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TANGENTIAL FIELDS IN MATHEMATICAL MODEL OF OPTICAL DIFFRACTION

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Abstract

We present the formulation of optical diffraction problem on periodic interface based on vector tangential fields, for which the system of boundary integral equations is established. Obtained mathematical model is numerically solved using boundary element method and applied to sine interface profile.

1. Introduction

Diffraction of optical wave on periodical interface between two media belongs to frequently solved problems, especially, when the grating period Λ is comparable with wavelength λ of incident beam. Among other, this phenomenon is studied and exploited by nanostructured optical elements design. Naturally, theoretical modelling is of great importance in such cases. One of possible approaches has been demonstrated in our previous paper [1], where the boundary integral equations (BIE) for tangential fields have been introduced. Unlike the usually used rigorous coupled waves algorithm (RCWA) advantageous in the far fields analysis [2], the BIE models enable effective modelling of near fields in the spatially modulated region.

2. Formulation of problem

Let $S : x_3 = f(x_1)$ in $\mathbb{R}^3$ be a smooth surface periodically modulated in the coordinate x_1 with period Λ and uniform in the x_2 direction. The interface S with normal vector $\boldsymbol{\nu}$ divides the space into two semi-infinite homogeneous regions $\Omega^{(1)} = \{(x_1, x_2, x_3) \in \mathbb{R}^3,\ x_3 > f(x_1)\}$, $\Omega^{(2)} = \{(x_1, x_2, x_3) \in \mathbb{R}^3,\ x_3 < f(x_1)\}$ with constant relative permittivities $\varepsilon^{(1)} \neq \varepsilon^{(2)}$, $\varepsilon^{(1)} \in \mathbb{R}$ and $\varepsilon^{(2)} \in \mathbb{C}$, $\mathrm{Re}\,(\varepsilon^{(2)}) > 0$, $\mathrm{Im}\,(\varepsilon^{(2)}) \geq 0$, and, the relative permeabilities $\mu^{(1)} = \mu^{(2)} = 1$ (both materials are magnetically neutral), see Fig.1.

We aim to solve optical diffraction problem for monochromatic plane wave with wavelength λ, i.e. with wave number $k_0 = 2\pi/\lambda$, incoming from $\Omega^{(1)}$ under the

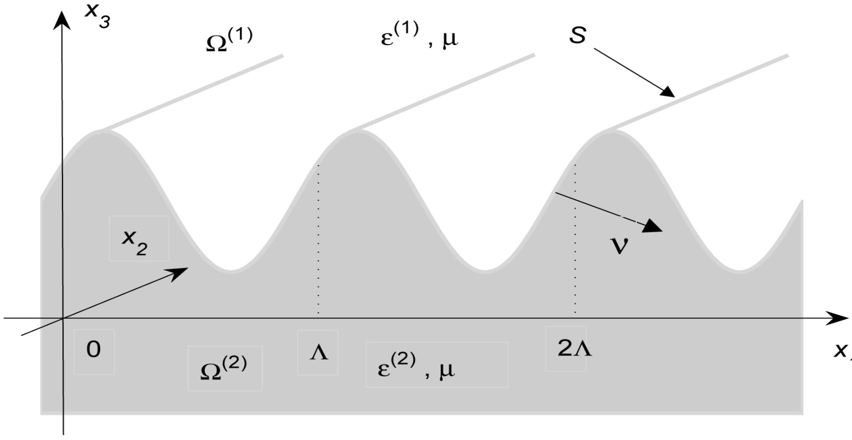

Figure 1: Structure of regions with common periodical boundary

angle of incidence θ measured from x_3 direction. We seek for space-dependent amplitudes $\boldsymbol{E}^{(j)} = \boldsymbol{E}|_{\Omega^{(j)}}$, $\boldsymbol{H}^{(j)} = \boldsymbol{H}|_{\Omega^{(j)}}$ of the electromagnetic field intensity vectors $\boldsymbol{E}(x_1, x_2, x_3)\mathrm{e}^{-\mathrm{i}\omega t}$, $\boldsymbol{H}(x_1, x_2, x_3)\mathrm{e}^{-\mathrm{i}\omega t}$, where $\omega = c/\lambda$ and c represents the light velocity in the free space. The unknown intensities can be written as

$$\boldsymbol{E} = \begin{cases} \boldsymbol{E}_0^{(1)} + \boldsymbol{E}^{(1)} & \text{in} \quad \Omega^{(1)}, \\ \boldsymbol{E}^{(2)} \quad \text{in} \quad \Omega^{(2)}, \end{cases} \qquad \boldsymbol{H} = \begin{cases} \boldsymbol{H}_0^{(1)} + \boldsymbol{H}^{(1)} & \text{in} \quad \Omega^{(1)}, \\ \boldsymbol{H}^{(2)} \quad \text{in} \quad \Omega^{(2)}, \end{cases} \tag{1}$$

where the subscript 0 denotes incident field. In the media without free charges, the vectors $\boldsymbol{E}^{(j)}$, $\boldsymbol{H}^{(j)}$, $j = 1, 2$ fullfill Maxwell equations (the free-space wave impedance is embedded in the vector $\boldsymbol{H}$) in the form

$$\nabla \times \boldsymbol{E}^{(j)} = \mathrm{i}k_0\mu\boldsymbol{H}^{(j)}\,, \qquad \nabla \times \boldsymbol{H}^{(j)} = -\mathrm{i}k_0\varepsilon^{(j)}\boldsymbol{E}^{(j)} \quad \text{in} \quad \Omega^{(j)}\,, \tag{2}$$

$$\nabla \cdot \boldsymbol{E}^{(j)} = 0, \qquad \nabla \cdot \boldsymbol{H}^{(j)} = 0 \quad \text{in} \quad \Omega^{(j)}\,. \tag{3}$$

The tangential components of the fields are continuous on the boundary, i.e.

$$\boldsymbol{\nu} \times (\boldsymbol{E}^{(1)} - \boldsymbol{E}^{(2)}) = \boldsymbol{o}\,, \qquad \boldsymbol{\nu} \times (\boldsymbol{H}^{(1)} - \boldsymbol{H}^{(2)}) = \boldsymbol{o} \qquad \text{on } S\,. \tag{4}$$

For the far fields, the well-known Sommerfeld's radiation convergence conditions hold that allow to consider the problem on the common interface S only [3].

We solve the problem (2)–(4) for the TM polarization of incident wave, therefore we set $\boldsymbol{E}^{(j)} = (E_1^{(j)}, 0, E_3^{(j)})$, $\boldsymbol{H}^{(j)} = (0, H_2^{(j)}, 0)$. To this purpose, we introduce tangential fields in the next section that enable to reformulate given problem as scalar integral equations at common boundary. Theoretical background of used approach is referred in the article [1]. The boundary element method (BEM) has been chosen to solve obtained system numerically (Sect. 4). Resulting algorithm is tested for sine interface profile in the Sect. 5.

3. Mathematical model

We formulate the problem (2)–(4) as boundary integral equations for tangential fields

$$\boldsymbol{J} = \boldsymbol{\nu} \times \boldsymbol{E}^{(1)} = \boldsymbol{\nu} \times \boldsymbol{E}^{(2)}, \qquad \boldsymbol{I} = -\boldsymbol{\nu} \times \boldsymbol{H}^{(1)} = -\boldsymbol{\nu} \times \boldsymbol{H}^{(2)} \ , \tag{5}$$

where $\boldsymbol{\nu}$ is an unit normal vector of the boundary S oriented as shown in Fig.1. Similarly, $\boldsymbol{\tau}$ represents an unit tangential vector of S. On the boundary we can write $\boldsymbol{J} = -J_2\boldsymbol{e}_2$, where $J_2 = \boldsymbol{\tau}\cdot\boldsymbol{E}^{(1)} = \boldsymbol{\tau}\cdot\boldsymbol{E}^{(2)}$; and, $\boldsymbol{I} = I_\tau\boldsymbol{\tau}$, where $I_\tau = -H_2^{(1)} = -H_2^{(2)}$.

We introduce a parametrization $\boldsymbol{\pi} : \langle 0, 2\pi\rangle \to \mathbb{R}^2$, $\boldsymbol{\pi}(t) = (p(t), q(t))$ of the curve $x_3 = f(x_1)$ having unit normal vector $\boldsymbol{\nu}(t)$ and corresponding tangential vector $\boldsymbol{\tau}(t)$ with the norm $\nu(t) = \sqrt{p'(t)^2 + q'(t)^2}$. Resulting system of boundary integral equations for scalar components I_τ and J_2 derived in [1] is of the following form:

$$J_2(s) = -J_{2,0}(s) - \mathrm{i}k_0\mu\boldsymbol{\tau}(s)\cdot\int_0^{2\pi} I_\tau(t)\boldsymbol{\tau}(t)\left(\Psi^{(1)}(s,t) - \Psi^{(2)}(s,t)\right)\ \nu(t)\ dt$$

$$-\ \frac{1}{\mathrm{i}k_0}\boldsymbol{\tau}(s)\cdot\int_0^{2\pi} I'_\tau(t)\nabla_t\left[\frac{1}{\varepsilon^{(1)}}\Psi^{(1)}(s,t) - \frac{1}{\varepsilon^{(2)}}\Psi^{(2)}(s,t)\right]\ dt$$

$$+\ \boldsymbol{\nu}(s)\cdot\int_0^{2\pi} J_2(t)\nabla_t\left[\Psi^{(1)}(s,t) - \Psi^{(2)}(s,t)\right]\ \nu(t)\ dt\ , \tag{6}$$

$$I_\tau(s) = -I_{\tau,0}(s) - \mathrm{i}k_0\int_0^{2\pi} J_2(t)\left(\varepsilon^{(1)}\Psi^{(1)}(s,t) - \varepsilon^{(2)}\Psi^{(2)}(s,t)\right]\nu(t)\ dt$$

$$+\int_0^{2\pi} I_\tau(t)\boldsymbol{\nu}(t)\cdot\nabla_t\left[\Psi^{(1)}(s,t) - \Psi^{(2)}(s,t)\right]\ \nu(t)\ dt\ . \tag{7}$$

In the kernels of integral operators, the parametrized periodical Green functions $\Psi^{(j)}(s,t)$, $j = 1, 2$ of Helmholtz equation play important role. We apply these by the relations [4]

$$\Psi^{(j)}(s,t) = \sum_{m=-\infty}^{\infty}\Psi_m^{(j)}(s,t)\,, \qquad \Psi_m^{(j)}(s,t) = \frac{1}{2\mathrm{i}\Lambda\beta_m}\ \mathrm{e}^{\mathrm{i}(\alpha_m(p(s)-p(t))+\beta_m|q(s)-q(t)|)}\ , \tag{8}$$

where α_m, β_m are the propagation constants defined as

$$\alpha_m = \alpha + (2\pi m)/\Lambda\ , \quad \alpha = k_0\sqrt{\varepsilon^{(1)}}\sin\theta\ , \quad \alpha_m^2 + \beta_m^2 = k_0^2\varepsilon\ . \tag{9}$$

Required properties of obtained operators have been established e.g. in references [4, 5]. Note, that the singularity of logarithmic type is of key importance, because it enables to split the operators into compact ones with continuous kernel and the other with logarithmic singularity:

$$\Psi^{(j)}(s,t) = \Psi_0^{(j)}(s,t) + \frac{1}{2\pi} \ln \left| 2\sin\frac{s-t}{2} \right| + \Psi_r^{(j)}(s,t) \tag{10}$$

with regular part

$$\Psi_r^{(j)}(s,t) = \sum_{m\in Z\,, m\neq 0} \left\{ \Psi_m^{(j)}(s,t) - \frac{1}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}m(s-t)}}{2|m|} \right\} \ . \tag{11}$$

In the way of existence and uniqueness of presented model we refer to the paper [6], where the properties of boundary operators are discussed in detail.

4. Numerical implementation

To solve the system of boundary integral equations (6),(7) we use collocation method with $2N+1$ equidistant collocation points $s_j = \frac{2\pi j}{2N}$, $j = 0, \ldots, 2N$.

We seek for discrete solutions

$$I_\tau(s) = \sum_{k=0}^{2N} c_k \phi_k(s) \quad \text{and} \quad J_2(s) = \sum_{k=0}^{2N} d_k \phi_k(s) \tag{12}$$

with interpolation basis $\{\phi_k\}_{k=0}^{2N}$. Thus, the system of trigonometric polynomials or linear splines (piecewise linear functions) is the usual choice of basis functions. Here, we prefer the last ones with nodes identical with collocation points ($\phi_k(s_j) = \delta_{kj}$). Note that an using of frequently applied cubic splines did not yield better results in the example demonstrated in the Sect. 5.

We find advantageous to take the order N of boundary discretization equal to the order of diffraction modes truncation in the Green function (8), so that

$$\Psi^{(j)}(s,t) \approx \sum_{m=-N}^{N} \Psi_m^{(j)}(s,t) \ , \quad j = 1, 2 \ . \tag{13}$$

Since the integral operators in the solved system are splitted by (10), we evaluate numerically the compact operators with continuous kernels – the trapezodial rule with nodes in collocation points (i.e. $t_j = s_j$) gives sufficiently accurate results. The logarithmic-type singular operators can be evaluated analytically.

5. Numerical results

As an example, we consider the smooth sine boundary

$$S: \ x_3 = \frac{h}{2}\left(1 + \cos\frac{2\pi x_1}{\Lambda}\right), \ x_1 \in \langle 0, \Lambda \rangle \ , \quad \Lambda = 500 \text{ nm}, \ h = 50 \text{ nm}$$

between two regions with indices of refraction $n_1 = 1$ (air) and $n_2 = 1.5$ (glass), $n_j = \sqrt{\varepsilon^{(j)}}$. Incident beam of wavelength $\lambda = 632.8$ nm propagates under given

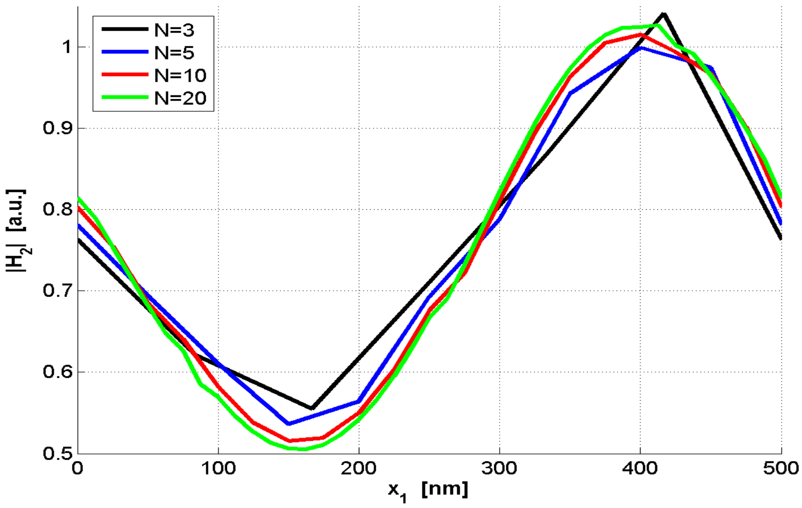

Figure 2: The convergence of used BEM algorithm (incidence angle $\theta = 40°$)

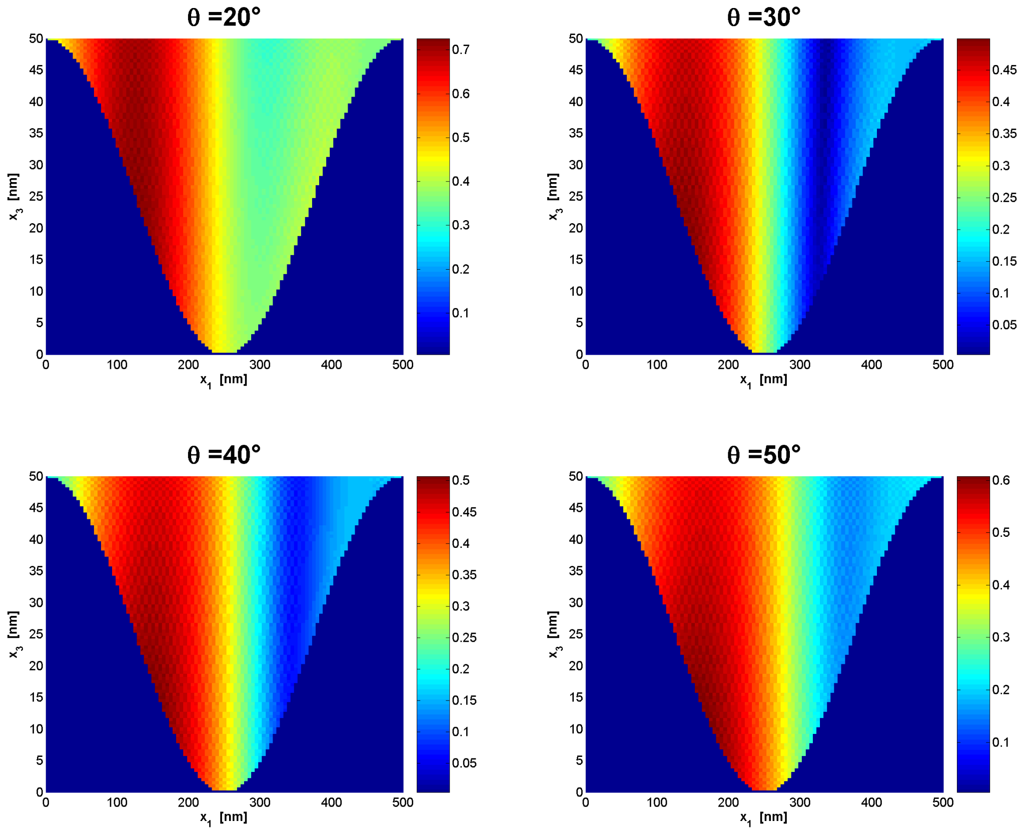

Figure 3: Reflected field $|H_2^{(1)}|$ for chosen incidence angle θ ($N = 50$).

angle of incidence θ. The Fig. 2 illustrates increasing accuracy of approximation with growing discretization order. We present here the absolute value of complex tangential component of the field $\boldsymbol{H}$ at one period of common boundary.

The reflected field $|H_2^{(1)}|$ is demonstrated at the Fig. 3 near to the boundary for several incidence angles. As the both materials are lossless, the field is nearly uniform in vertical direction.

6. Conclusion

The results obtained using presented BEM algorithm show possible applicability of the approach based on tangential fields to many problems, in which the detailed analysis of the diffracted optical field at an interface and/or in the near region is needed. We suppose to exploit this method in future to surface plasmon modelling.

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