Coupling of FEM and Fourier-mode expansion for the scattering by perfectly conducting gratings

Guanghui Hu[1] and Andreas Rathsfeld[1]

Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany
Guanghui.Hu@wias-berlin.de, Andreas.Rathsfeld@wias-berlin.de

Summary. To simulate the diffraction of planar waves by periodic surface structures, Huber et al. [2] have proposed to combine a Fourier-mode expansion over the half space with a finite element approximation of the electric field close to the surface. We analyze a slight modification of this mortar method and discuss an application to an inverse problem in scatterometry. In particular, we present a shape derivative formula for the derivative with respect to geometry parameters.

1 Boundary Value Problem for Gratings

Suppose the space $\mathbb{R}^3$ is filled with two materials separated by an interface Γ, which is a small perturbation of the $x_3 = 0$ plane and which is 2π-periodic in the x_l directions for $l = 1,2$. Furthermore, suppose the material below Γ is perfectly conducting and that in the domain Ω above Γ is lossless. To compute the diffraction of a time-harmonic plane wave $\mathbf{E}^{\text{in}}$ incident on Γ from above, we have to solve

$$\nabla\times\nabla\times\mathbf{E} - k^2\mathbf{E} = 0 \qquad \text{on } \Omega, \tag{1}$$

$$\nu\times\mathbf{E} = 0 \qquad \text{on } \Gamma, \tag{2}$$

$$\mathbf{E}(\mathbf{x}) - \mathbf{E}^{\text{in}}(\mathbf{x}) = \sum_{n\in\mathbb{Z}^2} \mathbf{E}_n e^{\mathrm{i}\mathbf{v}_n\cdot\mathbf{x}} \quad \text{for } x_3 > b. \tag{3}$$

Here ν is the unit normal vector on Γ, b is a fixed x_3 coordinate greater than those of Γ, and $\mathbf{v}_n$ are the vectors of the upward radiating (plane wave and evanescent) Fourier modes.

2 Mortar Method

It is natural, to approximate $\mathbf{E}$ for $x_3 > b$ by $\mathbf{E}^{\text{in}}$ plus a Fourier-mode expansion $\mathbf{E}^+$ like that on the right-hand side of (3). In the domain between the artificial surface $\Gamma_b' := \{\mathbf{x}\in\mathbb{R}^3 : \ x_3 = b\}$ and Γ, an FE approximation with quasi-periodic edge elements is possible. Clearly, the FEM can be restricted to the cell of periodicity $\Omega_b := \{\mathbf{x}\in\Omega : \ x_3 < b, \ 0\le x_l \le 2\pi, l = 1,2\}$ and the mode expansion to the bounded upper domain $\Omega_b^+ := \{\mathbf{x}\in\mathbb{R}^3 : \ b\le x_3 \le b+1, \ 0\le x_l\le 2\pi, l=1,2\}$ or even to $\Gamma_b := \{\mathbf{x}\in\Gamma_b : \ 0\le x_l\le 2\pi, l=1,2\}$. Following the idea of Huber et al. [2], we couple the two approximations by a mortar technique. More precisely, we replace the boundary value problem by the following variational equation

$$a\Big((\mathbf{E},\mathbf{E}^+),(\mathbf{V},\mathbf{V}^+)\Big) = -a\Big((0,\mathbf{E}^{\text{in}}),(\mathbf{V},\mathbf{V}^+)\Big),$$

required for all $\mathbf{V}\in H(\text{curl},\Omega_b)$ and $\mathbf{V}^+\in H(\text{curl},\Omega_b^+)$, where the sesquilinear form a is defined as the sum of

$$\int_{\Omega_b}\{\nabla\times\mathbf{E}\cdot\nabla\times\overline{\mathbf{V}} + \mathbf{E}\cdot\overline{\mathbf{V}}\}$$
$$-\int_{\Gamma_b}\nabla\times\mathbf{E}^+\cdot\nu\times\overline{\mathbf{V}} + \int_{\Gamma_b}\nu\times(\mathbf{E}-\mathbf{E}^+)\cdot\nabla\times\overline{\mathbf{V}}^+$$

plus a certain sesquilinear form corresponding to a finite rank operator. We get (cf. [4])

Theorem 1. *The operator corresponding to the variational equation is Fredholm of index zero. The solution of the sesquilinear form is equivalent to the boundary value problem (1)-(3).*

Unfortunately, there are examples of gratings such that the solution of the boundary value problem is non-unique. However, the scattered (non-evanescent) plane wave modes are always unique (cf. [4]).

Using Theorem 1, the justification of a coupled Fourier-mode-FE method should be possible (compare [1]). Simply, the E and V are to be replaced by edge finite elements and the E^+ and V^+ by truncated Fourier-mode expansions. Of course, the variational form is to be modified slightly. Frequently, in practical computations, only a small number of the Rayleigh coefficients $\mathbf{E}_n$ (cf. (3)) differ essentially from zero. Thus only a few terms in the Fourier-mode expansions are needed.

3 Inverse Problem in Scatterometry

To evaluation the fabrication process of lithographic masks, simple periodic or biperiodic structures must be measured. Using scatterometric techniques, the corresponding part of the surface is illuminated by a ray of laser light. The efficiencies (intensities) of the scattered plane wave modes are measured. Finally, a biperiodic surface structure is sought, the efficiencies of which coincide with the measured data, i.e., an inverse problem is to be solved.

Though this problem is severely ill-posed, we are looking for small deviations of the surface structure from the fabrication standard, i.e., for surfaces described by a small number of geometry parameters. The reduction to these parameters is like a regularization of the inverse problem, and the determination of the parameters with high accuracy should be possible. Note that we do not discuss the effect of modeling errors or random perturbations.

The numerical solution of the inverse problem can be realized minimizing a functional $\mathscr{F}(\mathbf{E})$, where $\mathscr{F}(\mathbf{E})$ is some measure for the deviation of the measured efficiencies and the efficiencies of the scattered field $\mathbf{E}$ corresponding to a grating structure with given parameters. Although the gratings are not perfectly conducting anymore, the scattered field $\mathbf{E}$ can be computed by an FEM similar to that of Sect. 3. Optimization schemes like the Gauß-Newton method or the Levenberg-Marquardt algorithm can be applied. However these local optimization routines require the Jacobian of the operator, mapping the set of geometry parameters to the vector of efficiency values. In other words, we need formulas for the derivatives of $\mathbf{E}$ with respect to the geometry parameters.

4 Shape Derivative

In the case of periodic gratings, i.e., for the two-dimensional Helmholtz equation, the classical methods for shape calculus apply. Unfortunately, for the time-harmonic Maxwell equation (1), an analogous procedure is not possible. Indeed, the underlying energy space $H(\mathrm{curl},\Omega_b)$ is not invariant under the transformations corresponding to a change of the geometry parameter.

On the other hand, in our optical applications the magnetic permeability μ is constant. For this case, it is known that the magnetic vector H is piecewise in the Sobolev space H^1. Using this fact, the shape calculus applies to the derivative of H. Switching now from the magnetic vector to the electric field, we can derive a formula for the derivative w.r.t. a geometry parameter p (cf. [3])

$$\partial_p \mathscr{F}(E) = \mathrm{Re}\ a_1(E, E_{\mathrm{adj}}). \tag{4}$$

Here $a_1(E,F)$ is a special sesquilinear form depending on the L^2 functions E, F, E, $\nabla \times E$, and $\nabla \times F$. The field E in (4) is the actual electric solution of the time-harmonic Maxwell equation. The field E_{adj} is the solution of the adjoint equation. In other words, E_{adj} is the solution of an equation with the adjoint FEM matrix and with a right-hand side depending on the functional $\mathscr{F}$.

In a numerical experiment, we have implemented a version of (4) discretized by FEM. The numerical algorithm for the inverse problem mentioned in Sect. 3, including the shape derivative based on (4), converges well.

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References

1. P. Monk. *Finite Element Method for Maxwell's Equations*. Oxford, Oxford Univ Press, 2003.
2. M. Huber, J. Schoeberl, A. Sinwel, and S. Zaglmayr. Simulation of diffraction in periodic media with a coupled finite element and plane wave approach. *SIAM J. Math. Anal.*, 43:1205–1231, 2009.
3. A. Rathsfeld. Shape derivatives for the scattering by biperiodic gratings. WIAS Preprint No. 1640, Berlin, 2011.
4. G. Hu and A. Rathsfeld. Scattering of time-harmonic electromagnetic plane waves by perfectly conducting diffraction gratings. WIAS Preprint No. 1694, Berlin, 2012.