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TANGENTIAL FIELDS IN OPTICAL DIFFRACTION PROBLEMS

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Abstract

Optical diffraction for periodical interface belongs to relatively fewer exploited application of boundary integral equations method. Our contribution presents the formulation of diffraction problem based on vector tangential fields, for which the periodical Green function of Helmholtz equation is of key importance. There are discussed properties of obtained boundary operators with singular kernel and a numerical implementation is proposed.

1. Introduction

Development of optical micro- and nanostructures with periodical ordering takes important place in many branches of integrated optics or nano-technology. The geometrical and material optimization of the sensors, switching elements and many other devices depends on the accurate control of their parameters. Besides less or more complicated experiments, theoretical studies are carried out including mathematical models of electromagnetic wave interaction with geometrically or material-wise modulated media. Generally, these models consist in the solving of Maxwell equations with appropriate boundary conditions. Diffraction of optical wave on an interface between two different media is one of frequently solved problem, where the rigorous choice of theoretical approach plays important role.

In the last two decades, there were published numerous works treating of optical diffraction in periodical structures - see [1] and references therein. One of relatively new approaches is based on Boundary Integral Equations (BIE), theoretical background of which is referred e.g. in [2]. In this article, we aim to show the especial integral formulation of the boundary problem for system of Maxwell equations. To this purpose, we introduce tangential vector fields and study the properties of derived integral operators.

2. Formulation of the problem

Let's denote $\boldsymbol{X} = (x_1, x_2, x_3) \in \mathbb{R}^3$ and further $S : x_3 = f(x_1)$ a surface which we consider to be smooth with normal vector $\boldsymbol{\nu}$ and periodically modulated in coordinate x_1 with period Λ and uniform in the x_2 direction, see Fig.1.

The interface S divides the space into two semi-infinite homogeneous regions $\Omega^{(1)} = \{\boldsymbol{X} \in \mathbb{R}^3,\ x_3 > f(x_1)\}$, $\Omega^{(2)} = \{\boldsymbol{X} \in \mathbb{R}^3,\ x_3 < f(x_1)\}$ 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, relative permeabilities $\mu^{(1)} = \mu^{(2)} = 1$ (materials are magnetically neutral).

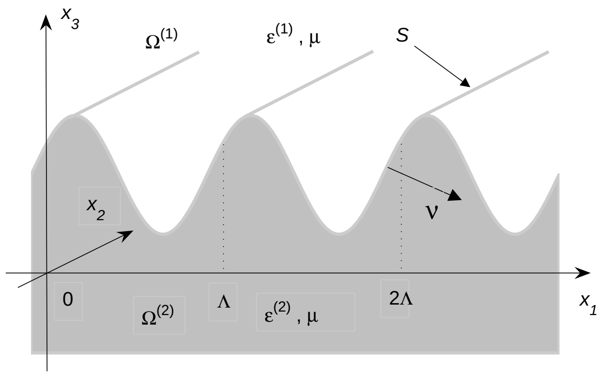

Figure 1: Structure of regions with common periodical boundary

We aim to solve optical diffraction problem for monochromatic plane wave with wavelength λ, i.e. with wave number $k_0 = 2\pi/\lambda$ that is incoming from $\Omega^{(1)}$ under the 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 $\boldsymbol{E}(\boldsymbol{X})\mathrm{e}^{-\mathrm{i}\omega t}$, $\boldsymbol{H}(\boldsymbol{X})\mathrm{e}^{-\mathrm{i}\omega t}$, where $\omega = c/\lambda$ and c represents the light velocity in the free space. Especially, we suppose the TM polarization of the incident wave, for which $\boldsymbol{E}^{(j)} = (E_1^{(j)},\ 0,\ E_3^{(j)})$, $\boldsymbol{H}^{(j)} = (0,\ H_2^{(j)},\ 0)$. Therefore, the Maxwell problem leads to the Helmholtz equations for the scalar components $H_2^{(j)}(\boldsymbol{X})$,

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

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

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

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

The incident field at zero diffraction order is characterized by the relation

$$\boldsymbol{H}_0^{(1-)} = \mathrm{e}^{-\mathrm{i}\omega t} \mathrm{e}^{\mathrm{i}(\alpha x_1 + \beta_0^{(1-)} x_3)} \boldsymbol{e}_2\ , \qquad \boldsymbol{e}_2 = (0, 1, 0)\ , \tag{3}$$

where $\alpha = k_0 \sqrt{\varepsilon^{(1)}} \sin\theta$ and $\beta_0^{(1-)}$ is the propagation constant defined below.

This optical beam is diffracted into reflected wave in $\Omega^{(1)}$ and transmitted one in $\Omega^{(2)}$, which are represented by countable sets of modes with wave vectors

$$\boldsymbol{k}_m^{(j\pm)} = (\alpha_m, 0, \beta_m^{(j\pm)}) \,, \quad \alpha_m = \alpha + 2\pi m/\Lambda, \quad (\beta_m^{(j\pm)})^2 = k_0^2 \varepsilon^{(j)} - \alpha_m^2 \,, \quad m \in \mathbb{Z}. \tag{4}$$

The sign in superscript denotes propagation direction with respect to the x_3 axis orientation: "+" means the forward wave (reflected), "–" the backward one (incident, transmitted). For example $\beta_m^{(j-)} < 0$, if $\beta_m^{(j-)} \in \mathbb{R}$, or, $\mathrm{Im}\,(\beta_m^{(j-)}) < 0$ otherwise with respect to radiation conditions and chosen convention $\mathrm{e}^{-\mathrm{i}\omega t}$ – see (3). In what follows stay 1 for 1+ and 2 for 2−.

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 [4]

$$\Psi^{(j)}(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2\mathrm{i}\Lambda} \sum_{m=-\infty}^{\infty} \Psi_m^{(j)}(\boldsymbol{x}, \boldsymbol{y}) \,, \qquad \Psi_m^{(j)}(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{\beta_m^{(j)}} \, \mathrm{e}^{\mathrm{i}(\alpha_m(x_1 - y_1) + \beta_m^{(j)}|x_3 - y_3|)} \,. \tag{5}$$

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

Theorem 1. *For both of the function $\Psi^{(j)}(\boldsymbol{x}, \boldsymbol{y})$ defined by (5) the difference (6) is continuous in $\mathbb{R}^2$.*

$$\Psi^{(j)}(\boldsymbol{x}, \boldsymbol{y}) - \frac{1}{2\pi} \ln \frac{1}{\|\boldsymbol{x} - \boldsymbol{y}\|} \tag{6}$$

3. Boundary integral equations

The aim of this section is to formulate boundary integral equations for tangential fields

$$\boldsymbol{J} = \boldsymbol{\nu} \times \boldsymbol{E}^{(1)} = \boldsymbol{\nu} \times \boldsymbol{E}^{(2)}, \qquad \boldsymbol{I} = -\boldsymbol{\nu} \times \boldsymbol{H}^{(1)} = -\boldsymbol{\nu} \times \boldsymbol{H}^{(2)} \,, \tag{7}$$

where $\boldsymbol{\nu} = (f', 0, -1)/\sigma$ with $\sigma = \sqrt{1 + f'^2}$ is an unit normal vector of the reduced boundary $S : \ x_3 = f(x_1)$ oriented as shown in Fig.1. Similarly, $\boldsymbol{\tau} = (1, 0, f')/\sigma$ represents an unit tangential vector of S.

Thus, 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, $\boldsymbol{I} = \sigma I_1 \boldsymbol{\tau} = I_\tau \boldsymbol{\tau}$, where $I_\tau = \sigma I_1 = -H_2^{(1)} = -H_2^{(2)}$.

For boundary points $\boldsymbol{\xi} = (\xi_1, \xi_3)$, $\boldsymbol{\eta} = (\eta_1, \eta_3)$ on the interface $S : \eta_3 = f(\eta_1)$, $\eta_1 \in \langle 0, \Lambda \rangle$ we obtain following system of boundary integral equations [5]

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

$$- \frac{1}{\mathrm{i}k_0} \boldsymbol{\tau}_\xi \cdot \int_S \frac{1}{\sigma} \frac{dI_\tau}{d\eta_1} \nabla_\eta \left(\frac{1}{\varepsilon^{(1)}} \Psi^{(1)} - \frac{1}{\varepsilon^{(2)}} \Psi^{(2)} \right) dl_\eta \, + \boldsymbol{\nu}_\xi \cdot \int_S J_2 \nabla_\eta (\Psi^{(1)} - \Psi^{(2)}) \, dl_\eta \,, \tag{8}$$

$$I_\tau(\boldsymbol{\xi}) = -I_0(\boldsymbol{\xi}) - \mathrm{i}k_0 \int_S J_2 (\varepsilon^{(1)} \Psi^{(1)} - \varepsilon^{(2)} \Psi^{(2)}) \, dl_\eta + \int_S I_\tau \, \boldsymbol{\nu}_\eta \cdot \nabla_\eta \left(\Psi^{(1)} - \Psi^{(2)} \right) dl_\eta \,, \tag{9}$$

where

$$J_0(\boldsymbol{\xi}) = -\boldsymbol{e}_2\cdot(\boldsymbol{\nu}_\xi\times\boldsymbol{E}_0^{(1-)}) = \boldsymbol{\tau}_\xi\cdot\boldsymbol{E}_0^{(1-)} \,, \qquad I_0(\boldsymbol{\xi}) = \boldsymbol{\tau}_\xi\cdot(\boldsymbol{\nu}_\xi\times\boldsymbol{H}_0^{(1-)}) = -H_{0,2}^{(1-)} \,, \tag{10}$$

thereby $\boldsymbol{E}_0^{(1-)}$, $\boldsymbol{H}_0^{(1-)}$ represent the incident wave in $\Omega^{(1)}$.

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

$$\int\limits_S g(\boldsymbol{\eta})\,\psi(\boldsymbol{x},\boldsymbol{\eta})\,dl_\eta \,, \qquad \int\limits_S g(\boldsymbol{\eta})\,\frac{\partial\psi(\boldsymbol{x},\boldsymbol{\eta})}{\partial\boldsymbol{\nu}}\,dl_\eta \,, \qquad \int\limits_S g(\boldsymbol{\eta})\,\nabla_\eta\psi(\boldsymbol{x},\boldsymbol{\eta})\,dl_\eta \tag{11}$$

with the kernel

$$\psi(\boldsymbol{x},\boldsymbol{\eta}) = \frac{1}{2\pi}\ln\frac{1}{\|\,\boldsymbol{x}-\boldsymbol{\eta}\,\|} \tag{12}$$

when crossing from the inner point $\boldsymbol{x}$ to the boundary point $\boldsymbol{\xi}$ in the normal direction (the superscript (j) is omitted for simplicity).

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

Theorem 2. *Let $\psi(\boldsymbol{x},\boldsymbol{\eta})$ is the function (12) and S is smooth boundary of the domain $\Omega\subset\mathbb{R}^2$ with unit outward normal $\boldsymbol{\nu}$. If $g\in\mathrm{C}(S)$, then*

$$\lim_{\boldsymbol{x}\to\boldsymbol{\xi}}\int\limits_S g(\boldsymbol{\eta})\,\nabla_\eta\psi(\boldsymbol{x},\boldsymbol{\eta})\,dl_\eta = \int\limits_S g(\boldsymbol{\eta})\,\nabla_\eta\psi(\boldsymbol{\xi},\boldsymbol{\eta})\,dl_\eta \pm \frac{1}{2}g(\boldsymbol{\xi})\boldsymbol{\nu}(\boldsymbol{\xi}) \,, \tag{13}$$

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

4. Operator form

Let $\boldsymbol{\pi}:\langle 0,2\pi\rangle\to\mathbb{R}^2$, $\boldsymbol{\pi}(t)=(p(t),q(t))$ be a parametrization of the boundary S. For the boundary points we have $\boldsymbol{\xi}=\boldsymbol{\pi}(s)$, $\boldsymbol{\eta}=\boldsymbol{\pi}(t)$, $s,t\in\langle 0,2\pi\rangle$ with corresponding unit normal vector $\boldsymbol{\nu}(t)=(\nu_1(t),\,\nu_3(t))=(q'(t),\,-p'(t))/\nu(t)$ and unit tangential vector $\boldsymbol{\tau}(t)=(p'(t),\,q'(t))/\nu(t)$, where $\nu(t)=\sqrt{p'(t)^2+q'(t)^2}$.

In the integral operators kernels the fundamental solution (5) of the Helmoltz equation takes place, hence the system (8), (9) can be written in operator form

$$\begin{bmatrix} \mathcal{V}_1+\mathcal{V}_2 & \mathcal{I}-\mathcal{V}_3 \\ \mathcal{I}-\mathcal{V}_4 & \mathcal{V}_5 \end{bmatrix}\begin{bmatrix} I_\tau \\ J_2 \end{bmatrix} = \begin{bmatrix} -J_{2,0} \\ -I_{\tau,0} \end{bmatrix} \,, \tag{14}$$

where $\mathcal{I}$ is the identity operator,

$$\mathcal{V}_1(I_\tau) = \frac{k_0}{2\Lambda\nu(s)}\int\limits_0^{2\pi} I_\tau(t)g_1(s,t)\sum_{m\in\mathbb{Z}}\left[\Psi_m^{(1)}(s,t)-\Psi_m^{(2)}(s,t)\right]dt \,, \tag{15}$$

$$\mathcal{V}_2(I_\tau) = \frac{\mathrm{i}}{2k_0\Lambda\nu(s)}\int\limits_0^{2\pi} I'_\tau(t)\sum_{m\in\mathbb{Z}}\left[\frac{g_{2,m}^{(1)}(s,t)}{\varepsilon^{(1)}}\Psi_m^{(1)}(s,t)-\frac{g_{2,m}^{(2)}(s,t)}{\varepsilon^{(2)}}\Psi_m^{(2)}(s,t)\right]dt \,, \tag{16}$$

$$\mathcal{V}_3(J_2) = \frac{1}{2\Lambda\nu(s)} \int_0^{2\pi} J_2(t) \sum_{m\in\mathbb{Z}} \left[g_{3,m}^{(1)}(s,t)\Psi_m^{(1)}(s,t) - g_{3,m}^{(2)}(s,t)\Psi_m^{(2)}(s,t) \right] \nu(t)\, dt \ , \quad (17)$$

$$\mathcal{V}_4(I_\tau) = \frac{1}{2\Lambda} \int_0^{2\pi} I_\tau(t) \sum_{m\in\mathbb{Z}} \left[g_{4,m}^{(1)}(s,t)\Psi_m^{(1)}(s,t) - g_{4,m}^{(2)}(s,t)\Psi_m^{(2)}(s,t) \right] dt \ , \quad (18)$$

$$\mathcal{V}_5(J_2) = \frac{k_0}{2\Lambda} \int_0^{2\pi} J_2(t) \sum_{m\in\mathbb{Z}} \left[\varepsilon^{(1)}\Psi_m^{(1)}(s,t) - \varepsilon^{(2)}\Psi_m^{(2)}(s,t) \right] \nu(t)\, dt \quad (19)$$

with

$$g_1(s,t) = \nu(s)\nu(t)\boldsymbol{\tau}(s)\cdot\boldsymbol{\tau}(t) \ , \qquad g_{2,m}^{(j)}(s,t) = \nu(s)\boldsymbol{\tau}(s)\cdot\boldsymbol{\kappa}_m^{(j)}(s,t) \ ,$$

$$g_{3,m}^{(j)}(s,t) = \nu(s)\boldsymbol{\nu}(s)\cdot\boldsymbol{\kappa}_m^{(j)}(s,t) \ , \qquad g_{4,m}^{(j)}(s,t) = \nu(t)\boldsymbol{\nu}(t)\cdot\boldsymbol{\kappa}_m^{(j)}(s,t) \ ,$$

$$\boldsymbol{\kappa}_m^{(j)}(s,t) = \Big(\alpha_m,\ \mathrm{sgn}(q(s)-q(t))\beta_m^{(j)}\Big) \quad (20)$$

The right-hand terms of (14) are obtained by parametrization of incident fields (10).

5. Properties of boundary integral operators

Now we need to discuss properties of integral operators kernels, which are written as differences $c_1\Psi^{(1)}(s,t) - c_2\Psi^{(2)}(s,t)$, or their gradients, where c_1, c_2 are generally complex constants. Because for $s \neq t$ this expression represents a continuous function, it suffices to analyse the singular case for $s = t$.

Theorem 3. *Let $c_1, c_2 \in \mathbb{C}$. Then for $s = t$ the functions*

$$c_1\Psi^{(1)}(s,t) - c_2\Psi^{(2)}(s,t) \ , \qquad \nabla_t\Big(c_1\Psi^{(1)}(s,t) - c_2\Psi^{(2)}(s,t)\Big) \quad (21)$$

are continuous for $c_1 = c_2$ and these have singularity of logarithmic type for $c_1 \neq c_2$.

The particular manner how to evaluate singular integrals depends on the choice of numerical method. The following theorems show one of possible methods - see [6], where also the proofs can be found ($\mathbb{Z}^* = \mathbb{Z} - \{0\}$).

Theorem 4. *Let $\boldsymbol{\pi} : \langle 0, 2\pi\rangle \to \mathbb{R}^2$ is a parametrization that satisfies*

$$p(0) = 0, \quad p(2\pi) = \Lambda, \quad q(0) = q(2\pi), \quad p(t+2\pi) = p(t) + \Lambda, \quad q(t+2\pi) = q(t).$$

Then

$$\ln\|\boldsymbol{\pi}(s) - \boldsymbol{\pi}(t)\| = \ln|2\sin\frac{s-t}{2}| = -\sum_{m\in\mathbb{Z}^*} \frac{\mathrm{e}^{-\mathrm{i}m(s-t)}}{2|m|} \ . \quad (22)$$

Theorem 5. *The series (23) is absolutely convergent.*

$$\sum_{m\in\mathbb{Z}^*} \left\{ \Psi_m^{(j)}(s,t) - \frac{1}{2\pi}\frac{\mathrm{e}^{-\mathrm{i}m(s-t)}}{2|m|} \right\} \quad (23)$$

These properties together with Theorem 1 allow us to split the fundamental solution as

$$\Psi^{(j)}(s,t) = \Psi_r^{(j)}(s,t) + \psi(s,t), \tag{24}$$

where

$$\Psi_r^{(j)}(s,t) = \Psi_0^{(j)}(s,t) + \sum_{m\in\mathbb{Z}^*} \left\{ \Psi_m^{(j)}(s,t) - \frac{1}{2\pi}\frac{\mathrm{e}^{-\mathrm{i}m(s-t)}}{2|m|} \right\} , \tag{25}$$

$$\psi(s,t) = \frac{1}{2\pi} \ln |2 \sin \frac{s-t}{2}| \, . \tag{26}$$

In numerical implementations we work separately with regular integral kernels and with singular integrals which can be evaluated analytically.

6. Conclusion

The presented formulation of diffraction problem represents appropriate background of numerical solution by the Boundary Elements Method (BEM). Specific problem to discuss is the choice of basis functions; trigonometric polynomials can be used [3], for instance. For further work we prefer piecewise linear boundary elements.

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References

[1] Bao, G., Cowsar, L. and Masters, W.: *Mathematical modeling in optical science.* SIAM, Philadelphia, 2001.

[2] Nedelec, J. C., Starling, F.: Integral equation methods in a quasi-periodic diffraction problem for the time-harmonic Maxwell's equations. SIAM, J. Math. Anal. **22** (1991), 1679–1701.

[3] Kleemann, B. H., Mitreiter, A. and Wyrowski, F.: Integral equation method with parametrization of grating profile. Theory and Experiments. J. Mod. Opt. **43** (7) (1996), 1323–1349.

[4] Linton, C. M.: The Green's function for the two-dimensional Helmholtz equation in periodic domains. J. Eng. Math. **33** (1998), 377–402.

[5] Dobson, D. C. and Cox, J. A.: An integral equation method for biperiodic diffraction structures. In: *Proc. of SPIE*, Vol. 1545, pp. 106-113, 1991.

[6] Žídek, A., Vlček, J., and Krček, J.: Solution of diffraction problems by boundary integral equations. In: *Proc. of 11th International Conference APLIMAT 2012, Febr. 7-9, 2012, Bratislava, Slovak Republic*, publ. by Faculty of Mechanical Engineering, Slovak University of Technology, Bratislava 2012, 221–229.