Finite Element Analysis of Induced Diffraction Gratings in Nonlinear Optics

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***Abstract*—In this paper, we present a multiharmonic model able to allow for general nonlinear optical media [1]. As a particular example, two- and three-photon processes are considered here. The numerical model is based on the finite element method that allows to take into account the inhomogeneities of the refraction index due to the nonlinearities. It consists of several harmonic equations at various frequencies coupled via some nonlinear terms. As an illustration we propose a simple homogeneous uniform slab made of non-linear material but illuminated by three plane waves in order to create an artificial periodic structure with a fictitious permittivity. This system exhibits a non trivial and quite complex behavior because of the induced diffraction grating.**

I. Multiharmonic nonlinear model

In this paper, we propose a numerical model for nonlinear optics based on a systematic approach of the nonlinearity in the frequency domain together with a very general setting via the finite element method. This model aims at applications in nanophotonics since the size of the scattering objects are of the same order of magnitude as the wavelength of the incident waves that are infrared or visible light. Considering a given incident monochromatic electric field of pulsation ω_I, we would like to solve the nonlinear vector wave equation:

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) + \partial_t^2 \mathbf{D} = 0,$$

for a given geometry and where the material properties are $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$ and $\mathbf{B} = \mu_0 \mathbf{H}$. We assume here that the polarization $\mathbf{P}$ is of the form:

$$\mathbf{P}(\mathbf{s},t) = \mathbf{P}^{(0)}(\mathbf{s}) + \sum_{n\in\mathbb{N}} \varepsilon_0 \int_{-\infty}^{\infty} d\omega_1 \cdots \int_{-\infty}^{\infty} d\omega_n \, \chi^{(n)}(\mathbf{s}, \omega_1, \cdots, \omega_n) \hat{\mathbf{E}}(\mathbf{s}, \omega_1) \cdots \hat{\mathbf{E}}(\mathbf{s}, \omega_n) e^{-i(\omega_1 + \cdots + \omega_n)t} ,$$

where $\hat{\mathbf{E}}(\mathbf{s}, \omega)$ is the Fourier transform of $\mathbf{E}$ with respect to time. We set $\mathbf{E}_p := \hat{\mathbf{E}}(\mathbf{s}, p\omega_I)$ and we note that $\mathbf{E}_{-p} = \overline{\mathbf{E}_p}$. The $\chi^{(n)}$ tensors describe the physical behavior of the media. We are interested here in the harmonic generation and therefore we now make the simplifying assumption that $\chi^{(n)}(\omega_1, \cdots, \omega_n) = 0$ if $\omega_i \neq p\omega_I$, $p \in \mathbb{Z}$ so that the electric field is $\mathbf{E}(\mathbf{s}, t) = \sum_{p\in\mathbb{Z}} \mathbf{E}_p(\mathbf{s}) e^{-ip\omega_I t}$. To further simplify and to obtain tractable problems, we set $\chi^{(n)} = 0$ if $n > 3$. We introduce the following notations for the nonlinear terms involving the $\chi^{(n)}$:

$$\lfloor \mathbf{E}_{p_1}, \cdots, \mathbf{E}_{p_n} \rfloor := \chi^{(n)}(p_1\omega_I, \cdots, p_n\omega_I) \mathbf{E}_{p_1} \cdots \mathbf{E}_{p_n}$$

and for the linear part $\mathcal{M}_p^{lin}$ of the wave operators:

$$\mathcal{M}_p^{lin}(\mathbf{E}_p) := -c^2 \nabla \times (\nabla \times \mathbf{E}_p) + (p\omega_I)^2 \varepsilon_r^{(1)}(p\omega_I) \mathbf{E}_p$$

where $\varepsilon_r^{(1)} = 1 + \chi^{(1)}$. With the previous assumptions, the time domain problem becomes an **infinite** set of **coupled** harmonic equations:

$$\mathcal{M}_p^{lin}(\mathbf{E}_p) + (p\omega_I)^2 \Big(\sum_{q\in\mathbb{Z}} \lfloor \mathbf{E}_q, \mathbf{E}_{p-q} \rfloor + \sum_{(q,r)\in\mathbb{Z}^2} \lfloor \mathbf{E}_q, \mathbf{E}_r, \mathbf{E}_{p-q-r} \rfloor \Big) = 0, \quad \text{for } p \in \mathbb{Z}.$$

Moreover, we limit our nonlinear phenomena to two- and three-photon processes. The corresponding problems are encountered in numerous nonlinear optics experiments involving second and third harmonic generation. Therefore we have $p \in \{-3, -2, -1, 1, 2, 3\}$, and a **system of three coupled nonlinear equations** is obtained.

II. Induced grating

We consider a simple uniform slab made of non-linear material but illuminated by three plane waves in order to create a periodic structure with an apparent permittivity. This system exhibits a non trivial and quite complex behavior because of the induced diffraction grating.

In our model, the geometry is invariant along the z-axis and an appropriate principal axis for the $\chi^{(n)}$ tensors is considered here together with a polarization of the electric field along the axis of invariance (the z-axis) in order to reduce the problem to a scalar two-dimensional one (in the $xy-$plane). The numerical implementation is performed in COMSOL Multiphysics by a direct coding of the weak formulation of the three coupled PDE. The discretization is performed with triangular finite elements. The incident field is a set of **three** plane waves imposed via a virtual antenna [2], [3], a special numerical technique specially designed for these nonlinear scattering problems.

We are interested in the direction along which the three harmonics of the field scatter and we can analyze the results in terms of the diffraction grating theory [4], [5]. Outside the slab (we are therefore in an homogeneous and linear media), each electric field component $\mathbf{E}_p$ satisfies a Helmholtz equation. We

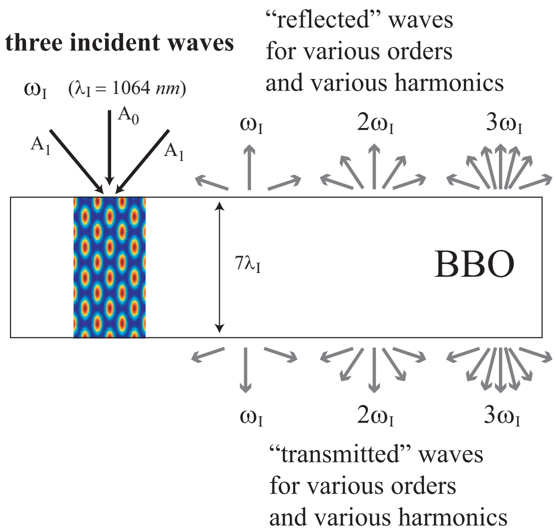

Fig. 1. The geometry of the system is an infinite slab. It is infinite along the z-axis, the invariance direction of the chosen incident field, and along the x-axis, the horizontal direction of the cross section shown here. Made up of β Barium Borate (BBO), it is illuminated by three plane waves, one with a normal incidence (amplitude A_0) and two with a symmetric oblique incidence (amplitude A_1) of 0.439 rad with respect to the normal. Along the finite dimension, the thickness is equal to $7\lambda_I$. Harmonics are generated in the nonlinear medium. Due to the interferences of the different waves oscillating at ω_I (the pattern of the field intensity of the incident waves is shown in color inside the slab), a structure (periodic along the x-axis and, therefore, equivalent to a diffraction grating or a finite photonic crystal) is induced in the cross section of the slab. This induced grating generates several orders for the fundamental frequency ω_I and for the higher harmonics.

write their propagating solutions as

$$\mathbf{E}_p(x,y) = \sum_{n\in\mathcal{U}_p} \{ b^{(r)}_{p,n} e^{i\left(\frac{2\pi n x}{d} + (k_p^2 - (\frac{2\pi n}{d})^2)^{1/2} y\right)} + b^{(t)}_{p,n} e^{i\left(\frac{2\pi n x}{d} - (k_p^2 - (\frac{2\pi n}{d})^2)^{1/2} y\right)} \} \hat{z},$$

with $k_p = p\omega_I/c$ and d is the period of the induced grating obtained from the incident waves. The coefficients $b^{(r)}_{p,n}$ (resp. $b^{(t)}_{p,n}$) denotes the complex amplitudes of the n-th order of the reflected (resp. transmitted) wave at pulsation $p\omega_I$, and $\mathcal{U}_p := \{n \in \mathbb{Z} : k_p^2 - (\frac{2\pi n}{d})^2 > 0\}$. We note that k_p^2 is larger for higher harmonics, so whereas only the orders -1, 0 and 1 are present in $\mathbf{E}_1$, the $\mathbf{E}_3$ harmonic contains orders from -3 to 3 (this depends on the wavelength and the tilts of the incident beams).

It is worth noting that the amplitude of the n-th order of the p-th harmonic (that is $b^{(r)}_{p,n}$ or $b^{(t)}_{p,n}$) is not monotonic with respect to the amplitude of the incident field, as is seen in the Figs. 2 and 3 where the third harmonic is taken as an example (due to the reflection symmetry along the y-axis of the system, $b^{(t)}_{3,-n} = b^{(t)}_{3,n}$). These functions present resonances, which means that higher incident intensities may give lower nonlinear effects. The coefficients are normalized so that $\sum_{n\in\mathcal{U}_3} \mid b^{(t)}_{3,n} \mid^2$ is equal to 1.

With a very simple system involving a non-linear optical material, we have shown that non-linear scattering problems in the resonant domain (*i.e.* when the size of the device is

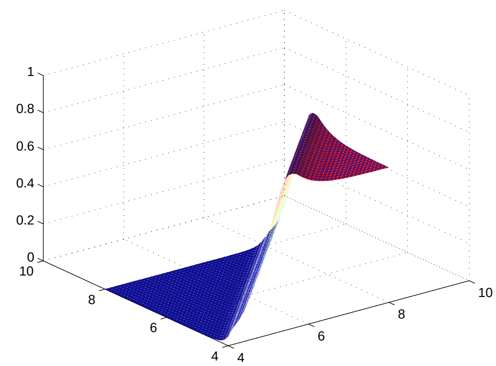

Fig. 2. The square of the modulus of coefficient $\mid b^{(t)}_{3,0} \mid^2$ of the order 0 transmitted propagating waves at the frequency $3\omega_I$ (vertical axis) as a function of the amplitude of the inclined incident field (left axis) and of the incident field orthogonally impinging on the slab (right axis).

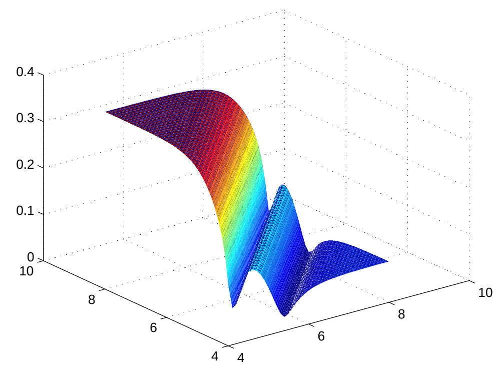

Fig. 3. The square of the modulus of coefficient $\mid b^{(t)}_{3,1} \mid^2$ of the order 1 transmitted propagating waves at the frequency $3\omega_I$ (vertical axis) as a function of the amplitude of the inclined incident field (left axis) and of the incident field orthogonally impinging on the slab (right axis).

similar to the wavelength) may exhibit a highly non trivial behavior.

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