Transfer-matrix method for second-order nonlinear processes with realistic beams

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Abstract

Accurate and fast modeling of electric fields in layered structures have a great scientific and practical value. Prevalent method for that is transfer-matrix method. However, transfer matrix method is limited to infinite plane wave calculations, which can become a limiting factor if a very narrow resonances, e.g. long range surface plasmon polaritons, are present in the structure. In this paper we extend the functionality of standard and nonlinear transfer-matrix method to include beams with arbitrary profile and propose applications for the method.

1. Introduction

Standard transfer-matrix method (TMM) is a very powerful and a fast method to solve the Maxwell equations in a layered structures [1, 2]. However, standard TMM is limited to linear optics and calculation of plane waves. In our previous paper (Ref. [3]) we extended standard TMM to second-order nonlinear processes (NL TMM) for calculation of plasmonic structures. This paper is devoted to extending the both standard and nonlinear TMM to use realistic beams with arbitrary profile. This communication will include all the details of the formulation used to extend the method. The improved method itself is made publicly available at github.com/ardiloot/NonlinearTMM.

The paper will begin with a short review to a standard TMM (Sec.2.1). Next the functionality of TMM is first extended to calculate the fields of the beam with arbitrary profile (Sec. 2.2.1 and 2.2.2) and then the theory for efficient calculation of the powers of the beams is developed (Sec. 2.2.3 and 2.2.4). Next, similar functionality is added to nonlinear TMM (Sec. 3). Finally, the paper is concluded and the possible applications of the method is outlined.

2. Standard TMM

This section will focus on the extending the standard TMM to employ realistic beams with arbitrary profile. This section begins with a short review to TMM (for more details see Refs. [1, 2, 3]), in Sec. 2.2 the theory to use realistic beams will be developed. The theory developed for standard TMM will be used in Sec. 3 to extend the NL TMM.

Figure 1: The usual layered structure for TMM calculations. The layers are defined by the thicknesses $d_i$ and refractive indices $n_i$. The input beam is incident from the left at a angle of incidence $\theta$, which correspond to the tangential wave vector $k_x$. In the case of standard TMM we have two plane waves $k^\pm_a$ is a single layer, however in case of NL TMM we have in addition nonlinear inhomogeneous waves denoted by $k^\pm_s$.

1. Review

The usual layered structure of TMM simulation is shown in Fig. 1. It consists of $N+1$ layers of different thickness $d_i$ and refractive index $n_i$. In every layer the electrical fields are described as a sum of forward- and backward-propagating waves (layer index $i$ omitted)

$$E = E^+ + E^- = A^+e^{ik^+_x r} + A^-e^{ik^-_x r},$$

(1)

where $+$ and $-$ denote the forward- and backward-propagating waves, $A^\pm$ is the amplitude, $k^\pm$ is the wave vector and $r$ is a standard position vector. The change of the amplitudes $A^\pm$ of the plane waves inside a single layer is described by a propagation matrix and the continuity relations on the boundary of the different layers are forced by transfer matrix [3].

The input beam is incident from the left (see Fig. 1) under angle of incidence $\theta$, which corresponds to the tangential wave vector component $k_x = 2\pi n_0/\lambda$ (same in every layer), where $\lambda$ is the wavelength of the light in vacuum.
2.2. Realistic beams

Standard TMM works with infinite plane waves, here we present the formulation to use beams with arbitrary profile. First, we develop the theory to calculate the field distribution in the case of realistic beams in an infinite homogeneous medium and then move to the calculation of the fields in the stratified structures. An extra care must be devoted to calculate the powers of arbitrary beams and it is explored in Sec. 2.2.3 and 2.2.4.

2.2.1. Fields in a infinite medium

![Coordinate system diagram]

Figure 2: The coordinate system of the wave $(x', z')$ and the coordinate system of the structure $(x, z)$. The wave is propagating at the angle of incidence $\theta$ in the structure.

Let's look at a wave with an arbitrary cross-sectional electrical field (wave profile) $E_{w}(x') = E(x', z' = 0)$ (defined at $z' = 0$) propagating in an infinite homogeneous medium under angle of incidence $\theta$ (see Fig. 2). Then, in the coordinate system of the wave $(x', z')$ we can easily express the electrical field through angular spectrum representation (see Ref. [4]) as

$$E(x', z') = \int_{-k}^{k} dk'_{x} \hat{E}_{w}(k'_{x}) e^{i(k'_{x}x' + k'_{z}z')},$$

where $(k'_{x}, k'_{z}) = \sqrt{k^{2} - k'_{z}^{2}}$ are the wave vector $x$ and $z$ components in the wave coordinate system, $k$ is the wave number and $E_{w}(k'_{z})$ is the Fourier transform of the wave profile

$$\hat{E}_{w}(k'_{z}) = \mathcal{F}[E_{w}(x')] = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx' E_{w}(x') e^{-ik'_{z}x'},$$

After rotation of coordinates by $-\theta$ we get

$$E(x, z) = \int_{-k}^{k} \frac{dk_{x}}{\cos(\theta)} \hat{E}_{w}(k'_{x}) e^{i(k_{x}x + k_{z}z)},$$

where $k'_{x} = \cos(\theta) k_{x} - \sin(\theta) k_{z}$. Eq. 4 together with Eq. 4 has a significant meaning: if we know the beam cross-sectional profile $E_{w}(x')$ we can find the electrical field of the wave everywhere under any angle of incidence $\theta$ by integration of plane waves in Eq. 4. This result must be now generalized to layered structures.

2.2.2. Fields in layered medium

Noticing, that $\hat{E}_{w}(k'_{z}) e^{i(k_{x}x' + k_{z}z)}$ is just a plane wave with amplitude $\hat{E}_{w}(k'_{z})$, which is easily calculated by standard TMM, it is evident, that using Eq. (4) allows to extend TMM for waves with arbitrary profile $E_{w}(x')$ through a single integral. In other words, for the input wave the amplitudes $E_{w}(k'_{z})$ are known from Eq. 3, and for the output waves the corresponding amplitudes are easily calculated by TMM and could be converted to final fields by Eq. 4 by integration.

In the case of Gaussian input wave the Fourier transform of the beam profile is given analytically by

$$\hat{E}_{w}(k_{x}) = E_{0} \frac{w_{0}}{2\sqrt{\pi}} e^{-k_{x}^{2}w_{0}^{2}/4},$$

where $E_{0}$ is the amplitude of the wave and $w_{0}$ is the waist size. However, we mainly use numerical calculation of Fourier transform, as in such way we are not limited to simple wave profiles, but can numerically input any field profiles.

In general, it is sufficient to use only 50 plane waves in the integration of Eq. 4 (trapezoidal integration) in order to represent common beam profiles reasonably well.

2.2.3. Power flow of s-polarized wave

In the case of s-polarized single plane wave the power flow through the rectangle with dimensions $L_{x} \times L_{y}$ is easily calculated from the electrical field amplitude

$$P_{s} = \frac{1}{2\omega\mu_{0}} |\mathcal{E}_{w}|^{2} L_{x} L_{y}. $$

However, such simple relationship is not applicable for waves consisting of many plane waves because the calculation of Poynting vector is a nonlinear operation. In this section, we derive formulas for calculation of power of s-polarized wave with arbitrary profile, the results of p-polarized wave are in Sec. 2.2.4.

First, to calculate the power through a rectangle in $xy$-plane, we only need to calculate the $z$-component of Poynting vector. Taking account that we are currently limited to $s$-polarization the Poynting vector is

$$\langle S \rangle_{z} = \frac{1}{2} \mathcal{R}[\mathbf{E} \times \mathbf{H}^{*}]_{z} = -\frac{1}{2} \mathcal{R}[E_{y} H_{z}^{*}]$$

and the corresponding power through the rectangle $(x_{0}...x_{1}, 0...L_{y})$ with dimensions $L_{x} \times L_{y}$ is

$$P_{s} = \frac{L_{x} L_{y}}{2} \mathcal{R} \int_{x_{0}}^{x_{1}} dx E_{y} H_{z}^{*}.$$  

Analogous to Eq. (4) the electric fields can be expressed as
where $E_{0y}(k_x)$ is the amplitude of plane wave calculated by TMM. The magnetic field follows from
\[ H = \frac{1}{\omega \mu_0} (k \times E) \]
and the complex conjugate of the $x$-component is expressed as
\[ H^*_x = \frac{-1}{\omega \mu_0} \int_{-k}^{k} dk_x k_z E_{0y}^*(k_x) e^{-i(k_xx + k_zz)}. \]
Thus, the power of the beam is represented by the triple integral over the $x$-coordinate and two over $x$-component of the wave-vector. Numerical calculation of such integral requires a fair amount of computational power, especially for higher-order nonlinear processes. Fortunately, after rearrangement of integrals it is possible to analytically calculate the integral over $x$-coordinate. The expression for the power of the beam then becomes
\[ P_x = \frac{L_y}{2\omega \mu_0} \Re \left[ I_{ks} \right] \]
where $I_{ks} = \int_{-k}^{k} dk_x dk'_x k'_z E_{0y}^*(k'_x) \hat{E}_{0y}(k_x) F_x F_z$, $F_x$ and $F_z$ describe the interference between the plane waves in $x$- and $z$-direction, respectively. Those coefficients are defined by
\[ F_x (\Delta k) = \int_{x_0}^{x_1} dx e^{i\Delta k x} = \frac{-i}{\Delta k} e^{i\Delta k x} \bigg|_{x_0}^{x_1} \]
\[ F_z (k_x, k'_x) = e^{i(k_x - k'_x)z}, \]
where $\Delta k = k_z - k'_z$. Int the limit $\Delta k \to 0$, the Eq. (13) becomes
\[ \lim_{\Delta k \to 0} F_x (\Delta k) = x_1 - x_0 = L_z. \]
Calculation of double integral in Eq. (12) is readily done by numerical methods. The calculation of powers is included to the code of NLTMM and is available at github.com/ardiloot/NonlinearTMM.

### 2.2.4. Power flow of $p$-polarized wave

In case of $p$-polarization, the derivation stays the same, however now the main field component is given by $H_y$. The power of the wave is given by
\[ P_p = \frac{L_y}{2\varepsilon_0 \omega \mu_0} \Re \left[ I_{kp} \right] \]
\[ I_{kp} = \int_{-k}^{k} dk_x dk'_x H_{0y} (k_x) k_z \hat{H}_{0y}^* (k'_x) F_x F_z, \]
where $F_x$ and $F_z$ are given by Eqs. (13) and (14).

### 3. Nonlinear transfer-matrix method

Standard TMM is used by NLTMM to calculate the electrical fields of the input beams (non-depleted pump-wave approximation), so the functionality derived in Sec. 2 is also essential for NLTMM for realistic beams. However, the calculation of the generated beam in NLTMM significantly differs from the calculation of the input beams and is reviewed here.

#### 3.1. Review

NLTMM directly solves the Maxwell equations in any nonlinear layered structure (see Fig. 1) in the limit of non-depleted pump wave approximation. Our focus is devoted to the second-order nonlinear processes (e.g. second-harmonic, sum-frequency, difference-frequency generation), but in general, the method could be extended to the higher-order nonlinear processes. The main equation for electrical field in nonlinear homogeneous isotropic medium directly follows from Maxwell equations and is given by
\[ \nabla^2 E + \frac{\omega^2}{c^2} \varepsilon (\omega) E = -\frac{\omega^2}{\varepsilon_0 c^2} P_{NL} + \nabla (\nabla \cdot E), \]
where $P_{NL}$ denotes the nonlinear polarization, which is the driving term for the generation of nonlinear wave [5]. Symbol $\nabla$ is Nabla-operator, $c$ is the absolute speed of light and $\varepsilon (\omega) = \varepsilon_0 (\omega)^2$ is the relative permittivity of the medium. Eq. 17 describes the fields in a homogeneous layer (layer index omitted, see Fig. 1), between the different layers the fields must connected to match the continuity conditions [3, 4]. For comprehensive review of NLTMM see Ref. [6].

#### 3.2. Absorption

In the case of standard TMM the calculation of absorption could be easily done through the powers of incident, reflected and transmitted beam. The calculation of absorption of the generated beam is not possible in a similar manner because the “incident/source” power in not known. In order to calculate the absorption of the generated wave the NLTMM was extended. As the nonlinear mediums in this study are always non-absorbing, it is sufficient to calculate the absorption of generated fields in linear absorbing layers. The absorbed energy in rectangular box $(0..L_x, 0..L_y, 0..z_0)$ is given by (coordinates defined in Fig. 1, layer index $i$ omitted)
\[ A = \frac{1}{2} \varepsilon_0 Im [\varepsilon] \omega L_x L_y \int_{z_0}^{z_1} E \cdot E^* dz, \]
where $\varepsilon_0$ is the permittivity of the vacuum (layer index is omitted) [4]. The integral in Eq. 18 could be easily analytically solved if the expression (Eq. 1) for the electrical field vector is substituted into Eq. 18 and taking into account that $\exp (ik^2 \cdot r) = \exp (ik_x x \pm ik_z z)$ in our geometry (see Fig. 1) we arrive to
The possibility to calculate the absorption of the generated nonlinear wave allows to calculate the out-coupling efficiency, to characterize the ratio between the power of absorbed (lost) and out-coupled (detected) light.

3.3. Realistic beams

The calculation of the fields and powers of the generated beam of second-order nonlinear process is similar to standard TMM. However, the single integral in Eq. 4 is replaced by a double integral over both input waves $k_{x1}$ and $k_{x2}$. The plane wave amplitudes $\hat{E}_w(k'_{x1}, k'_{x2})$ could be readily calculated by NL TMM (Sec. 3).

The calculation of the powers of the generated beam is even simpler as the formulas described in Sec. 2.2.3 and 2.2.4 depend only on $\hat{E}_0y(k_x)$ and $\hat{H}_0y(k_x)$. Those dependencies is readily calculable by NLTM. Otherwise, the formulas to calculate the power of s- and p-polarized beam with arbitrary profile stays exactly the same.

4. Discussion and conclusions

This paper focuses on extending the widely used transfer-matrix method, used for modeling of layered structures, to beams with realistic dimensions. The formulations are described in the detail and the code is freely available at github.com/ardiloot/NonlinearTMM. In addition to the extension of the standard TMM also nonlinear TMM (developed in Ref. [3]) is extended to incorporate the excitation with beams with any profile.

Acknowledgement

The research was supported by the Estonian research project IUT2-27.

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