We consider a "diffractive optic" to be a biperiodic surface separating two half-spaces, each having constant constitutive parameters; within a unit cell of the periodic surface and across the transition zone between the two half-spaces, the constitutive parameters can be a continuous, complex-valued function. Mathematical models for diffractive optics have been developed, and implemented as numerical codes, both for the "direct" problem and for the "inverse" problem. In problems of the "direct" class, the diffractive optic is specified, and the full set of Maxwell's equations is cast in a variational form and solved numerically by a finite element approach. This approach is well-posed in the sense that existence and uniqueness of the solution can be proved and specific convergence conditions can be derived. An example of a metallic grating at a Wood anomaly is presented as a case where other approaches are known to have convergence problems. In problems of the "inverse" class, some information about the diffracted field (e.g., the far-field intensity) is given, and the problem is to find the periodic structure in some optimal sense. Two approaches are described: phase reconstruction in the far-field approximation; and relaxed optimal design based on the Helmholtz equation. Practical examples are discussed for each approach to the inverse problem, including array generators in the far-field case and antireflective structures for the relaxed optimal design.
Mathematical Modeling for Diffractive Optics

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Outline

Need
Statement of Problem
Overview of Approaches
Examples
Mathematical Modeling for Diffractive Optics

Classes of Problems

● The Direct Problem

Given the incident field and grating structure
Predict the behavior of the outgoing fields
Solve Maxwell’s equations rigorously

● The Inverse Problem

Given the incident field and the desired output field
Calculate the optimum structure
Model a scalar wave equation with simplifications
Definition of the Direct Problem

Time Harmonic, Source-free
Maxwell’s Eqs

\[ \nabla \times E - i\omega H = 0 \]

\[ \nabla \times H + i\omega \varepsilon E = 0 \]

\[ \varepsilon \in L_{\infty}(\Omega_0) \quad \varepsilon = \varepsilon_1 \text{ in } \Omega_1 \quad \varepsilon = \varepsilon_2 \text{ in } \Omega_2 \]

Find
Quasiperiodic Solutions
with Bounded Outgoing Waves

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Survey of Approaches to the Direct Problem

**Comments**

- Discretized grating profile
- PDE embedded in infinite set of coupled linear eqs
- Numerical implementation
  - truncate set of linear eqs
  - solve $Ax = b$
- Smooth grating profile
  - Infinite Taylor series for Rayleigh coef. (recursion)
  - Padé approximant sum of series

<table>
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<th>Approach</th>
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<td>1. Integral Method</td>
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<td>2. Differential Method</td>
<td>(coupled waves)</td>
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<td>3. Coupled Modes</td>
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<td>4. Variational Method</td>
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<td>5. Riemann-Hilbert Problem</td>
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<td>6. Analytic Continuation</td>
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Mathematical Modeling for Diffractive Optics

Honeywell / IMA Program

The Direct Problem

1. Integral Method (Maxcoll)  Dobson & Friedman  Singly periodic grating
                                 Simple profile(graph)

2. Variational Method (Maxfelm)  Dobson  Biperiodic grating
                                 General profile

3. Analytic Continuation (TBD)  Bruno & Reitich  Biperiodic grating
                                    Simple profile(function)

The Inverse Problem

1. Phase Reconstruction (Phaseopt)  Dobson  Scalar field / Fraunhofer approx
                                      Nonperiodic structures
                                      Nonlinear least squares method

2. Relaxed Optimization (Profopt)  Dobson  Scalar field / Helmholtz eq
                                      Singly periodic grating
                                      Complex profile
Mathematical Modeling for Diffractive Optics

Examples

The Direct Problem

1. Reflective Polarization Beamsplitter
2. LIGA Grating
3. Mixed Index Biperiodic Grating

The Inverse Problem

1. Phase Reconstruction  - Hypercube Beamsplitter
2. Relaxed Optimization  - Angle Optimized Motheye Structure
Reflective Polarization Beamsplitter

$\lambda = 0.78 \, \mu m$

$\theta = 45^\circ$

Maximize reflectivity

TE polarization (-1 order)

TM polarization (0 order)
Variational Method vs Coupled Waves Method

Variational Method
* - TE
+ - TM

Coupled Waves
o - TE
x - TM
Variational Method (Maxfelm) Example
LIGA Grating

\[ \lambda = 10.6 \, \mu m \]
TM polarization

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Variational Method (Maxfelm) Example

Mixed Index Biperiodic Grating

$\lambda = 0.55 \mu m$ (E $\parallel x_2$)

$\theta = 30^\circ$

$\Lambda = 0.5 \mu m$

X$_1$ or X$_2$

X$_3$
Fig. 2. Cross-section of the amplitude $|H|$, taken through the metal region in the $(x_2, x_3)$ plane.

Fig. 3. Cross-section of the amplitude $|H|$, taken through the non-absorptive region in the $(x_1, x_3)$ plane.
FIG. 4. Cross-section of the amplitude $|H|$, taken through the metal region in the $(x_1, x_2)$ plane.

FIG. 5. Cross-section of the amplitude $|H|$, taken below the metal region in the $(x_1, x_2)$ plane.
Dobson Method

Gerchberg Saxton Method
Relaxed Optimization (Profopt) Example

Optimized Moth Eye Grating

\[ \theta = \pm 70^\circ \]

\[ \lambda = 1.0 \, \mu m \]

Find structure of zero order grating to minimize reflectivity over range of incident angles

\[ n = 1.6 \]

\[ \Lambda = 0.5 \, \mu m \]
Relaxed Optimization (Profopt) Example
Mathematical Modeling for Diffractive Optics

Summary

The Direct Problem

Variational Approach with Finite Elements Method
- exhibits good convergence, numerical stability
- treats complicated biperiodic structures
- can be computationally intensive

Analytic Continuation Approach
- elegant solution
- limited domain of convergence and biperiodic structures
- computationally very fast

The Inverse Problem

Phase Reconstruction - comparable to other approaches

Relaxed Optimization - potential to identify new structures