Inverse problems for the scatterometric measuring of grating structures

Hermann Groß, Andreas Rathsfeld
Outline

1 Scatterometry.

2 Direct Problem: Diffraction by Grating Structures.

3 Reconstruction of Periodic Surface Structures.

4 Shape Derivatives.

5 Numerical Example.

6 Statistics and Further Issues.

7 Conclusions.
Outline

1. Scatterometry.

2. Direct Problem: Diffraction by Grating Structures.


4. Shape Derivatives.

5. Numerical Example.


7. Conclusions.
Lithography

chip production like old-fashioned photography:
photoresist layer illuminated by light scattered from mask,
development: baking and etching procedures $\rightarrow$ chip

standard test configurations:
- periodic line-space structure (lines formed by bridges with
trapezoidal cross section)
- biperiodic array of trapezoidal blocks resp. holes
Scatterometry

Spectroscopic Reflectrometer, Operating Range $\approx 13$ nm, BESSY II, PTB
Outline

1 Scatterometry.

2 Direct Problem: Diffraction by Grating Structures.

3 Reconstruction of Periodic Surface Structures.

4 Shape Derivatives.

5 Numerical Example.

6 Statistics and Further Issues.

7 Conclusions.
Periodic Grating

Incoming field: \((\vec{E}_i, \vec{H}_i)\)

Reflected modes

Transmitted modes

Periodic gratings

Details of surface geometry in size of wavelength
Biperiodic (Doubly Periodic) Grating

biperiodic surface structures (period $d_j$ in $x_j$-direction, $j = 1, 2$)
details of surface geometry in size of wavelength
Plane-wave illumination. 3D time-harmonic Maxwell's equations reduce to:

- **Curl-Curl** equation for three-dimensional amplitude factor of time harmonic electric field (i.e. \( E(x_1, x_2, x_3, t) = E(x_1, x_2, x_3)e^{-i\omega t} \))

\[
\nabla \times \nabla \times E(x_1, x_2, x_3) - k^2 E(x_1, x_2, x_3) = 0
\]

Here: wave number \( k := \omega \sqrt{\mu \varepsilon} \)

- scalar 2D Helmholtz equation if geometry is constant in \( x_3 \) direction and if direction of incoming plane wave is in \( x_1 - x_2 \) plane

\[
\nabla^2 v(x_1, x_2) + k^2 v(x_1, x_2) = 0, \ v = E_3, H_3
\]

- two coupled scalar 2D Helmholtz equations if geometry is constant in \( x_3 \) direction but direction of incoming plane wave is not in \( x_1 - x_2 \) plane (conical diffraction)
Plane-wave illumination. 3D time-harmonic Maxwell's equations reduce to:

- **Curl-Curl** equation for three-dimensional amplitude factor of time harmonic electric field (i.e. \( E(x_1, x_2, x_3, t) = E(x_1, x_2, x_3)e^{-i\omega t} \))

\[
\nabla \times \nabla \times E(x_1, x_2, x_3) - k^2 E(x_1, x_2, x_3) = 0
\]

Here: wave number \( k := \omega \sqrt{\mu \varepsilon} \)

- scalar 2D Helmholtz equation if geometry is constant in \( x_3 \) direction and if direction of incoming plane wave is in \( x_1 - x_2 \) plane

\[
\Delta v(x_1, x_2) + k^2 v(x_1, x_2) = 0, \quad v = E_3, H_3
\]

- two coupled scalar 2D Helmholtz equations if geometry is constant in \( x_3 \) direction but direction of incoming plane wave is not in \( x_1 - x_2 \) plane (conical diffraction)
Boundary Value Problem

Domain of Computation:
Rectangular box over one periodic cell $\Omega$

Non–local boundary condition:
Including radiation condition
Mortaring with Fourier mode sol.
(Coupling with boundary elements or Absorbing bound.cond. PML)

Transmission conditions:
Continuous tangential traces
Continuous tangential traces of curl

Quasiperiodic boundary condition:
\[ v(x_1+d_1, x_2, x_3) = v(x_1, x_2, x_3) \exp(i\alpha d_1) \]
\[ v(x_1, x_2+d_2, x_3) = v(x_1, x_2, x_3) \exp(i\beta d_2) \]
Rayleigh Series Expansion Below/Above Computational Domain

incident plane wave (inspecting w.): 
\[ E^{\text{inc}}(x_1, x_2, x_3) \exp(-i\omega t), \]
\[ E^{\text{inc}}(x_1, x_2, x_3) := A^{\text{inc}} \exp \left( i k^{\text{inc}} \cdot (x_1, x_2, x_3)^\top \right) \]
\[ k^{\text{inc}} = k^+(\sin \theta \cos \phi, \sin \theta \sin \phi, -\cos \theta)^\top \]

\[ E(x_1, x_2, x_3) = \sum_{j,l=-\infty}^{\infty} A^{-}_{j,l} \exp \left( i k^{-}_{j,l} \cdot (x_1, x_2, x_3)^\top \right), \quad x_3 < x_{\text{min}}, \]
\[ \alpha_j := k^+ \sin \theta \cos \phi + \frac{2\pi}{d_1} j, \]
\[ k^{-}_{j,l} := (\alpha_j, \beta_l, \gamma^{-}_{j,l})^\top, \quad \beta_l := k^+ \sin \theta \sin \phi + \frac{2\pi}{d_2} l, \]
\[ \gamma^{-}_{j,l} := -\sqrt{[k^-]^2 - [\alpha_j]^2 - [\beta_l]^2} \]

Rayleigh series: Rayleigh coefficients \( A_{j,l}^- \in \mathbb{C}^3, \ A_{j,l}^- \perp k^-_{j,l} \), with \( k = k^- \) for \( x_3 < x_{\text{min}} \) (similarly, coefficients \( A_{j,l}^+ \) for expansion with \( x_3 > x_{\text{max}} \), where \( k = k^+ \))

Efficiency \( \mathcal{E}_{j,l}^\pm \) of \((j, l)\) -th mode: ratio of energy radiated into direction of mode

\[ \mathcal{E}_{j,l}^\pm := (\gamma_{j,l}^\pm / \gamma_{0,0}^+) |A_{j,l}^\pm|^2 \]
Rayleigh Series Expansion Below/Above Computational Domain

incident plane wave (inspecting w.): \( E^{\text{inc}}(x_1, x_2, x_3) \exp(-i\omega t) \),
\[
E^{\text{inc}}(x_1, x_2, x_3) := A^{\text{inc}} \exp \left( i k^{\text{inc}} \cdot (x_1, x_2, x_3)^\top \right)
\]
\[
k^{\text{inc}} = k^+ (\sin \theta \cos \phi, \sin \theta \sin \phi, -\cos \theta)^\top
\]
\[
E(x_1, x_2, x_3) = \sum_{j,l=-\infty}^{\infty} A_{j,l}^- \exp \left( i k_{j,l}^- \cdot (x_1, x_2, x_3)^\top \right), \quad x_3 < x_{\text{min}},
\]
\[
\alpha_j := k^+ \sin \theta \cos \phi + \frac{2\pi}{d_1} j,
\]
\[
k_{j,l}^- := (\alpha_j, \beta_l, \gamma_{j,l}^-)^\top, \quad \beta_l := k^+ \sin \theta \sin \phi + \frac{2\pi}{d_2} l,
\]
\[
\gamma_{j,l}^- := -\sqrt{[k^-]^2 - [\alpha_j]^2 - [\beta_l]^2}
\]

Rayleigh series: Rayleigh coefficients \( A_{j,l}^- \in \mathbb{C}^3 \), \( A_{j,l}^- \perp k_{j,l}^- \), with \( k = k^- \) for \( x_3 < x_{\text{min}} \) (similarly, coefficients \( A_{j,l}^+ \) for expansion with \( x_3 > x_{\text{max}} \), where \( k = k^+ \))

Efficiency \( \mathcal{E}_{j,l}^\pm \) of \((j, l)\)–th mode: ratio of energy radiated into direction of mode
\[
\mathcal{E}_{j,l}^\pm := (\gamma_{j,l}^\pm / \gamma_{0,0}^+) |A_{j,l}^\pm|^2
\]
Variational Equation 1

\[ \int_\Omega \nabla \times E \cdot \nabla \times F - \int_\Omega k^2 E \cdot \overline{F} - \int_{\Gamma^+} \nabla \times E^+ \cdot \nu \times \overline{F} + \int_{\Gamma^+} \nu \times (E - E^+) \cdot \nabla \times \overline{F}^+ \\
- \int_{\Gamma^-} \nabla \times E^- \cdot \nu \times \overline{F} + \int_{\Gamma^-} \nu \times (E - E^-) \cdot \nabla \times \overline{F}^- + \text{finite rank terms} \\
= \int_{\Gamma^+} \nabla \times E^{\text{inc}} \cdot \nu \times \overline{F} + \int_{\Gamma^-} \nu \times E^{\text{inc}} \cdot \nabla \times \overline{F}^+ + \text{finite rank term}, \quad \forall F, \forall F^{\pm} \]

\[ a\left( (E, E^+, E^-), (F, F^+, F^-) \right) = F\left( (F, F^+, F^-) \right), \quad \forall F \in H(\text{curl}, \Omega), \quad \forall F^{\pm} \text{Rayleigh expansions} \]

with solution \((E, E^+, E^-): E \in H(\text{curl}, \Omega)\) and \(E^{\pm}\) Rayleigh expansions in \(H_{\text{loc}}(\text{curl})\)

\(\Omega\) domain of computation, \(\Gamma^{\pm}\) upper/lower boundary face, \(\nu\) normal at \(\Gamma^{\pm}\)

\(H(\text{curl}, \Omega) := \{ F \in [L^2(\Omega)]^3 : F \text{ quasi-per., piecewise } \nabla \times F \in [L^2(\Omega)]^3, \nu \times F \text{ continuous over interfaces} \}\)

Theorem (Hu, R. ’12)

For profile gratings with perfectly conducting substrate: operator corresponding to sesqui-linear form a takes the form \( \begin{pmatrix} A_0 & 0 \\ 0 & -A_1 \end{pmatrix} + T \), where \( A_0, A_1 \) strongly elliptic and \( T \) compact.
Variational Equation 1

\[
\int_{\Omega} \nabla \times E \cdot \nabla \times F - \int_{\Omega} k^2 E \cdot F - \int_{\Gamma^+} \nabla \times E^+ \cdot \nu \times F + \int_{\Gamma^+} \nu \times (E - E^+) \cdot \nabla \times F^+ \\
- \int_{\Gamma^-} \nabla \times E^- \cdot \nu \times F + \int_{\Gamma^-} \nu \times (E - E^-) \cdot \nabla \times F^- + \text{finite rank terms}
\]

\[
= \int_{\Gamma^+} \nabla \times E^{\text{inc}} \cdot \nu \times F + \int_{\Gamma^-} \nu \times E^{\text{inc}} \cdot \nabla \times F^+ + \text{finite rank term}, \quad \forall F, \forall F^\pm
\]

\[
a \left( (E, E^+, E^-), (F, F^+, F^-) \right) = \mathcal{F} \left( (F, F^+, F^-) \right), \quad \forall F \in H(\text{curl}, \Omega), \forall F^\pm \text{Rayleigh expansions}
\]

with solution \((E, E^+, E^-): E \in H(\text{curl}, \Omega)\) and \(E^\pm\) Rayleigh expansions in \(H_{\text{loc}}(\text{curl})\)

\(\Omega\) domain of computation, \(\Gamma^\pm\) upper/lower boundary face, \(\nu\) normal at \(\Gamma^\pm\)

\(H(\text{curl}, \Omega) := \{ F \in [L^2(\Omega)]^3: F\text{ quasi-per., piecewise } \nabla \times F \in [L^2(\Omega)]^3, \nu \times F \text{ continuous over interfaces} \}\)

Theorem (Hu, R. ’12)

For profile gratings with perfectly conducting substrate: operator corresponding to sesqui-linear form \(a\) takes the form

\[
\begin{pmatrix}
A_0 & 0 \\
0 & -A_1
\end{pmatrix}
+ T, \text{ where } A_0, A_1 \text{ strongly elliptic and } T \text{ compact.}
\]
finite rank term to cope with the case of plane-wave modes in Rayleigh expansion propagating
in the direction of the $x_1 - x_2$ plane,
(i.e., for $k^\pm := \omega \sqrt{\mu \varepsilon^\pm}$, there exist indices $j, l$ with $\gamma_j^\pm, l = 0$)

\[
\text{finite rank term} := \\
\eta \sum_{(j,l) \in \Upsilon^\pm} \int_{\Gamma^\pm} \nu \times (E - E^\pm) \cdot (\nu \times U_{j,l}) \int_{\Gamma^\pm} \nu \times (E - E^\pm) \cdot (\nu \times U_{j,l})
\]

where: $\Upsilon^\pm$ is any fixed finite index set containing all $(j, l)$ with $\gamma_j^\pm, l = 0$
\(\eta\) is a fixed constant
$U_{j,l}$ is special mode in Rayleigh expansion defined by

\[
U_{j,l}(x_1, x_2, x_3) := \frac{1}{\sqrt{\alpha_j^2 + \beta_l^2}} (-\beta_l, \alpha_j, 0)^\top \exp \left( i k_j^\pm \cdot (x_1, x_2, x_3)^\top \right)
\]
Inverse problems for scatterometric measuring of gratings · IPMS, 23 May 2012 · Page 14 (42)
Finite Element Methods and Alternatives

- **2D theory**: H. Urbach, G. Bao, D.C. Dobson, J.A. Cox, J. Elschner, R. Hinder, and G. Schmidt

  - generalized finite elements (trial space of piecewise Helmholtz solutions) for faster convergence and for highly oscillating solutions

- **3D theory**: G. Schmidt for the approximation of the divergence free magnetic field


- **alternatives**: rigorous coupled wave analysis (RCWA) and integral equation methods (BEM, e.g., B. Bugert and G. Schmidt)
Outline

1. Scatterometry.
2. Direct Problem: Diffraction by Grating Structures.
4. Shape Derivatives.
5. Numerical Example.
7. Conclusions.
Inverse Problem

- **Given**: the diffraction properties of grating (e.g. efficiencies $E_{j,l}^{\pm}$)
- **Seek**: the grating, i.e., the geometry of the domains filled with different materials and the refractive indices of these materials

- **severely ill-posed problem**: small errors in data lead to large errors for the solution


- contributions to 3D case by H. Ammari, G. Bao, Z. Zhou, H. Zhang, and J. Zou,
Uniqueness Theorem 3D

**perfectly conducting profile grating (PCPG):**

two materials, perfectly conducting substrate, dielectric cover material, interface graph
\[ \{(x', x_3) \in \mathbb{R}^3 : x_3 = f(x')\} \]
of a function \( f \)

- PCPG with small \( f \) with finite number of Fourier modes, Rayleigh coefficients measured for propagating plane-wave modes: uniqueness by Ammari
- general grating, Rayleigh coefficients measured for propagating reflected plane-wave modes (even for all angles of incidence): no reconstruction, 2D counter example by Kirsch
- PCPG with small and smooth function, electric field measured over plane above interface: certain uniqueness by Bao/Zhou
- PCPG with polyhedral function, single incoming plane wave, electric field measured over plane above interface: interface not identifiable if in one of 7 classes of Bao/Zhang/Zou

---

**Theorem (Bao, Zhang, Zou ’11)**

*Two polyhedral PCPGs. One interface has two faces forming an angle different from \( \pi/4, \pi/3, \pi/2, \) and \( 2\pi/3 \). For single incoming wave, corresponding reflected fields coincide over plane above interfaces. Then: PCPGs coincide.*
Uniqueness Theorem 3D

perfectly conducting profile grating (PCPG):
two materials, perfectly conducting substrate, dielectric cover material, interface graph
\{ (x', x_3) \in \mathbb{R}^3 : x_3 = f(x') \} of a function f

- PCPG with small $f$ with finite number of Fourier modes, Rayleigh coefficients measured for propagating plane-wave modes: uniqueness by Ammari
- general grating, Rayleigh coefficients measured for propagating reflected plane-wave modes (even for all angles of incidence): no reconstruction, 2D counter example by Kirsch
- PCPG with small and smooth function, electric field measured over plane above interface: certain uniqueness by Bao/Zhou
- PCPG with polyhedral function, single incoming plane wave, electric field measured over plane above interface: interface not identifiable if in one of 7 classes of Bao/Zhang/Zou

Theorem (Bao, Zhang, Zou ’11)

Two polyhedral PCPGs. One interface has two faces forming an angle different from $\pi/4$, $\pi/3$, $\pi/2$, and $2\pi/3$. For single incoming wave, corresponding reflected fields coincide over plane above interfaces. Then: PCPGs coincide.
Class of Gratings

avoid full inverse problems by using more a priori information on the grating:

- seek grating in class defined by a few parameters $h = (h_j)_{j=1}^{J}$
  (parameter identification)
Class of Gratings

Reasonable initial values for optimizations

- bottomCD: ~140 nm
- hTaO: 12 nm, SWA: 82.6°
- hTaN: 54.9 nm, SWA: 90°
- hGla(buff): 8 nm, SWA: 90°
- hGla(capping): 1.246 nm
- hSi(capping): 12.536 nm

50x h [0.5–2.259–1.263–3.077 nm]

mask for EUV lithography: wavelength of inspecting light 13 nm

Inverse problems for scatterometric measuring of gratings · IPMS, 23 May 2012 · Page 20 (42)
Equivalent Optimization Problem

measured data, efficiencies or phase shifts: \( \mathcal{E}^{meas} = (\mathcal{E}_{m}^{meas})_{m \in \mathcal{M}} \)

computed data corresponding to parameters \( h \): \( \mathcal{E}(h) = (\mathcal{E}_{m}(h))_{m \in \mathcal{M}} \)

minimize objective functional

\[
\mathcal{F}(\mathcal{E}_{m}(h)) \rightarrow \text{inf}
\]

\[
\mathcal{F}(E) := \mathcal{F}(\mathcal{E}(h)) := \sum_{m \in \mathcal{M}} \omega_{m} |\mathcal{E}_{m}(h) - \mathcal{E}_{m}^{meas}|^{2}, \quad \omega_{m} := \frac{1}{\sigma(\mathcal{E}_{m}^{meas})^{2}}
\]

standard deviation of measurement: \( \sigma(\mathcal{E}_{m}^{meas}) \)

box constraints \( h_{j}^{\text{min}} \leq h_{j} \leq h_{j}^{\text{max}} \)

use: conjugate gradients method, interior point method, Levenberg-Marquardt algorithm or SQP
Convergence of Gauß-Newton iteration (SQP)

- similar to statistics: least squares estimator
- proposed by Drège, Al-Assad, Byrne for grating reconstruction without box constraints
- convergence properties:
  - limit satisfies KKT condition necessary for minimum
  - if measurement data is exact: $\|h^{k+1} - h^{sol}\| \leq c\|h^k - h^{sol}\|^2$
  - small error in measurement data: $\|h^k - h^{sol}\| \leq cq^k$, $0 < q < 1$
  - large error $\varepsilon$ in measurement data: $\|h^k - h^{sol}\| \leq c\varepsilon$ if $k \geq k_0$
- advantages in comparison to gradient based method for optimization of objective functional:
  - fast: small number of iterations, no line search
  - no trouble with computation of small gradients at iterates close to optimum
  - more robust w.r.t. nonoptimal scaling
Convergence of Gauß-Newton iteration (SQP)

- similar to statistics: least squares estimator
- proposed by Drège, Al-Assad, Byrne for grating reconstruction without box constraints
- convergence properties:
  - limit satisfies KKT condition necessary for minimum
  - if measurement data is exact: \( \| h^{k+1} - h^{sol} \| \leq c \| h^k - h^{sol} \|^2 \)
  - small error in measurement data: \( \| h^k - h^{sol} \| \leq cq^k, \ 0 < q < 1 \)
  - large error \( \varepsilon \) in measurement data: \( \| h^k - h^{sol} \| \leq c\varepsilon \) if \( k \geq k_0 \)

- advantages in comparison to gradient based method for optimization of objective functional:
  - fast: small number of iterations, no line search
  - no trouble with computation of small gradients at iterates close to optimum
  - more robust w.r.t. nonoptimal scaling
similar to statistics: least squares estimator

proposed by Drège, Al-Assad, Byrne for grating reconstruction without box constraints

convergence properties:

- limit satisfies KKT condition necessary for minimum
- if measurement data is exact: \( \|h^{k+1} - h^{sol}\| \leq c\|h^k - h^{sol}\|^2 \)
- small error in measurement data: \( \|h^k - h^{sol}\| \leq cq^k, \ 0 < q < 1 \)
- large error \( \varepsilon \) in measurement data: \( \|h^k - h^{sol}\| \leq c\varepsilon \) if \( k \geq k_0 \)

advantages in comparison to gradient based method for optimization of objective functional:

- fast: small number of iterations, no line search
- no trouble with computation of small gradients at iterates close to optimum
- more robust w.r.t. nonoptimal scaling
Outline

1 Scatterometry.

2 Direct Problem: Diffraction by Grating Structures.

3 Reconstruction of Periodic Surface Structures.

4 Shape Derivatives.

5 Numerical Example.

6 Statistics and Further Issues.

7 Conclusions.
vector field on \( \Omega \) vanishing on boundary \( \partial \Omega \): \( \chi(\vec{x}) \)
generates family of automorphisms of domain \( \Omega \): \( \Phi_t(\vec{x}) := \vec{x} + t\chi(\vec{x}), 0 \leq t < 1 \)
generates family of solutions over transformed domain: \( E_t \) solution of time-harmonic Maxwell equation with coefficient \( k \) replaced by \( k_t := k \circ \Phi_t^{-1} \)
material derivative of \( F(E) \) w.r.t. \( \chi \):

\[
\partial_t[F(E_t)]|_{t=0} := \lim_{t \to 0} \frac{F(E_t) - F(E_0)}{t}
\]

If grating geometry is polyhedral,
if the only non-vanishing component of \( \chi \) is \( \chi x_i \),
if \( \chi x_i \) is piecewise linear and linear over all faces of the grating geometry,
if \( \chi x_i(P) = 1 \) for the vertex \( P \), and
if \( \chi x_i(Q) = 0 \) for all other vertices \( Q \),
then
\[
\partial_t[F(E_t)]|_{t=0} \text{ is the shape derivative of } F(E) \text{ w.r.t. the } x_i\text{-component of the vertex } P
\]
classical techniques of shape derivatives (cf. e.g. Sokolowski/Zolesio)

unfortunately, energy space $H(\text{curl}, \Omega)$ not invariant w.r.t. transform $\Phi_t$

fortunately, magnetic permeability is constant and magnetic field is in $H^1(\Omega)$ over each subdomain filled with one material

derive shape derivative for the magnetic solution by classical method and, in the final formula, replace magnetic field by electric field
Shape-Derivative Formula

\[ a_1(E, F) := \int_{\Omega} k^2 E \cdot F \ \nabla \cdot \chi - \int_{\Omega} \nabla \times E \cdot \nabla \times F \ \nabla \cdot \chi \]

\[ + \int_{\Omega} k^2 E \cdot \left( \nabla x_1 \cdot F, \nabla x_2 \cdot F, \nabla x_3 \cdot F \right)^\top + \int_{\Omega} k^2 \left( \nabla \chi x_1 \cdot F, \nabla \chi x_2 \cdot F, \nabla \chi x_3 \cdot F \right)^\top \cdot \nabla \times F \]

\[ + \int_{\Omega} \left[ \nabla \times E \right] \cdot \left[ \nabla \times F \right] x_1 \nabla \chi x_1 + \left[ \nabla \times F \right] x_2 \nabla \chi x_2 + \left[ \nabla \times F \right] x_3 \nabla \chi x_3 \]

\[ + \int_{\Omega} \left[ \nabla \times E \right] x_1 \nabla \chi x_1 + \left[ \nabla \times E \right] x_2 \nabla \chi x_2 + \left[ \nabla \times E \right] x_3 \nabla \chi x_3 \cdot \nabla \times F \]

differentiated sesqui-linear form

\[ a\left( (E, E^+, E^-), (F_{ad}, F_{ad}^+, F_{ad}^-) \right) = \int_{\Gamma^+} [\nu \times E] \cdot \bar{\psi}, \ \forall E, E^+, E^- \]

\[ \psi := \sum_{m \in M} c_m \omega_m \sqrt{\varepsilon_m} \left[ \varepsilon_m - \varepsilon_m^{meas} \right] \]

adjoint solution \((F_{ad}, F_{ad}^+, F_{ad}^-)\) (here \(c_m\) certain constants)

final formula:

\[ \partial_t [F(E_t)]_{t=0} = -\Re a_1(E_0, F_{ad}) \]
Shape-Derivative Formula

\[ a_1(E, F) := \int_{\Omega} k^2 E \cdot F \nabla \chi - \int_{\Omega} \nabla \times E \cdot \nabla \times F \nabla \cdot \chi \]

\[ + \int_{\Omega} k^2 E \cdot \left( \nabla x_1 \cdot F, \nabla x_2 \cdot F, \nabla x_3 \cdot F \right)^\top + \int_{\Omega} k^2 \left( \nabla \chi x_1 \cdot F, \nabla \chi x_2 \cdot F, \nabla \chi x_3 \cdot F \right)^\top \cdot F \]

\[ + \int_{\Omega} [\nabla \times E] \cdot \left[ [\nabla \times F] x_1 \nabla \chi x_1 + [\nabla \times F] x_2 \nabla \chi x_2 + [\nabla \times F] x_3 \nabla \chi x_3 \right] \]

\[ + \int_{\Omega} \left[ [\nabla \times E] x_1 \nabla \chi x_1 + [\nabla \times E] x_2 \nabla \chi x_2 + [\nabla \times E] x_3 \nabla \chi x_3 \right] \cdot \left[ \nabla \times F \right] \]

differentiated sesqui-linear form

\[ a \left( (E, E^+, E^-), (F_{ad}, F_{ad}^+, F_{ad}^-) \right) = \int_{\Gamma^+} [\nu \times E] \cdot \overline{\psi}, \quad \forall E, E^+, E^- \]

\[ \psi := \sum_{m \in M \Psi} c_m \omega_m \sqrt{\varepsilon_m} \left[ \varepsilon_m - \varepsilon_{m\text{meas}} \right] \]

adjoint solution \((F_{ad}, F_{ad}^+, F_{ad}^-)\) (here \(c_m\) certain constants)

final formula:

\[ \partial_t [\mathcal{F}(E_t)] \big|_{t=0} = -\Re a_1(E_0, F_{ad}) \]
Shape-Derivative Formula

\[ a_1(E, F) := \int_{\Omega} k^2 E \cdot \bar{F} \nabla \cdot \chi \quad - \int_{\Omega} \nabla \times E \cdot \nabla \times F \nabla \cdot \chi \]
\[ + \int_{\Omega} k^2 E \cdot \left( \nabla x_1 \cdot F, \nabla x_2 \cdot F, \nabla x_3 \cdot F \right)^\top \quad + \int_{\Omega} k^2 \left( \nabla \chi x_1 \cdot F, \nabla \chi x_2 \cdot F, \nabla \chi x_3 \cdot F \right)^\top \cdot \bar{F} \]
\[ + \int_{\Omega} [\nabla \times E] \cdot [\nabla \times F] x_1 \nabla \chi x_1 \quad + \nabla \times F] x_2 \nabla \chi x_2 \quad + \nabla \times F] x_3 \nabla \chi x_3 \]
\[ + \int_{\Omega} \left[ [\nabla \times E] x_1 \nabla \chi x_1 \quad + \nabla \times E] x_2 \nabla \chi x_2 \quad + \nabla \times E] x_3 \nabla \chi x_3 \right] \cdot \overline{[\nabla \times F]} \]

differentiated sesqui-linear form

\[ a\left((E, E^+, E^-), (F_{ad}, F_{ad}^+, F_{ad}^-)\right) = \int_{\Gamma^+} [\nu \times E] \cdot \bar{\psi}, \quad \forall E, E^+, E^- \]
\[ \psi := \sum_{m \in \mathcal{M}} c_m \omega_m \sqrt{\varepsilon_m} \left[ \varepsilon_m - \varepsilon_{m}^{meas} \right] \]

adjoint solution \((F_{ad}, F_{ad}^+, F_{ad}^-)\) (here \(c_m\) certain constants)

final formula:
\[ \partial_t [\mathcal{F}(E_t)]|_{t=0} = - \Re a_1(E_0, F_{ad}) \]
Outline

1 Scatterometry.

2 Direct Problem: Diffraction by Grating Structures.

3 Reconstruction of Periodic Surface Structures.

4 Shape Derivatives.

5 Numerical Example.

6 Statistics and Further Issues.

7 Conclusions.
Parameters to be Reconstructed

reconstruct the three parameters $a$, $b$, and $c$ for array of contact holes, contact hole symmetric frustum of pyramid in middle of periodic cell $\Omega$

$$3.15 \, \text{nm} \leq a \leq 3.85 \, \text{nm}, \quad 4.55 \, \text{nm} \leq b \leq 5.25 \, \text{nm}, \quad 3.85 \, \text{nm} \leq c \leq 4.55 \, \text{nm}$$

period in $x$- and $y$- direction: 16.8 nm and 14 nm
inspecting wave length: 13.7 nm
side material SiO$_2$, substrate layer Ta, lower multilayer system Mo and Si
normal incidence, five “measured” efficiencies $E_m$ of order (-1,0), (0,-1), (0,0), (0,1), (1,0)
corresponding weights $\omega_m$: 1000, 2000, 4, 2000, 1000
## Convergence of Reconstruction Algorithm

Number of iterations and reconstruction of parameters for contact hole.

<table>
<thead>
<tr>
<th>mesh size</th>
<th>nmb.of its.</th>
<th>(a) in nm</th>
<th>(b) in nm</th>
<th>(g) in nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>initial vals.</td>
<td></td>
<td>3.90000</td>
<td>4.60000</td>
<td>3.90000</td>
</tr>
<tr>
<td>2.95</td>
<td>8</td>
<td>3.52643</td>
<td>4.89211</td>
<td>4.20601</td>
</tr>
<tr>
<td>1.47</td>
<td>5</td>
<td>3.49339</td>
<td>4.90394</td>
<td>4.20270</td>
</tr>
<tr>
<td>0.73</td>
<td>5</td>
<td>3.49984</td>
<td>4.90018</td>
<td>4.20011</td>
</tr>
<tr>
<td>exact</td>
<td></td>
<td>3.50000</td>
<td>4.90000</td>
<td>4.20000</td>
</tr>
</tbody>
</table>
Sensitivity analysis: Optimize choice of measurement data and weights using the Jacobians

- Given distribution and variance of measurement values: estimate uncertainties (standard deviation) of reconstructed values
  - Covariance matrix estimates by inverse Jacobians
  - Monte Carlo methods

- Estimate the impact of model errors on the reconstruction, Maximum-likelihood methods
  - Stochastic deviations of the widths in the multilayer system
  - Corner roundings and footage
  - Linewidth roughness (LWR) and lineedge roughness (LER) of line-space structures
Analysis Done for 2D Case

- Sensitivity analysis: Optimize choice of measurement data and weights using the Jacobians
- Given distribution and variance of measurement values: estimate uncertainties (standard deviation) of reconstructed values
  - covariance matrix estimates by inverse Jacobians
  - Monte Carlo methods
- Estimate the impact of model errors on the reconstruction, Maximum-likelihood methods
  - Stochastic deviations of the widths in the multilayer system
  - Corner roundings and footage
  - Linewidth roughness (LWR) and lineedge roughness (LER) of line-space structures
Sensitivity analysis: Optimize choice of measurement data and weights using the Jacobians

Given distribution and variance of measurement values: estimate uncertainties (standard deviation) of reconstructed values
  - covariance matrix estimates by inverse Jacobians
  - Monte Carlo methods

Estimate the impact of model errors on the reconstruction,
  Maximum-likelihood methods
  - Stochastic deviations of the widths in the multilayer system
  - Corner roundings and footage
  - Linewidth roughness (LWR) and lineedge roughness (LER) of line-space structures
Lineedge Roughness and Linewidth Roughness

stochastic perturbation in line space structure

Lineedge roughness (LER)
Linewidth roughness (LWR)
Simple 2D Simulation of LWR/LER

- simplifying assumption: assume perturbation of lines is slow in the direction of the lines
- locally: like geometry of perfect parallel lines with perturbations in line widths and distances between lines
- approximated by periodic grating: super cell with large period containing many (e.g. 48) lines with variable line widths and distances

Cross section of super cell

Cross section of single line
Simple 2D Simulation of LWR/LER

- Simplifying assumption: assume perturbation of lines is slow in the direction of the lines.
- Locally: like geometry of perfect parallel lines with perturbations in line widths and distances between lines.
- Approximated by periodic grating: super cell with large period containing many (e.g., 48) lines with variable line widths and distances.

Inverse problems for scatterometric measuring of gratings · IPMS, 23 May 2012 · Page 34 (42)
Monte-Carlo Results for LER: Systematic Error

(a) Normalized deviations from the efficiencies of the unperturbed reference line structure, depicted as circles; diamonds represent the mean over the deviations of all 100 samples; dashed lines indicate the mean efficiency ± standard deviation; random perturbations of the center positions (LER): $\sigma_{x_i} = 5.6 \text{ nm}$. (b) Standard deviations relative to the mean perturbed efficiencies shown as circles for the given example; diamonds depict best approximation by an exponential function.

FEM results: $\sigma_{x_i} = 5.6 \text{ nm}$

$[1-\exp(-\sigma_r^2k_j^2/3)]/\sqrt{2}$

$\sigma_r = 5.55 \text{ nm}$; $k_j = 2 \pi n_j/d$

d = 280 nm (period)
Monte-Carlo Results for LWR: Systematic Error

(a) Normalized deviations from the efficiencies of the unperturbed reference line structure, depicted as circles; diamonds represent the mean over the deviations of all 100 samples; dashed lines indicate the mean efficiency ± standard deviation; random perturbations of the line widths (LWR): $\sigma_{CDi} = 5.6 \text{ nm}$. (b) Standard deviations relative to the mean perturbed efficiencies shown as circles for the given example; diamonds depict an approximation by an exponential function.

FEM results: $\sigma_{CDi} = 5.6 \text{ nm}$

$[1-\exp(-\sigma_r^2k_j^2/3)]/\sqrt{2}$

$\sigma_r = 2.74 \text{ nm}; k_j = 2\pi n_j/d$

d = 280 nm (period)
A. Kato and F. Scholze: formula for impact of LER/LWR if Fraunhofer approximation applies

\[ \mathcal{E}_{j, \text{pert}}^+ \approx \exp \left( - \left( \frac{2\pi j}{d} \right)^2 \sigma \right) \mathcal{E}_{j, \text{no pert}}^+ \]

where:  
- \( d \) period,  
- \( j \) order of mode,  
- \( \sigma \) is the standard deviation of the stochastic perturbation of the line edges.

- similar exponential function for variances  
- by our experiments: formulas confirmed for rigorous Maxwell's equations and slow perturbation along the lines  
- knowing the LER/LWR perturbation: incorporate formula into numerical reconstruction algorithm
Correction Factor for LER/LWR Perturbations

A. Kato and F. Scholze: formula for impact of LER/LWR if Fraunhofer approximation applies

\[ E_{j,\text{pert}}^+ \approx \exp \left( -\left( \frac{2\pi j}{d} \right)^2 \sigma \right) E_{j,\text{no pert}}^+ , \]

where: \( d \) period,
\( j \) order of mode,
\( \sigma \) is the standard deviation of the stochastic perturbation of the line edges.

- similar exponential function for variances
- by our experiments: formulas confirmed for rigorous Maxwell’s equations and slow perturbation along the lines
- knowing the LER/LWR perturbation: incorporate formula into numerical reconstruction algorithm
Correction Factor for LER/LWR Perturbations

A. Kato and F. Scholze: formula for impact of LER/LWR if Fraunhofer approximation applies

\[ E_{j, \text{pert}}^+ \approx \exp \left( - \left( \frac{2\pi j}{d} \right)^2 \sigma \right) E_{j, \text{no pert}}^+ \]

where: $d$ period,

$j$ order of mode,

$\sigma$ is the standard deviation of the stochastic perturbation of the line edges.

- similar exponential function for variances
- by our experiments: formulas confirmed for rigorous Maxwell’s equations and slow perturbation along the lines
- knowing the LER/LWR perturbation: incorporate formula into numerical reconstruction algorithm
Improved Numerical Reconstruction

$\sigma_2^2: 1.62 \text{ nm} \quad \sigma_6: 0.04 \text{ nm} \quad \sigma_7: 0.48 \text{ nm}$

$\sigma_2^2: 0.73 \text{ nm} \quad \sigma_6: 0.20 \text{ nm} \quad \sigma_7: 0.35 \text{ nm}$

$\sigma_{\text{SWA}}: 1.82^\circ \quad \text{SWA}_{\text{mean}}: 95.05^\circ \quad \sigma_{\text{SWA}}: 0.82^\circ \quad \text{SWA}_{\text{mean}}: 90.20^\circ$

1% standard deviation of edges with LER/LWR, left reconstruction without correction factor, right with correction factor, deviation around nominal value.
Outline

1 Scatterometry.

2 Direct Problem: Diffraction by Grating Structures.

3 Reconstruction of Periodic Surface Structures.

4 Shape Derivatives.

5 Numerical Example.

6 Statistics and Further Issues.

7 Conclusions.
Conclusions

- Simulation of scattered field by biperiodic grating possible with FEM and mortar method (unfortunately: slow)
- Shape derivatives can be computed by FEM
- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Uncertainties of reconstructed parameters can be estimated even by fast covariance-matrix method
- To get results closer to those obtained by alternative measurement methods: model errors need to be analyzed, e.g., LER, LWR

For more details:
S. Heidenreich: today’s talk, M10, Salon B, 16:50–17:15
Conclusions

- Simulation of scattered field by biperiodic grating possible with FEM and mortar method (unfortunately: slow)
- Shape derivatives can be computed by FEM
- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Uncertainties of reconstructed parameters can be estimated even by fast covariance-matrix method
- To get results closer to those obtained by alternative measurement methods: model errors need to be analyzed, e.g., LER, LWR

For more details:
S. Heidenreich: today’s talk, M10, Salon B, 16:50–17:15
Conclusions

- Simulation of scattered field by biperiodic grating possible with FEM and mortar method (unfortunately: slow)
- Shape derivatives can be computed by FEM
- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Uncertainties of reconstructed parameters can be estimated even by fast covariance-matrix method
- To get results closer to those obtained by alternative measurement methods: model errors need to be analyzed, e.g., LER, LWR

For more details:
S. Heidenreich: today’s talk, M10, Salon B, 16:50–17:15
Conclusions

- Simulation of scattered field by biperiodic grating possible with FEM and mortar method (unfortunately: slow)
- Shape derivatives can be computed by FEM
- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Uncertainties of reconstructed parameters can be estimated even by fast covariance-matrix method

To get results closer to those obtained by alternative measurement methods: model errors need to be analyzed, e.g., LER, LWR

For more details:
S. Heidenreich: today’s talk, M10, Salon B, 16:50–17:15
Conclusions

- Simulation of scattered field by biperiodic grating possible with FEM and mortar method (unfortunately: slow)
- Shape derivatives can be computed by FEM
- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Uncertainties of reconstructed parameters can be estimated even by fast covariance-matrix method
- To get results closer to those obtained by alternative measurement methods: model errors need to be analyzed, e.g., LER, LWR

For more details:
S. Heidenreich: today’s talk, M10, Salon B, 16:50–17:15
Conclusions

- Simulation of scattered field by biperiodic grating possible with FEM and mortar method (unfortunately: slow)
- Shape derivatives can be computed by FEM
- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Uncertainties of reconstructed parameters can be estimated even by fast covariance-matrix method
- To get results closer to those obtained by alternative measurement methods: model errors need to be analyzed, e.g., LER, LWR

For more details:
**S. Heidenreich**: today's talk, M10, Salon B, 16:50–17:15


Acknowledgment

The research has been supported by the BMBF (Federal Ministry of Education and Research):
- BMBF-Project CDuR 32: Schlüsseltechnologien zur Erschliessung der Critical Dimension (CD) und Registration (REG) Prozess- und Prozesskontrolltechnologien für die 32 nm-Maskenlithographie

We appreciate the cooperation/consultation with:


Thank you for your attention!