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Simulation, Optimization, and Reconstruction of Diffractive Structures

Leibniz Gemeinschaft

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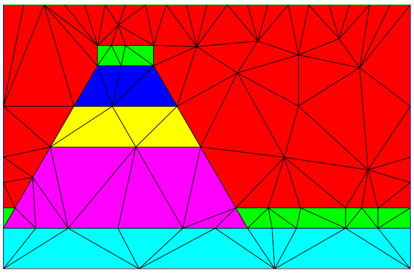
Simulation



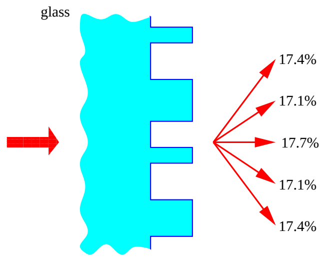
Cross section of trapezoidal grating with FEM triangulation

Mathematical Model: ▹ diffraction grating: surface geometry constant in one surface direction, periodic in the other
▹ Maxwell's system reduces to boundary value problem for 2D Helmholtz equation over the cross section
▹ boundary integral operators to include radiation condition
▹ equivalent variational formulation
Numerical Algorithm: ▹ finite element method (FEM) over triangular grid, capable to simulate general multilayered gratings with smooth or polygonal interfaces
▹ generalized FEM to reduce the pollution in the case of large wave numbers
▹ rigorous method, no Rayleigh series expansion, no slicing

Optimal Design

$DH_n^{\pm}$ - derivative of coefficient of reflected/transmitted mode of n-th order
k - piecewise constant wave number
Λ - curve separating substrate and cover material
u - field solution of diffraction problem
v - solution of dual problem
ν - normal to profile curve
$\partial_{\nu,\alpha}$ - $\nu_1\partial_1 + \nu_2\partial_2 + \nu_1 \mathbf{i}(\alpha, 0)$
$\partial_{\tau,\alpha}$ - $-\nu_2\partial_1 + \nu_1\partial_2 - \nu_2 \mathbf{i}(\alpha, 0)$
α - horizontal component of wave vector
χ - $\Lambda_h = \Phi_h(\Lambda),\ \Phi_h(x) = x + h\chi(x)$

Objectives of Geometrical Design:
▹ optimize the energies of certain reflected/transmitted modes
▹ approximate a prescribed far field pattern
▹ approximate a prescribed phase shift between the TE and TM polarized modes (elliptic or linear polarization)
▹ realize optical functions over a certain range of incident angles or wave lengths
Mathematical Methods: ▹ proof of smooth dependence of objective functionals on geometrical data
▹ sensitivity analysis based on the concept of the material derivative
▹ analytical formulas for the gradient in form of contour integr.
▹ convergence of gradient based minimization algorithms
▹ implementation of conjugate gradient method and interior point method
▹ efficient FEM-BEM solution of direct and dual problems

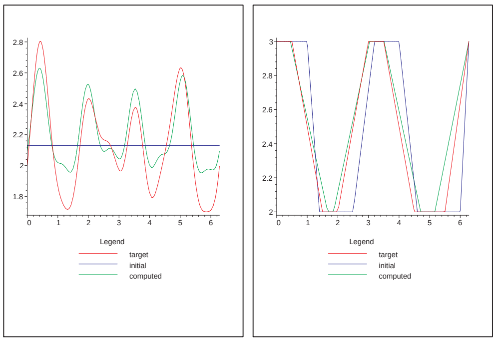


Beam splitter

$$DH_n^{\pm} = \int_\Lambda (\chi, \nu) \left[\frac{1}{k^2} \left(\partial_{\nu,\alpha} u \overline{\partial_{\nu,\alpha} v} - \partial_{\tau,\alpha} u \overline{\partial_{\tau,\alpha} v} \right) \right]_\Lambda$$

Profile Reconstruction

φ - unknown density function in potential representation
f - unknown profile function
u_F - measured far field data
u_f^{in} - incoming wave on profile curve
$T\varphi$ - far field corresponding to density φ
$S_f\varphi$ - field on profile corresponding to density φ
γ - regularization parameter



Reconstruction of Fourier and piecewise linear grating

$$\left\| T\varphi - u_F \right\|_{L^2}^2 + \gamma \left\| \varphi \right\|_{L^2[0,2\pi]}^2 + \left\| u_f^{in} - S_f\varphi \right\|_{L^2}^2 \longrightarrow \min$$

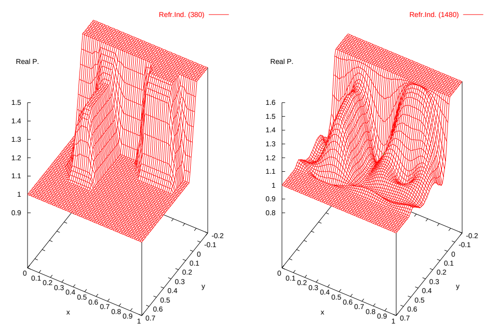
Given: ▹ cover and substrate material of unknown grating
▹ one or more incident plane waves
▹ measured far field (either efficiencies and phase shifts of reflected modes or field at certain distance from grating)
Sought: ▹ periodic profile curve separating the substrate material from the cover material
Theoretical Results: ▹ uniqueness for Lipschitz profiles
▹ conditional stability
▹ equivalence to least squares problem
Numerical Methods:
▹ potential representation of far field data and solution
▹ discretization of least squares functional for non-linear optimization
▹ splitting of problem in non-linear well-posed and linear ill-posed parts
▹ Tikhonov regularization for severely ill-posed and Levenberg-Marquardt algorithm for non-linear part

Inverse Media Reconstruction

u - unknown field solution
R - unknown refractive index function
Ω - domain of grating
u_F - measured far field data
u^{in} - incoming wave on upper boundary of Ω
B_R - preconditioned operator of field
Tu - far field values of field u
$\gamma_{1/2}$ - regularization parameters

Given: ▹ rectangular domain of a grating consisting of different materials of unknown refractive index and location
▹ one or more incident plane waves
▹ measured far field (either efficiencies and phase shifts of reflected modes or field at certain distance from)
Sought: ▹ shape and material distribution, i.e. refractive indices of the several parts of the grating represented by a refractive index function depending on the location point
▹ identification of manufacturing defects
Numerical Methods: ▹ reformulation of the reconstruction problem as an optimization of a functional including all the constraint conditions in form of penalty terms
▹ discretization of the objective functional using FEM
▹ solution of the discrete non-linear optimization problem by the conjugate gradient method or by the SQP method
▹ use analytic formulas for the gradients

$$\left\| B_R u - u^{in} \right\|_{L^2}^2 + \left\| Tu - u_F \right\|_{L^2}^2 + \gamma_1 \left\| R^2 \right\|_{H^{1/2}}^2 + \gamma_2 \left\| u \right\|_{H^1}^2 \longrightarrow \min$$



Reconstruction of refractive index function for lamellar grating

Future Activities:
▹ optimization and design of polygonal gratings
▹ global optimization methods
▹ reconstruction of gratings with non-perfectly conducting substrate material

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