis along with some general considerations concerning the simultaneous use, for the study of grating couplers in nonlinear optics, of the coupled-mode formalism and of the *linear* diffraction theory. The case of the undepleted pump plane wave is considered in Sect. 3. The question of phase matching, using space harmonics, is also treated in this section. Numerical results, concerned with guided wave and surface plasmon enhanced SHG at grating couplers, are presented in Sect. 4 not only for the guided wave intensity at the SH frequency but also for the *radiated* diffracted orders at this frequency. These results are compared with the corresponding ones derived using the full numerical method 1.

2. Theory

The system under consideration is depicted in Figs. 1. A pump beam of circular frequency ω is incident, under incidence θ_i , on a coated grating with periodicity d and groove depth δ . The coating layer is a χ^2 nonlinear medium. This grating coupler may support guided waves or surface plasmons: Fig. 1a corresponds to an interaction between guided modes at the pump (ω) and at the SH (2ω) circular frequencies, whereas in Fig. 1b surface plasmons are involved at these two frequencies.

Throughout this paper $\partial/\partial z = 0$. Thus the solu-

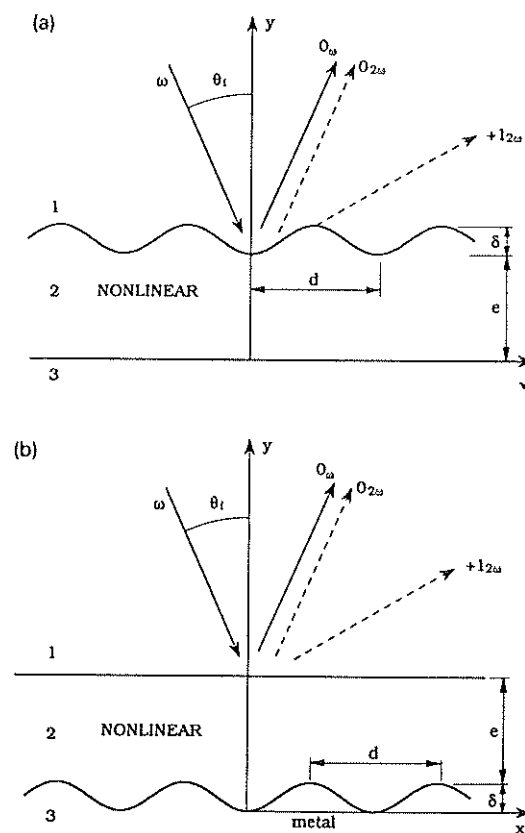


Fig. 1. Geometry and notations for SHG at grating couplers: (a) when guided modes are involved at ω and at 2ω , (b) when surface plasmons are involved at ω and at 2ω . The specular diffracted order at pump frequency is called O_ω ; $O_{2\omega}$ and $+1_{2\omega}$ represent the 0 and +1 diffracted orders at the SH frequency. With the numerical values used in Figs. 3 and 4, these two diffracted orders are radiated.

tions at the pump and at the SH frequencies are either TE or TM polarized and are characterized by $\delta_z(x, y)$ and $\mathcal{H}_z(x, y)$ respectively.

2.1. The requirements of the coupled-mode formalism

In order to use the coupled mode formalism [4,5], one has:

- (a) to define the unperturbed structure and to look for its normal modes,
- (b) to specify the source terms,
- (c) to write down the equations of evolution of the normal modes amplitude at ω and at 2ω .

In the case of SHG at grating couplers (Figs. 1), the situation is the following:

Point a: the unperturbed structure and its normal modes.

The unperturbed system is constituted by the grating coupler without any incident beam.

For a mode m at the SH frequency, let us define:

$$\begin{aligned} \Phi_m(2\omega, x, y) &= \delta_{z,2,m}(x, y), \quad \text{in the TE case,} \\ &= \mathcal{H}_{z,2,m}(x, y), \quad \text{in the TM case.} \end{aligned} \quad (1a)$$

It is convenient to consider first the associated smooth structures i.e., the ones which are deduced from those in Figs. 1 by letting the groove depth δ goes to zero. In this case, Φ_m has the following form

$$\Phi_m(2\omega, x, y) = c_{2,m} \psi_{2,m}(y) \exp(i\gamma_{2,m}x). \quad (1b)$$

In Eq. (1b), $c_{2,m}$ is the amplitude of mode m .

When the groove depth is different from zero, due to the periodicity along x , $\psi_{2,m}$ is no longer a function of only the y -coordinate but becomes also x -dependent with periodicity d . Thus $\psi_{2,m}$ can be expanded in Fourier series and Eq. (1b) becomes

$$\begin{aligned} \Phi_m(2\omega, x, y) \\ = c_{2,m} \sum_n \varphi_{2,m,n}(y) \exp[i(\gamma_{2,m} + n\sigma)x], \end{aligned} \quad (1c)$$

where $\sigma = 2\pi/d$.

It is shown in Ref. [6] that outside the modulated region $\varphi_{2,m,n}$ has a known exponential dependence with respect to y . Thus, in regions 1 and 3, Φ_m can be expressed as a Rayleigh expansion which writes

$$\begin{aligned} \Phi_m(2\omega, x, y) &= c_{2,m} \sum_n a_{q,2,m,n} \\ &\times \exp\{i[(\gamma_{2,m} + n\sigma)x + \alpha_{q,2,m,n}y]\}, \end{aligned} \quad (1d)$$

with $q = 1, 3$,

$$\begin{aligned} \alpha_{q,2,m,n}^2 + (\gamma_{2,m} + n\sigma)^2 &= k_q^2(2\omega), \\ k_q(2\omega) &= \sqrt{\epsilon_q(2\omega)} (2\omega/c), \end{aligned} \quad (1e)$$

ϵ_q is the relative permittivity of medium q , $a_{q,2,m,n}$, $\gamma_{2,m}$ and $\alpha_{q,2,m,n}$ are known from the solution of the linear homogeneous problem [6].

Inside the modulated region, no simple expression exists for the y -dependence of the n th space harmonic: the y -dependence of Φ_m is obtained using the rigorous theory of diffraction [6].

At circular frequency ω , for the quantity $\Phi_p(\omega, x, y)$ associated to mode p , one has to make the substitution $(2, m, n) \rightarrow (1, p, s)$.

Due to the existence of the grating, each mode is a sum of an infinite number of space harmonics, or equivalently, of diffracted orders with longitudinal wavevector component:

$$\tilde{\gamma}_{1,p,s} = \gamma_{1,p} + s\sigma$$

for the space harmonic s of mode p at ω ,

$$\tilde{\gamma}_{2,m,n} = \gamma_{2,m} + n\sigma$$

for the space harmonic n of mode m at 2ω .

Since the device is leaky [6], $\gamma_{1,p}$ and $\gamma_{2,m}$ are complex numbers even in the absence of dielectric losses.

Notice that the diffracted orders n , for which $\gamma_{2,m} + n\sigma < k_1(2\omega)$, are radiated in the upper medium.

Point b: the source terms.

There are two source terms:

- one of them, called $\mathcal{P}^L(x, y)$ in what follows, describes the in-coupling of the pump beam,
- the other ones account for the nonlinear polarization at ω and at 2ω and will respectively be denoted by $\mathcal{P}^{NL}(\omega, x, y)$ and $\mathcal{P}^{NL}(2\omega, x, y)$. When the undepleted pump approximation applies, the nonlinear polarization at ω is neglected.

According to Ref. [7], the nonlinearity of the metal (Fig. 1b) is small as compared to the one of the dielectric which coats the grating. Thus in the case of

Fig. 1b, only the nonlinearity of the dielectric is taken into account.

Point c: the equations of evolution.

It is shown in Refs. [4,5] that the existence of source terms leads to x -dependent mode amplitudes. A brief demonstration of the equation obeyed by these amplitudes is given in the appendix.

Throughout this paper, it is assumed that the electromagnetic (EM) fields at circular frequencies ω and 2ω are such that a space harmonic s_0 of mode p at ω and a space harmonic n_0 of mode m at 2ω are excited close to resonance. This means that the phase-matching condition is nearly fulfilled (nearly: within the width of the resonance curves respectively at ω and at 2ω). This is the most interesting situation. These two space harmonics are the dominant ones in the EM field expansion Eq. (1c). Thus in the equations of evolution of the mode amplitudes, only these resonant, i.e. phase-matched, space harmonics are retained.

2.2. Amplitude of the diffracted orders

2.2.1. The guided wave

From Eq. (A7) of the appendix, the following equations are obtained

- at the pump frequency for the mode amplitude $c_{1,p}(x)$:

$$N_{1,p,s_0} \frac{dc_{1,p}}{dx} = -i\omega \langle E_{1,p,s_0}^{\dagger}(y) \cdot \mathcal{P}^{NL}(\omega, x, y) \rangle \times \exp(i\tilde{\gamma}_{1,p,s_0}^{\dagger} x) - i\omega \langle E_{1,p,s_0}^{\dagger}(y) \cdot \mathcal{P}^L(x, y) \rangle \exp(i\tilde{\gamma}_{1,p,s_0}^{\dagger} x) \quad (2a)$$

- at the SH frequency for the mode amplitude $c_{2,m}(x)$:

$$N_{2,m,n_0} \frac{dc_{2,m}}{dx} = -i2\omega \langle E_{2,m,n_0}^{\dagger}(y) \cdot \mathcal{P}^{NL}(2\omega, x, y) \rangle \times \exp(i\tilde{\gamma}_{2,m,n_0}^{\dagger} x). \quad (2b)$$

In Eqs. (2):

(i) E_{2,m,n_0} and H_{2,m,n_0} represent the y -dependence of the electric and magnetic fields corresponding to the space harmonic (m, n_0) ,

(ii) the superscript \dagger denotes the adjoint structure deduced from the original one by transposition of the

dielectric permittivity and the magnetic permeability matrices [4]; the quantity $\tilde{\gamma}_{2,m,n_0}^{\dagger}$ fulfills:

$$\tilde{\gamma}_{2,m,n_0}^{\dagger} + \tilde{\gamma}_{2,m,n_0} = 0. \quad (3a)$$

For the space harmonic (p, s_0) at circular frequency ω , one has to make the substitution: $(2, m, n_0) \rightarrow (1, p, s_0)$.

(iii) The brackets including the nonlinear polarization $\mathcal{P}^{NL}(x, y)$ account for the nonlinear effect in the guiding layer for which:

$$\mathcal{P}_h^{NL}(\omega, x, y) = \epsilon_0 \chi_{h,i,j}(\omega = 2\omega - \omega) \times E_{2,m,n_0,i}(y) E_{1,p,s_0,j}^{\dagger}(y) c_{2,m}(x) c_{1,p}^{\dagger}(x) \times \exp[i(\tilde{\gamma}_{2,m,n_0} - \tilde{\gamma}_{1,p,s_0}^{\dagger})x], \quad (3b)$$

$$\mathcal{P}_l^{NL}(2\omega, x, y) = \epsilon_0 \chi_{l,i,j,h}(2\omega = \omega + \omega) E_{1,p,s_0,j}(y) \times E_{1,p,s_0,h}(y) c_{1,p}^{\dagger}(x) \exp(i2\tilde{\gamma}_{1,p,s_0}^{\dagger} x). \quad (3c)$$

In Eqs. (3b) and (3c), a summation over the repeated cartesian indices i, j, h is understood. The other bracket at circular frequency ω in Eq. (2a) describes the incoupling of the pump beam. The corresponding source polarization $\mathcal{P}^L(x, y)$ takes into account the finite width of the pump beam. No incident beam is assumed at the SH frequency.

According to Eqs. (3b) and (3c), Eqs. (2) can be rewritten as:

$$\frac{dc_{1,p}}{dx} = -i\omega \xi_1^{\dagger}(x) c_{2,m} c_{1,p}^{\dagger} \times \exp[-i(\tilde{\gamma}_{1,p,0} + \tilde{\gamma}_{1,p,0}^{\dagger} - \tilde{\gamma}_{2,m,n_0})x] - i\tau_1 \mathcal{A}_1(x) \exp[i(\beta_0 + r_0 \sigma - \tilde{\gamma}_{1,p,0})x], \quad (4a)$$

$$\frac{dc_{2,m}}{dx} = -i2\omega \xi_2^{\dagger}(x) c_{1,p}^{\dagger} \exp[i(2\tilde{\gamma}_{1,p,0} - \tilde{\gamma}_{2,m,n_0})x]. \quad (4b)$$

In Eqs. (4)

- the quantity $\mathcal{A}_1(x)$ represents the x -dependence of the finite-width pump beam;

- $\beta_0 = k_1(\omega) \sin \theta_1$

- r_0 is the integer which labels the resonantly excited evanescent diffracted order at the pump frequency; the labelling of the space harmonics at circular frequency ω is such that it is the space harmonic $s_0 = 0$ which is associated to this diffracted order r_0 ;

$$\tau_1 \mathcal{A}_1(x) \exp[i(\beta_0 + r_0 \sigma)x] = \omega \frac{\langle E_{1,p,0}^{\dagger} \cdot \mathcal{P}^L(x, y) \rangle}{N_{1,p,0}}, \quad (4c)$$

thus τ_i denotes the in-coupling coefficient associated to the resonantly excited diffracted order r_0 at the pump circular frequency ω ;

- the star "*" means the complex conjugate;

$$\xi_1(x) = \epsilon_0 \times \frac{\langle \chi_{h,i,j}(\omega, x, y) E_{1,p,0,h}^1(y) E_{2,m,n_0,i}(y) E_{1,p,0,j}^*(y) \rangle}{N_{1,p,0}}, \quad (4d)$$

$$\xi_2(x) = \epsilon_0 \times \frac{\langle \chi_{i,j,h}(2\omega, x, y) E_{2,m,n_0,i}^1(y) E_{1,p,0,j}(y) E_{1,p,0,h}(y) \rangle}{N_{2,m,n_0}}. \quad (4e)$$

Eqs. (4d) and (4e) show that the quantities $\xi_1(x)$ and $\xi_2(x)$ are nonlinear coefficients directly related to the overlap integral [4,5]. The existence of a modulated region in the grating coupler explains the (x, y) dependence of the elements of the nonlinear susceptibility tensor $[\chi]$ and thus the x -dependence of $\xi_1(x)$ and $\xi_2(x)$.

According to the fact that the transverse field maps (along y) at the pump and at the SH frequencies are known and correspond to the one of the *linear* regime, the calculation of the in-coupling coefficient τ_i and of the nonlinear coefficients $\xi_1(x)$ and $\xi_2(x)$ is achieved using the *linear* theory of diffraction developed in Ref. [6].

It is worth noticing that the value of τ_i , $\xi_1(x)$ and $\xi_2(x)$ depends neither on the shape of the input beam nor on the fact that the undepleted pump approximation is made or not. Thus the in-coupling coefficient τ_i is calculated assuming an undepleted pump plane wave and the determination of $\xi_1(x)$ and $\xi_2(x)$ only requires the knowledge of the normal modes at ω and 2ω .

The simplification introduced by this modal analysis, where the diffraction phenomenon is accounted for using only the rigorous *linear* theory of diffraction, can be better appreciated by comparing with the rigorous theory of diffraction in nonlinear optics developed in Ref. [1]: instead of the complicated flow chart Fig. 5 of Ref. [1] which is given here for the sake of convenience (Fig. 2), the SH amplitude $c_{2,m}$ is deduced from Eqs. (4). As already stated, the only computations correspond to a *linear* diffraction study

at ω and 2ω in order to get the numerical values of τ_i , $\xi_1(x)$ and $\xi_2(x)$.

When solved, Eqs. (4) yield the guided wave amplitude at the pump and at the SH frequencies. But these equations tell nothing concerning the *radiated* diffracted orders which are directly accessible to experiments. It is the object of the next section to determine their amplitudes.

2.2.2. The diffracted orders

The diffracted SH amplitude is obtained by noting that once $c_{2,m}(x)$ is known, Eq. (1d) gives the amplitude of a diffracted order n in medium q ($q=1, 3$ in Fig. 1) at the ordinate y . Let us call this amplitude $\mathcal{C}_{2,m,n}(x, y)$. Eq. (1d) shows that $\mathcal{C}_{2,m,n}(x, y)$ is given by the following expression:

$$\mathcal{C}_{2,m,n}(x, y) = c_{2,m}(x) a_{q,2,m,n} \exp(i\alpha_{q,2,m,n}y). \quad (5)$$

In Eq. (5), n is an integer, equal or different from n_0 , which labels the space harmonics.

The quantity $a_{q,2,m,n} \exp(i\alpha_{q,2,m,n}y)$ is known from the solution of the *linear* homogeneous problem of diffraction at 2ω developed in Ref. [6] and $c_{2,m}(x)$ is obtained by resolving Eqs. (4). Thus Eq. (5) leads to the x -dependence of the amplitude of any diffracted order at the SH frequency in medium q . Eq. (5) provides the link between the resonantly excited evanescent diffracted order and the amplitudes of the diffracted orders at the SH frequency whatever their nature may be: evanescent or radiated.

3. An example of solution: the undepleted pump plane wave case

3.1. The calculation

Let us derive the modes amplitude $c_{1,p}(x)$ and $c_{2,m}(x)$ assuming that the incident field is a plane wave and that the undepleted pump approximation holds.

In this case, $\xi_1(x) = 0$ and Eq. (4a) becomes:

$$\frac{dc_{1,p}}{dx} = -i\tau_i \mathcal{A}_i \exp[i(\beta_0 + r_0\sigma - \tilde{\gamma}_{1,p,0})x]. \quad (6a)$$

Thus:

$$c_{1,p}(x) = \mathcal{A}_i C_{r_0} \exp[i(\beta_0 + r_0\sigma - \tilde{\gamma}_{1,p,0})x],$$

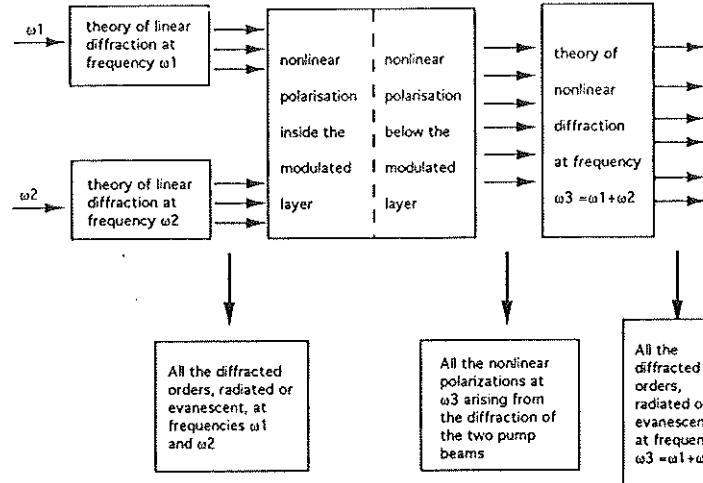


Fig. 2. Flow chart of the theory of SHG at grating couplers according to Ref. [1]. In this reference, the general case of an interaction of the type: $(\omega_1, \omega_2) \rightarrow \omega_3 = \omega_1 + \omega_2$ is considered.

with

$$C_{r_0} = - \frac{\tau_i}{\beta_0 + r_0\sigma - \tilde{\gamma}_{1,p,0}} \quad (6b)$$

In general, the nonlinear medium includes a modulated region and a homogeneous one. Thus $\xi_2(x)$ is the sum of two terms, one for each region:

$$\xi_2(x) = \xi_2^{(1)}(x) + \xi_2^{(2)}, \quad (7a)$$

where the first term of the right hand side of Eq. (7a) refers to the modulated region of thickness δ . According to the periodicity of the grating, $\xi_2^{(1)}(x)$ can be expanded in Fourier series:

$$\xi_2^{(1)}(x) = \sum_l \xi_{2,l}^{(1)} \exp(i\sigma x). \quad (7b)$$

Use of Eqs. (7a) and (4b) shows that:

$$c_{2,m} = c_{2,m}^{(1)} + c_{2,m}^{(2)}, \quad (8a)$$

with:

$$c_{2,m}^{(1)} = -2\omega_i \mathcal{A}_i^2 \sum_l \xi_{2,l}^{(1)} \times \frac{\tau_i^2}{(\beta_0 + r_0\sigma - \tilde{\gamma}_{1,p,0})^2 [2\beta_0 + (2r_0 + l)\sigma - \tilde{\gamma}_{2,m,n_0}]} \times \exp\{i[2\beta_0 + (2r_0 + l)\sigma - \tilde{\gamma}_{2,m,n_0}]x\}, \quad (8b)$$

$$c_{2,m}^{(2)} = -2\omega_i \mathcal{A}_i^2 \xi_2^{(2)} \times \frac{\tau_i^2}{(\beta_0 + r_0\sigma - \tilde{\gamma}_{1,p,0})^2 [2(\beta_0 + r_0\sigma) - \tilde{\gamma}_{2,m,n_0}]} \times \exp\{i[2(\beta_0 + r_0\sigma) - \tilde{\gamma}_{2,m,n_0}]x\}. \quad (8c)$$

3.2. Phase-matching

Let $n_{eff,1}$ and $n_{eff,2}$ be the complex effective indices respectively for the mode $(p, 0)$ at ω and for the mode (m, n_0) at 2ω .

Eq. (8b) shows that phase matching occurs for the pairs (n_0, l) satisfying:

$$\text{Re}\{n_{eff,2}\} - \text{Re}\{n_{eff,1}\} = (l - n_0)\lambda/2d, \quad (9)$$

Re{...}: real part of {...}.

This means that when Eq. (9) is satisfied, resonance takes place for $c_{2,m}^{(1)}$ both at the pump frequency for the evanescent diffracted order r_0 and at the SH frequency for the space harmonic n_0 of mode m . According to Eq. (9), n_0 depends on l : $n_0 = n_0(l)$.

But all the pairs (n_0, l) satisfying Eq. (9) do not play the same role. First of all, let us notice that for the pairs $(n_0, l \neq 0)$ the overlap integral has to be calculated over the thickness of the modulated region only since $c_{2,m}^{(2)}$ is non resonant. The simultaneous resonance of $c_{2,m}^{(1)}$ and $c_{2,m}^{(2)}$ occurs for the pair $(n_0, 0)$,

i.e. involving the fundamental $l=0$ Fourier-component of the nonlinear susceptibility. For this pair, there is phase-matching not only for $c_{2,m}^{(1)}$ but also for $c_{2,m}^{(2)}$. Thus the overlap integral is to be carried out over *all* the thickness of the nonlinear medium, i.e. including in addition to the modulated region, as for the pairs $(n_0, l \neq 0)$, the homogeneous part of the nonlinear waveguide (region 2 of Fig. 1). Therefore the couple $(n_0, 0)$ is of special interest in view of efficient SH processes.

Such a phase matching scheme, based on the use of space harmonics, has already been pointed out in Ref. [8]. But it was in a geometry where resonance at the pump frequency is not possible contrary to the situation considered in this paper.

We remind the reader that the calculation of $\xi_{2,0}^{(1)}$

is achieved using the rigorous theory of diffraction in linear optics [6] at ω and 2ω .

4. Numerical results and comparison with method 1

Calculations have been performed in the undepleted pump plane wave case considering two different types of interactions:

- (i) between TE₀ modes at the pump and the second harmonic frequencies (Fig. 1a),
- (ii) between surface plasmons at the pump and the second harmonic frequencies (Fig. 1b).

Figs. 3 and 4 respectively represent the interactions (i) and (ii). Each of these figures is a plot of the amplitude of the guided wave (case i) or surface

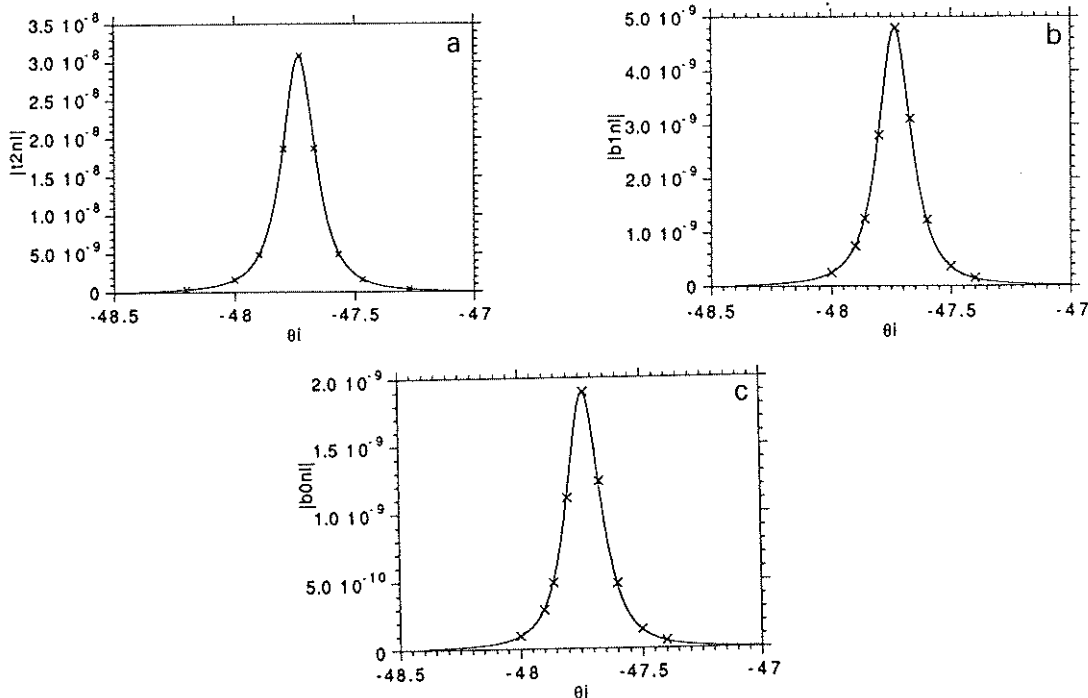


Fig. 3. Second harmonic generation at the grating coupler Fig. 1a coated by a χ^2 guiding layer. All the numerical values correspond to fictitious media. The refractive indices of the different layers of the grating coupler have been chosen in such a way that phase matching occurs for the TE₀ modes at ω and at 2ω . Solid curves: simplified theory presented here. Crosses: full numerical method [1-3]. Pump wavelength 1.06 μm . Grating profile: sinusoidal, periodicity $d=0.4 \mu\text{m}$, groove depth $\delta=0.12 \mu\text{m}$. χ^2 waveguide: thickness: $e=0.58 \mu\text{m}$, the only nonzero χ^2 element is $\chi_{zzz}=\epsilon_0$, refractive indices of the different media: (i) at the pump frequency: substrate 1.7; χ^2 waveguide $2+i0.0005$; upper medium 1, (ii) at the second harmonic frequency: substrate 1.7; χ^2 waveguide $1.94175+i0.0005$; upper medium 1. (a) Absolute value of the guided wave amplitude, $|t_{2nl}|$ at $y=0$, at 2ω as a function of the angle of incidence of the pump field. (b) Same as (a) but for the absolute value, $|b_{1nl}| = |\xi_{2,m,1}(y=\delta+e)|$ of the amplitude of the +1 radiated diffracted order at 2ω . (c) Same as (a) but for the absolute value, $|b_{0nl}| = |\xi_{2,m,0}(y=\delta+e)|$ of the amplitude of the zero radiated diffracted order at 2ω .

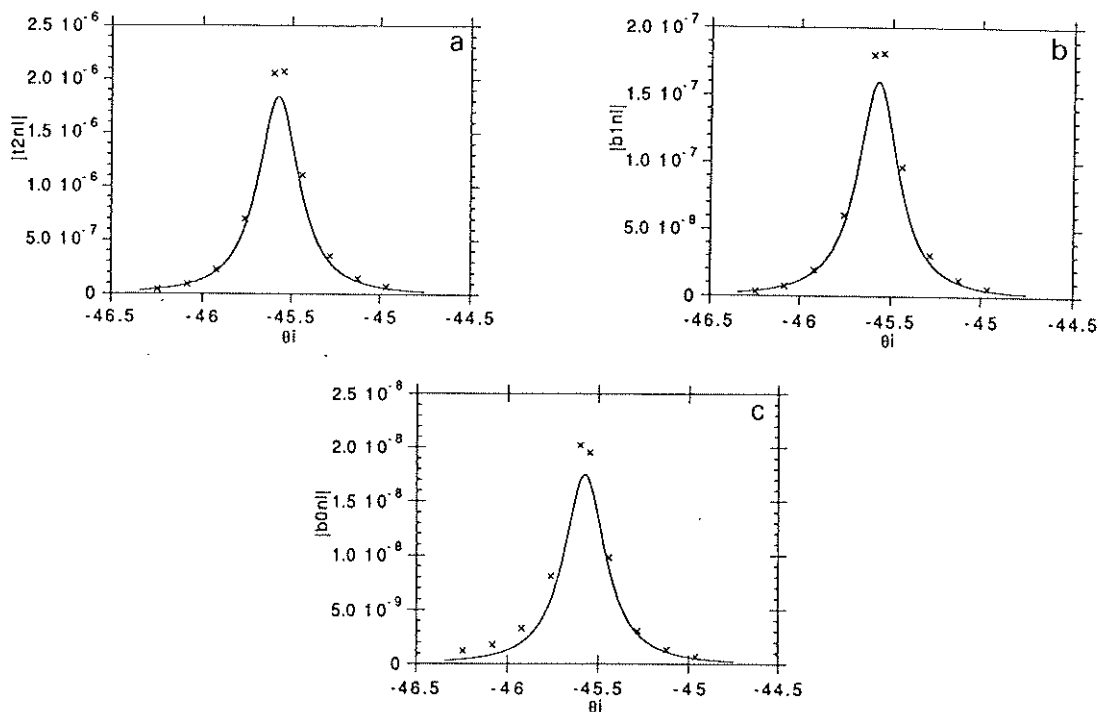


Fig. 4. Second harmonic generation at the grating coupler Fig. 1b coated by a χ^2 layer. All the numerical values correspond to fictitious media. The refractive indices the different layers of the grating coupler have been chosen in such a way that phase matching occurs for the surface plasmons at ω and at 2ω . Metal: silver. Solid curves: simplified theory presented here. Crosses: full numerical method [1-3]. Pump wavelength 1.06 μm . Grating profile: sinusoidal, periodicity $d=0.4 \mu\text{m}$, groove depth $\delta=0.0154 \mu\text{m}$. χ^2 layer: thickness $e=0.01 \mu\text{m}$, the only nonzero χ^2 element is $\chi_{yyy}=\epsilon_0$. Refractive indices of the different media: (i) at the pump frequency: substrate $0.3+i9.5$; χ^2 waveguide 1.534; upper medium 1.534, (ii) at the second harmonic frequency: substrate $0.05+i3.14$; χ^2 waveguide 1.39184; upper medium 1.39184. (a) Absolute value of the surface plasmon amplitude, $|t_{2n}|$ at $y=0$, at 2ω as a function of the angle of incidence of the pump field. (b) Same as (a) but for the absolute value, $|b_{1n}| = |\zeta_{2,m,1}(y=\delta+e)|$ of the amplitude of the +1 radiated diffracted order at 2ω . (c) Same as (a) but for the absolute value, $|b_{0n}| = |\zeta_{2,m,0}(y=\delta+e)|$ of the amplitude of the zero radiated diffracted order at 2ω .

plasmons (case ii) and of the +1 and zero radiated diffracted orders at the second harmonic frequency as a function of the angle of incidence of the pump field:

- the solid curves correspond to the new method presented here. The set of Eqs. (8b) and (8c) yield the guided wave or surface plasmon amplitude whereas Eq. (5) was used to derive the amplitude of the +1 and zero radiated diffracted orders.

- the crosses are obtained from the full numerical theory [1-3].

The agreement between both methods can be considered as excellent when guided modes are involved. Other results, not reported here, with a TE_0 pump mode and a TE_1 SH mode show the same type of agreement as for Figs. 3.

In the case of a surface plasmon-surface plasmon interaction (Fig. 1b), there is a small discrepancy (of the order of 10%) between the modal theory developed here and method 1. Moreover, calculations have shown that this discrepancy increases with the losses of silver. To understand this result, one has to remember that, according to Eq. (4e), in the calculation of the nonlinear coefficient ζ_2 only the resonant space harmonics at ω and 2ω are retained. But the higher the losses and the refractive index steps between the different media constituting the grating coupler, the more important the contribution of the other space harmonics n . Thus the nonlinear quantity ζ_2 is undervalued. This explains the fact that the modal method yields lower values than method 1 and that the agreement is much better for the "low

loss full dielectric" grating considered in Figs. 3 than with the lossy metallic coated grating of Figs. 4.

5. Conclusion

It has been shown that the simultaneous use of the coupled mode formalism and of the rigorous theory of diffraction in *linear* optics provides a very convenient mean to study second harmonic generation at grating couplers. Eqs. (4) and (5) are important. Indeed they constitute the basic set of nonlinear equations for SHG at a grating coupler on a χ^2 guiding structure supporting surface plasmon or guided waves. These equations describe the diffraction process in nonlinear optics at the pump and at the SH frequencies taking into account both the depletion and the finite width of the pump beam: Eqs. (4) and (5) respectively account for the angular dependence and spatial evolution of the guided wave and of all the other diffracted orders at 2ω whatever their type may be: evanescent or radiated. The fact that a problem of diffraction in *nonlinear* optics, namely at the second harmonic frequency, is studied using only the *linear* diffraction theory [6] is worth noticing. This possibility arises because these grating couplers are used close to resonance. In the case of stationary plane wave studies, *analytical* expressions are obtained whereas the full numerical theory [1-3] requires heavy computer calculations. In addition to the simplification, the obvious advantage is that an easy physical insight is gained. It is worth noticing that the existence of a phase matching scheme where the overlap integral involves the *whole* χ^2 guiding structure has been demonstrated. Finally, the simplicity of this method not only allows the investigation of new solutions arising from the finite width and the depletion of the pump beam but also the optimisation of second harmonic generators. Thus this theory constitutes a powerful tool for the study of second harmonic generation at grating couplers.

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Appendix

The derivation of the equation of evolution of the mode amplitude closely follows the method of Ref. [4].

In the presence of a source term, \mathcal{P} , the electric and magnetic fields (respectively \mathcal{E} and \mathcal{H}) satisfy the following Maxwell equations at a frequency ω (an $\exp(-i\omega t)$ time dependence is assumed):

$$\text{rot } \mathcal{E} = i\omega[\mu]\mathcal{H}, \tag{A.1}$$

$$\text{rot } \mathcal{H} = -i\omega[\epsilon]\mathcal{E} - i\omega\mathcal{P}, \tag{A.2}$$

$[\epsilon]$ and $[\mu]$ being respectively the dielectric permittivity and the magnetic permeability matrices whose elements may depend on the transverse coordinates.

Besides, let us introduce the adjoint structure deduced from the original one by transposition of the dielectric permittivity and magnetic permeability matrices. The electric and magnetic fields \mathcal{E}_n^* and \mathcal{H}_n^* of the adjoint mode n (that is to say the n th mode of the adjoint structure without the source term \mathcal{P}) satisfy:

$$\text{rot } \mathcal{E}_n^* = i\omega^*[\mu]\mathcal{H}_n^*, \tag{A.3}$$

$$\text{rot } \mathcal{H}_n^* = -i\omega^*[\epsilon]\mathcal{E}_n^*. \tag{A.4}$$

From Eqs. (A.1)-(A.4), we get:

$$\text{div}(\mathcal{E} \times \mathcal{H}_n^* - \mathcal{E}_n^* \times \mathcal{H}) = -i\omega\mathcal{E}_n^* \cdot \mathcal{P}. \tag{A.5}$$

Integrating Eq. (A.5) over a cross-section plane and keeping in mind that the mode n (guided wave or surface plasmon) vanishes at infinity yields:

$$(d/dx)\langle u \cdot (\mathcal{E} \times \mathcal{H}_n^* - \mathcal{E}_n^* \times \mathcal{H}) \rangle = -i\omega\langle \mathcal{E}_n^* \cdot \mathcal{P} \rangle, \tag{A.6}$$

where:

(i) $\langle \dots \rangle$ stands for an integral in the cross-section plane:

$$\langle \dots \rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \dots dy dz \text{ in the most general case,}$$

(ii) u is the unit vector along the x -axis.

Let c_n be the mode amplitude, use of the orthogonality relation [4] allows to write Eq. (A.6) under the following form:

$$N_n \frac{dc_n}{dx} = -i\omega \langle \mathcal{E}_n^i \cdot \mathcal{P} \rangle. \quad (\text{A.7})$$

In Eq. (A.7), $N_n = \langle \mathbf{u} \cdot (\mathcal{E}_n \times \mathcal{H}_n^i - \mathcal{E}_n^i \times \mathcal{H}_n) \rangle$.

Eq. (A.7) is the desired result. In order to go from this equation to Eqs. (2), one has:

- (i) to use the fact that $\mathcal{E}(x, y) = E(y) \exp(i\gamma x)$,
- (ii) to write down the expression of the source term: $\mathcal{P} = \mathcal{P}^{\text{NL}} + \mathcal{P}^{\text{L}}$.

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