Mathematical modelling of periodic diffraction problems in optics

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Abstract: The optical diffraction on a periodical interface belongs to relatively less exploited applications of the boundary integral equations method. This contribution presents a less frequent formulation of the diffraction problem based on vector tangential fields. There are discussed properties of obtained boundary operators with singular kernel and several problems related to a numerical implementation.

Keywords: optical diffraction, tangential fields, boundary elements method.

1 Introduction

The diffraction of an optical wave on a periodical interface between two media belongs to frequently solved problems, especially, when the grating period Λ is comparable with the wavelength λ of the incident beam. Among other, these phenomena are studied and exploited for nanostructured optical elements design. Naturally, the theoretical modelling is of great importance in such cases. In the last two decades, there were published numerous works treating of the optical diffraction in periodical structures - see [1] and references therein. One of the relatively new approaches is based on the Boundary Integral Equations (BIE). In this article, we present one special integral formulation of the boundary problem for the system of the Maxwell equations based on the tangential vector fields and propose a numerical implementation. Unlike the usually used rigorous coupled waves algorithm (RCWA) advantageous in the far fields analysis [1], 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 that is periodically modulated in the coordinate x_1 with the period Λ and uniform in the x_2 direction. The interface S with the normal vector $\boldsymbol{\nu}$ divides the space into two semi-infinite homogeneous domains

$$\Omega^{(1)} = \{(x_1, x_2, x_3) \in \mathbb{R}^3,\ x_3 > f(x_1)\}, \quad \Omega^{(2)} = \{(x_1, x_2, x_3) \in \mathbb{R}^3,\ x_3 < f(x_1)\}$$

with the 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 the materials are magnetically neutral), see Fig.1.

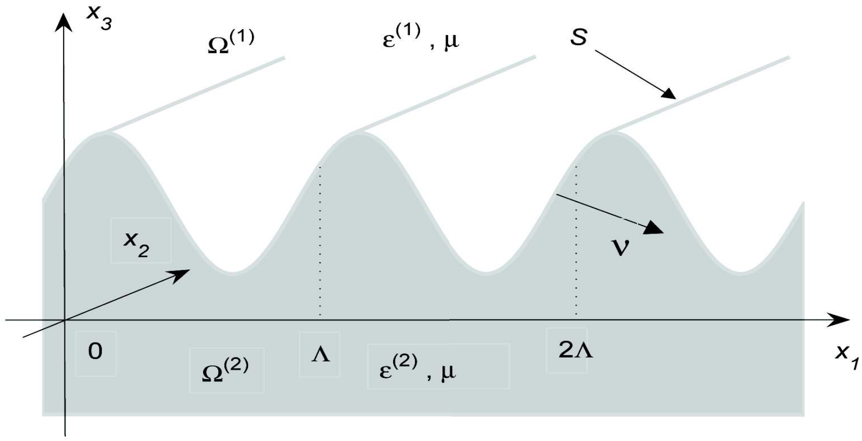

Figure 1: Semi-infinite domains with common periodical boundary

We aim to solve the optical diffraction problem for a monochromatic plane wave with the wavelength λ, i.e. with the wave number $k_0 = 2\pi/\lambda$, that is incoming from the domain $\Omega^{(1)}$ under the angle of incidence θ measured from the x_3 direction. We seek for the 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 (the subscript 0 denotes the incident field)

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

In the media without free charges, the vectors $\boldsymbol{E}^{(j)}$, $\boldsymbol{H}^{(j)}$, $j = 1, 2$ fulfil the Maxwell equations

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

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

and their tangential components are continuous on the boundary

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

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

In the following we solve the problem (2)–(4) for the transverse magnetic (TM) polarization of the incident wave for which $\boldsymbol{E}^{(j)} = (E_1^{(j)}, 0, E_3^{(j)})$, $\boldsymbol{H}^{(j)} = (0, H_2^{(j)}, 0)$. The Maxwell equations (2),(3) lead to the Helmholtz equations for the scalar components $H_2^{(j)}$,

$$\Delta H_2^{(j)} + k_0^2\varepsilon^{(j)}H_2^{(j)} = 0 \qquad \text{on} \quad \Omega^{(j)}\,, \quad j = 1, 2. \tag{5}$$

Denoting $\boldsymbol{x} = (x_1, x_3)$, $\boldsymbol{y} = (y_1, y_3)$, the periodical fundamental solution of the Helmholtz equation in $\Omega^{(j)}$ can be written as [7]

$$\Psi^{(j)}(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{2\mathrm{i}\Lambda}\sum_{m=-\infty}^{\infty}\Psi^{(j)}_m(\boldsymbol{x},\boldsymbol{y})\,, \qquad \Psi^{(j)}_m(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{\beta^{(j)}_m}\,\mathrm{e}^{\mathrm{i}(\alpha_m(x_1-y_1)+\beta^{(j)}_m|x_3-y_3|)}\,, \tag{6}$$

where α_m, $\beta^{(j)}_m$ are the propagation constants defined as

$$\alpha_m = \alpha + (2\pi m)/\Lambda\,, \quad \alpha = k_0\sqrt{\varepsilon^{(1)}}\sin\theta\,, \quad \alpha_m^2 + \left(\beta^{(j)}_m\right)^2 = k_0^2\varepsilon^{(j)}\,. \tag{7}$$

In further considerations we exploit the following property of the functions $\Psi^{(j)}$.

Theorem 1. *For both of the function $\Psi^{(j)}(\boldsymbol{x},\boldsymbol{y})$ defined by (6) and for an arbitrary but fixed $\boldsymbol{x} \in \mathbb{R}^2$ the difference*

$$\tilde{\Psi}^{(j)}(\boldsymbol{y}) = \Psi^{(j)}(\boldsymbol{x},\boldsymbol{y}) - \frac{1}{2\pi}\ln\frac{1}{\|\boldsymbol{x}-\boldsymbol{y}\|} \tag{8}$$

is continuous in $\mathbb{R}^2$.

The proof of this theorem was presented in [9].

3 Mathematical model

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

$$\boldsymbol{J} = \boldsymbol{\nu}\times\boldsymbol{E}^{(1)} = \boldsymbol{\nu}\times\boldsymbol{E}^{(2)}, \qquad \boldsymbol{I} = -\boldsymbol{\nu}\times\boldsymbol{H}^{(1)} = -\boldsymbol{\nu}\times\boldsymbol{H}^{(2)}\,, \tag{9}$$

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 $I_\tau = -H_2^{(1)} = -H_2^{(2)}$.

For the boundary points $\boldsymbol{\xi} = (\xi_1, \xi_3)$, $\boldsymbol{\eta} = (\eta_1, \eta_3)$ on the interface $S_\Lambda : \eta_3 = f(\eta_1)$, $\eta_1 \in \langle 0, \Lambda\rangle$ we obtain the following system of the boundary integral equations [4]

$$J_2(\boldsymbol{\xi}) = -J_0(\boldsymbol{\xi}) - \mathrm{i}k_0\boldsymbol{\tau}_\xi\cdot\int_{S_\Lambda} I_\tau\boldsymbol{\tau}_\eta(\Psi^{(1)}-\Psi^{(2)})\,dl_\eta$$

$$-\frac{1}{\mathrm{i}k_0}\boldsymbol{\tau}_\xi\cdot\int_{S_\Lambda}\frac{1}{\sigma}\frac{dI_\tau}{d\eta_1}\nabla_\eta\left(\frac{1}{\varepsilon^{(1)}}\Psi^{(1)} - \frac{1}{\varepsilon^{(2)}}\Psi^{(2)}\right)dl_\eta + \boldsymbol{\nu}_\xi\cdot\int_{S_\Lambda} J_2\nabla_\eta(\Psi^{(1)}-\Psi^{(2)})\,dl_\eta\,, \tag{10}$$

$$I_\tau(\boldsymbol{\xi}) = -I_0(\boldsymbol{\xi}) - \mathrm{i}k_0\int_{S_\Lambda} J_2(\varepsilon^{(1)}\Psi^{(1)} - \varepsilon^{(2)}\Psi^{(2)})\,dl_\eta + \int_{S_\Lambda} I_\tau\,\boldsymbol{\nu}_\eta\cdot\nabla_\eta\left(\Psi^{(1)}-\Psi^{(2)}\right)dl_\eta\,, \tag{11}$$

where the terms $J_0(\boldsymbol{\xi})$ and $I_0(\boldsymbol{\xi})$ represent the incident wave in $\Omega^{(1)}$.

To derive these equations it was necessary to study properties of the integral operators

$$\boldsymbol{\mathcal{V}}^{(j)}v(\boldsymbol{x}) = \int_{S_\Lambda} v(\boldsymbol{\eta})\Psi^{(j)}(\boldsymbol{x},\boldsymbol{\eta})\,dl_\eta\,, \qquad \boldsymbol{\mathcal{W}}^{(j)}v(\boldsymbol{x}) = \int_{S_\Lambda} v(\boldsymbol{\eta})\frac{\partial\Psi^{(j)}(\boldsymbol{x},\boldsymbol{\eta})}{\partial\boldsymbol{\nu}_\eta}\,dl_\eta\,,$$

$$\boldsymbol{\mathcal{L}}^{(j)}v(\boldsymbol{x}) = \int\limits_{S_\Lambda} v(\boldsymbol{\eta})\nabla_\eta \Psi^{(j)}(\boldsymbol{x},\boldsymbol{\eta})\ dl_\eta\ , \qquad j=1,2 \tag{12}$$

when the inner point $\boldsymbol{x}$ tends to the boundary point $\boldsymbol{\xi}$ in the normal direction.

Whereas the first and the second of them are the well-known single and double layer potentials, the third one is worth to mention.

Theorem 2. *If S is the smooth boundary of the domain $\Omega \subset \mathbb{R}^2$ with the unit outward normal $\boldsymbol{\nu}$ and $v \in \mathrm{C}(S)$, then*

$$\lim_{\boldsymbol{x}\to\boldsymbol{\xi}} \boldsymbol{\mathcal{L}}^{(j)}v(\boldsymbol{x}) = \int\limits_{S_\Lambda} v(\boldsymbol{\eta})\nabla_\eta \Psi^{(j)}(\boldsymbol{\xi},\boldsymbol{\eta})\ dl_\eta \pm \frac{1}{2}v(\boldsymbol{\xi})\boldsymbol{\nu}_\xi\ , \tag{13}$$

where $\boldsymbol{\xi} \in S$, minus holds for $\boldsymbol{x} \in \Omega$ and plus for $\boldsymbol{x} \in \mathbb{R}^2 \setminus \bar{\Omega}$.

This theorem is the vector generalization of the well-known statements for scalar integral operators, see e.g. [8] , Chapter 6.

To simplify calculations we introduce the parametrization

$$\boldsymbol{\pi} : \langle 0, 2\pi\rangle \to \mathbb{R}^2\ , \quad \boldsymbol{\pi}(t) = (p(t), q(t)) \tag{14}$$

of the curve $x_3 = f(x_1)$ having the unit normal vector $\boldsymbol{\nu}(t)$ with the norm $\nu(t) = \sqrt{p'(t)^2 + q'(t)^2}$.

The resulting system of the boundary integral equations for the scalar components I_τ and J_2 derived in [4] is of the following form:

$$\begin{aligned}
&-\mathrm{i}k_0\mu\boldsymbol{\tau}(s)\cdot\int\limits_0^{2\pi} I_\tau(t)\boldsymbol{\tau}(t)\left(\Psi^{(1)}(s,t) - \Psi^{(2)}(s,t)\right)\ \nu(t)\ dt \\
&- \frac{1}{\mathrm{i}k_0}\boldsymbol{\tau}(s)\cdot\int\limits_0^{2\pi} \rho I_\tau(t)\nabla_t\left[\frac{1}{\varepsilon^{(1)}}\Psi^{(1)}(s,t) - \frac{1}{\varepsilon^{(2)}}\Psi^{(2)}(s,t)\right]\nu(t)\ dt \\
&+ J_2(s) - \boldsymbol{\nu}(s)\cdot\int\limits_0^{2\pi} J_2(t)\nabla_t\left[\Psi^{(1)}(s,t) - \Psi^{(2)}(s,t)\right]\ \nu(t)\ dt\ =\ -J_{2,0}(s)\ ,
\end{aligned} \tag{15}$$

$$\begin{aligned}
&I_\tau(s) + \mathrm{i}k_0\int\limits_0^{2\pi} J_2(t)\left(\varepsilon^{(1)}\Psi^{(1)}(s,t) - \varepsilon^{(2)}\Psi^{(2)}(s,t)\right]\nu(t)\ dt \\
&-\int\limits_0^{2\pi} I_\tau(t)\boldsymbol{\nu}(t)\cdot\nabla_t\left[\Psi^{(1)}(s,t) - \Psi^{(2)}(s,t)\right]\ \nu(t)\ dt\ =\ -I_{\tau,0}(s)\ ,
\end{aligned} \tag{16}$$

where the functions $\Psi^{(j)}(s,t)$ in the operators kernels are the parametrized periodical fundamental solutions (6) of the Helmholtz equation (5) in $\Omega^{(j)}$.

Note, that the singularity of the logarithmic type is of the key importance, because it enables to split the operators into the compact ones with the continuous kernels and the other with the logarithmic singularity:

$$\Psi^{(j)}(s,t) = \Psi_r^{(j)}(s,t) + \psi(s,t) \tag{17}$$

with the regular part

$$\Psi_r^{(j)}(s,t) = \Psi_0^{(j)}(s,t) + \sum_{\substack{m \in \mathbb{Z} \\ m \neq 0}} \left(\Psi_m^{(j)}(s,t) - \frac{1}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}m(s-t)}}{2|m|} \right) , \tag{18}$$

and, the sigular one

$$\psi(s,t) = \frac{1}{2\pi} \ln \left| 2 \sin \frac{s-t}{2} \right| = \frac{1}{2\pi} \sum_{\substack{m \in \mathbb{Z} \\ m \neq 0}} \frac{\mathrm{e}^{-\mathrm{i}m(s-t)}}{2|m|} . \tag{19}$$

4 Numerical implementation

To solve the system of the boundary integral equations (15),(16) we use the collocation method with $2N+1$ equidistant collocation points $s_j = \frac{2\pi j}{2N}$, $j = 0, \dots, 2N$.

We seek for the discrete solutions

$$I_\tau(s) = \sum_{k=0}^{2N} c_k \phi_k(s) , \qquad J_2(s) = \sum_{k=0}^{2N} d_k \phi_k(s) \tag{20}$$

with an interpolation basis $\{\phi_k\}_{k=0}^{2N}$. The choice of the best basis functions system appears to be very important. The system of trigonometric polynomials, linear splines (piecewise linear functions) or cubic splines are the usual choices of basis functions. After experiments with mentioned basis functions we prefer the system of trigonometric polynomials with the nodes identical with the collocation points ($\phi_k(s_j) = \delta_{kj}$), i.e.

$$\phi_k(t) = \frac{1}{2N+1} \sum_{\ell=-N}^{N} \mathrm{e}^{-\frac{2\pi \mathrm{i} \ell k}{2N+1}} \mathrm{e}^{\mathrm{i}\ell t} , \qquad k = 0, 1, 2 \dots, 2N . \tag{21}$$

Furthermore, we find advantageous to take the order N of the boundary discretization equal to the order of the diffraction modes truncation in the Green function (6), so that

$$\Psi^{(j)}(s,t) \approx \frac{1}{2\mathrm{i}\Lambda} \sum_{m=-N}^{N} \Psi_m^{(j)}(s,t) , \quad j = 1, 2 . \tag{22}$$

Since the integral operators in the solved system are splitted by (17), we evaluate numerically the compact operators with the continuous kernels – the trapezoidal rule with the nodes in the collocation points (i.e. $t_j = s_j$) gives sufficiently accurate results. The logarithmic-type singular operators can be evaluated analytically [6].

5 Numerical results

As an example, we consider the smooth sine boundary

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

between two regions with the indices of refraction $n_1 = 1$ (air) and $n_2 = 1.5$ (glass), $n_j = \sqrt{\varepsilon^{(j)}}$. The incident beam of the wavelength $\lambda = 632.8$ nm propagates under the given angle of incidence θ. The Fig. 2 illustrates the increasing accuracy of approximation with growing discretization order. As analytical solution of the problem is not available we compare numerical solutions for various values of N.

Obtained results are demonstrated by the absolute value of the complex tangential component of the field $\boldsymbol{H}$ at one period of the common boundary. The low discretization orders enable more perspicuous view because the data calculated at collocation points are nearly equal (in the graph) roughly for $N \geq 30$. Note that we aimed to functionality verification of presented model as well as of proposed algorithm.

The distribution of reflected field $|H_2^{(1)}|$ in the superstrate is demonstrated at the Fig. 3 near to the boundary for several incidence angles.

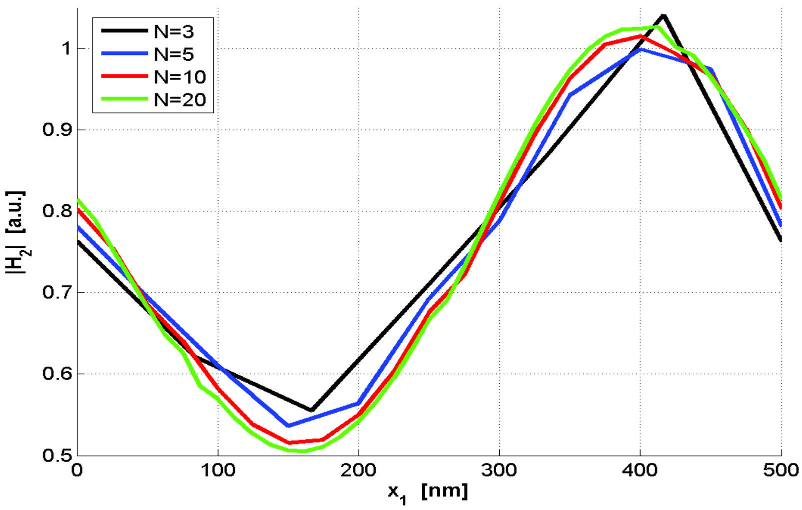

Figure 2: The convergence of the used BEM algorithm (incidence angle $\theta = 40°$).

Conclusion

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

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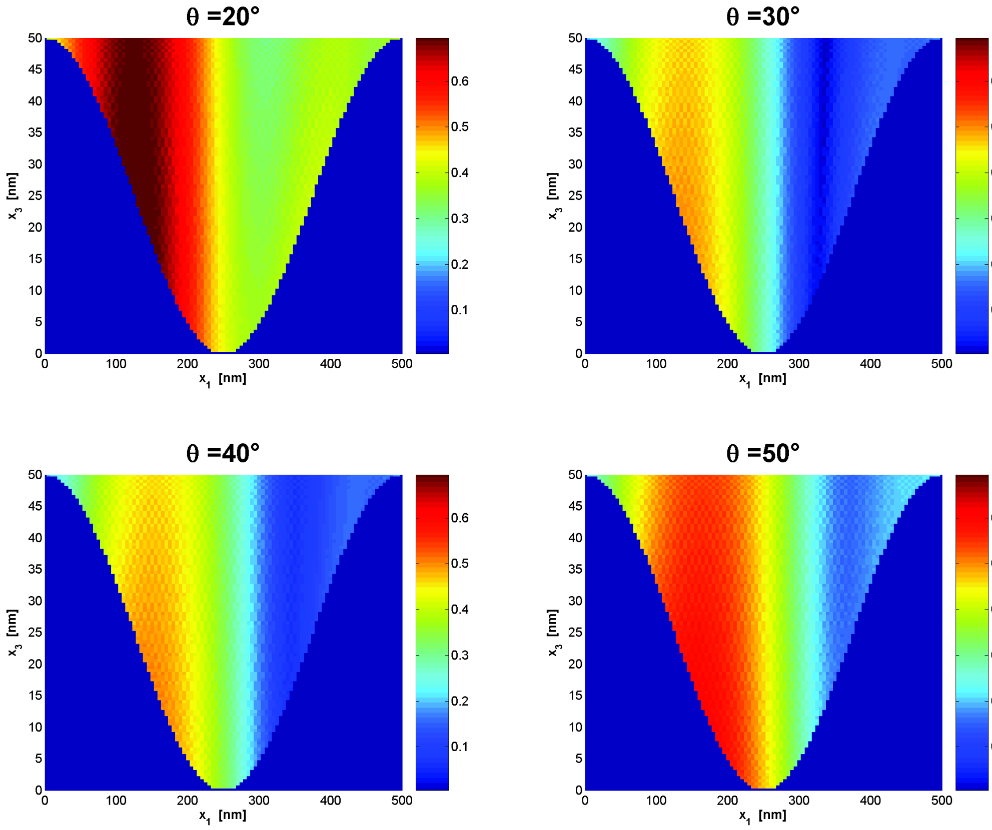

Figure 3: Reflected field $|H_2^{(1)}|$ for chosen incidence angle θ ($N = 50$).

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Matematické modelování periodických difrakčních úloh v optice

Abstrakt: Optická difrakce na periodckém rozhraní patří k relativně málo prouzkoumaným aplikacím metody hraničních integrálních rovnic. V příspěvku je popsána méně obvyklá formulace difrakční úlohy pomocí vektorových tečných polí. Dále jsou diskutovány vlastnosti odvozených integrálních operátorů se singulárním jádrem stejně jako některé problémy související s numerickou implementací.

Klíčová slova: optická difrakce, tečná pole, metoda hraničních prvků.