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### Abstract

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**

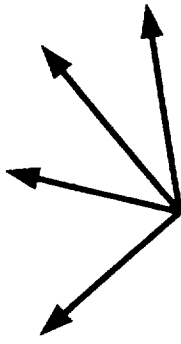
**Given the incident field and grating structure  
Predict the behavior of the outgoing fields  
Solve Maxwell's equations rigorously**

- **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

Reflected Orders



Time Harmonic, Source-free  
Maxwell's Eqs

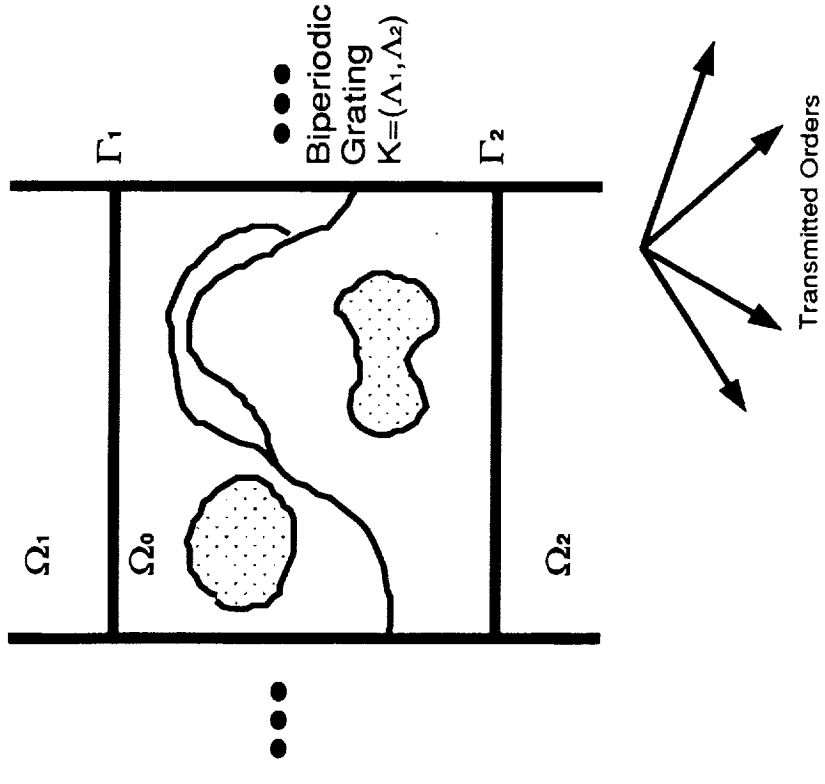
$$\nabla \times \mathbf{E} - i\omega \mathbf{H} = \mathbf{0}$$

$$\nabla \times \mathbf{H} + i\omega \epsilon \mathbf{E} = \mathbf{0}$$


$$\epsilon \in L^\infty(\Omega_0) \quad \epsilon = \epsilon_1 \text{ in } \Omega_1 \quad \epsilon = \epsilon_2 \text{ in } \Omega_2$$

Find

Quasiperiodic Solutions  
with Bounded Outgoing Waves



# Survey of Approaches to the Direct Problem

Approach	Comments
1. Integral Method	
2. Differential Method (coupled waves)	
3. Coupled Modes	
4. Variational Method	
5. Riemann-Hilbert Problem	
6. Analytic Continuation	
	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

# Mathematical Modeling for Diffractive Optics

## Honeywell / IMA Program

### The Direct Problem

- |                                    |                   |  |
|------------------------------------|-------------------|--|
| 1. Integral Method<br>(Maxcoll)    | Dobson & Friedman | Singly periodic grating<br>Simple profile(graph) |
| 2. Variational Method<br>(Maxfelm) | Dobson            | Biperiodic grating<br>General profile            |
| 3. Analytic Continuation<br>(TBD)  | Bruno & Reitich   | Biperiodic grating<br>Simple profile(function)   |

### The Inverse Problem

- |                                       |        |  |
|---------------------------------------|--------|--|
| 1. Phase Reconstruction<br>(Phaseopt) | Dobson | Scalar field / Fraunhofer approx<br>Nonperiodic structures<br>Nonlinear least squares method |
| 2. Relaxed Optimization<br>(Profopt)  | Dobson | Scalar field / Helmholtz eq<br>Singly periodic grating<br>Complex profile                    |

# Mathematical Modeling for Diffractive Optics

## Examples

### The Direct Problem

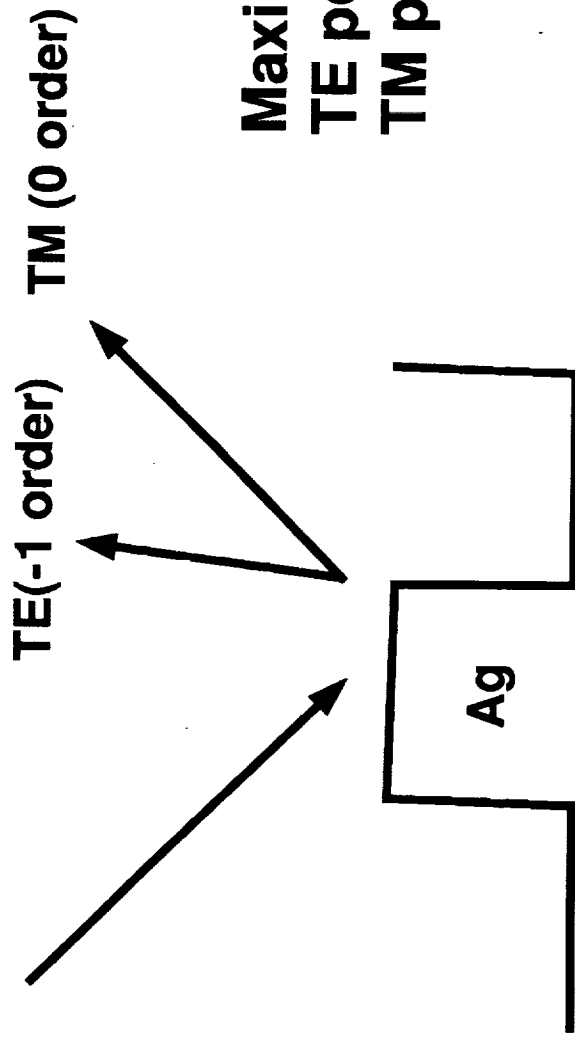
1. Reflective Polarization Beamsplitter
2. LIGA Grating
3. Mixed Index Biperiodic Grating

### The Inverse Problem

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

# Reflective Polarization Beamsplitter

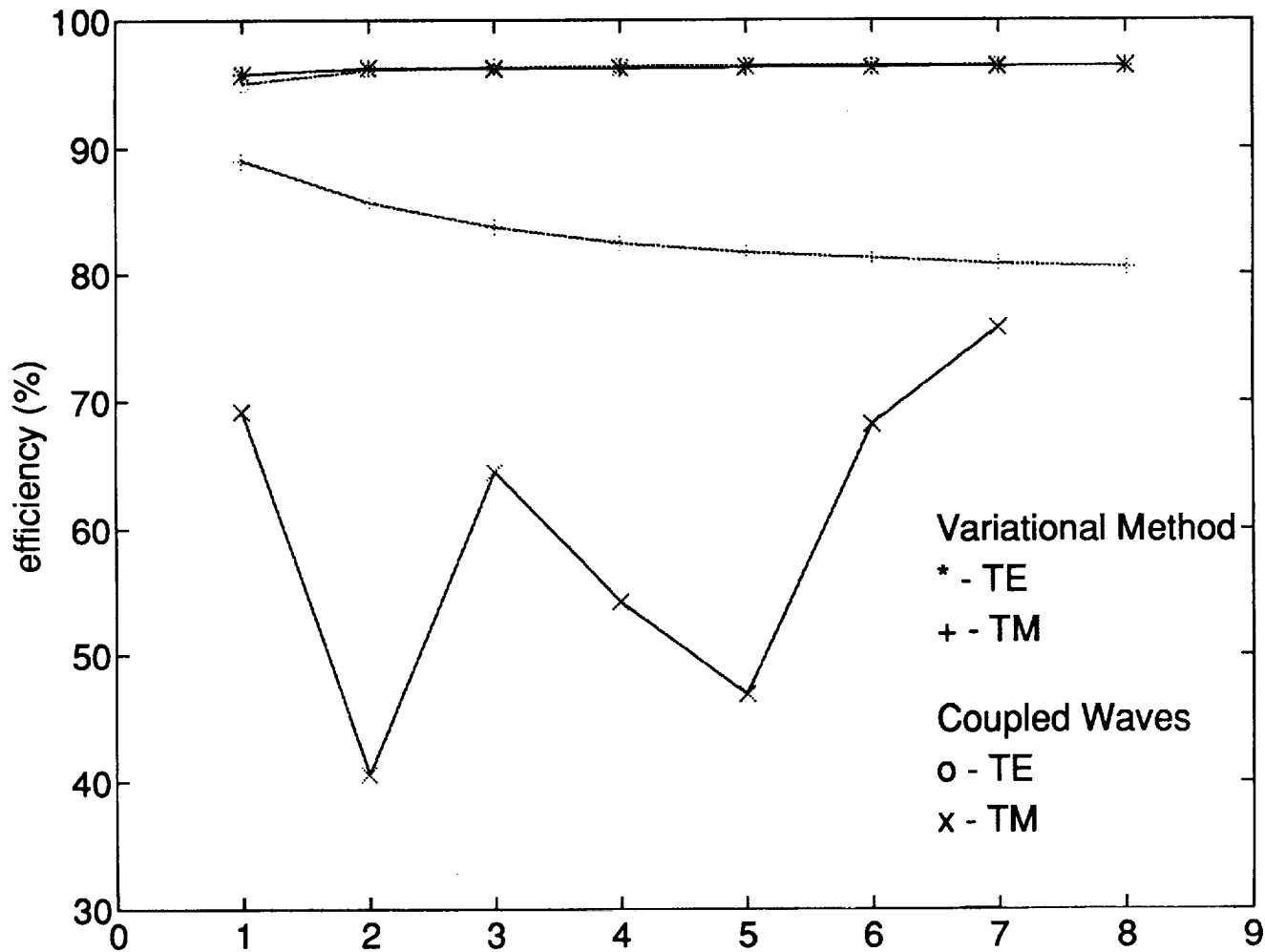
$\lambda = 0.78 \mu\text{m}$   
 $\theta = 45^\circ$



Maximize reflectivity  
TE polarization (-1 order)  
TM polarization (0 order)

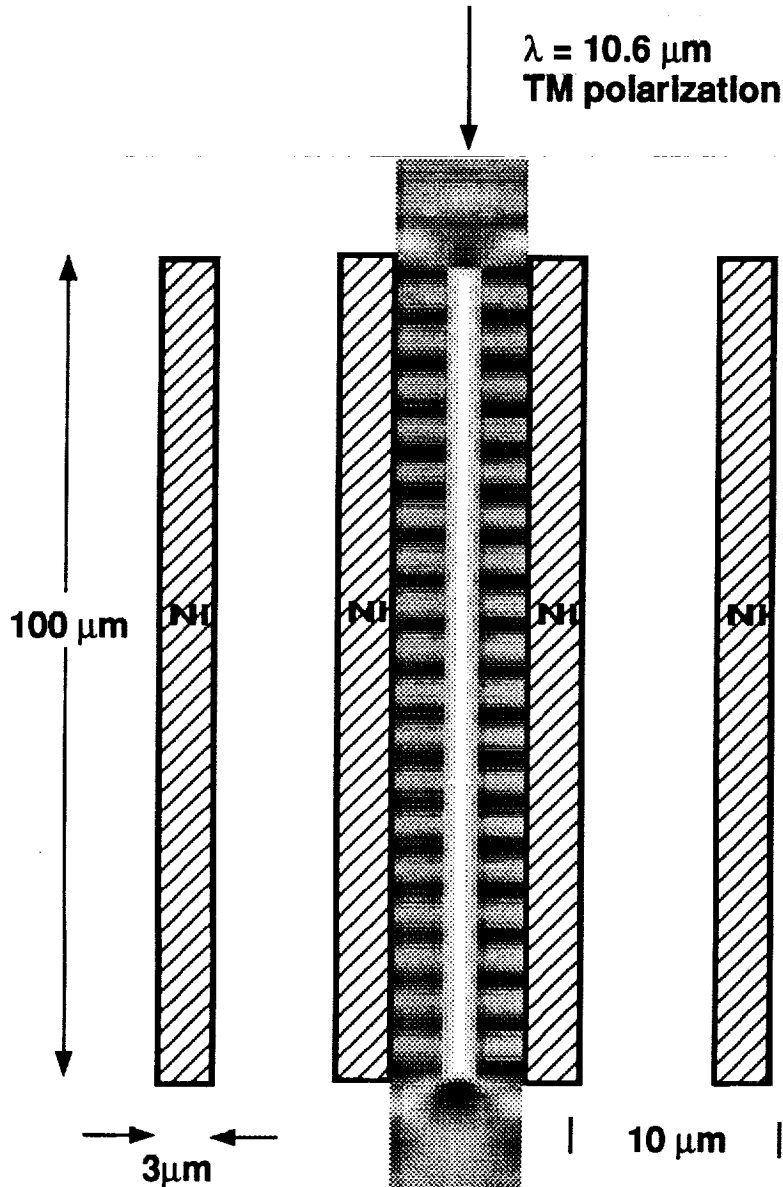


Variational Method vs Coupled Waves Method



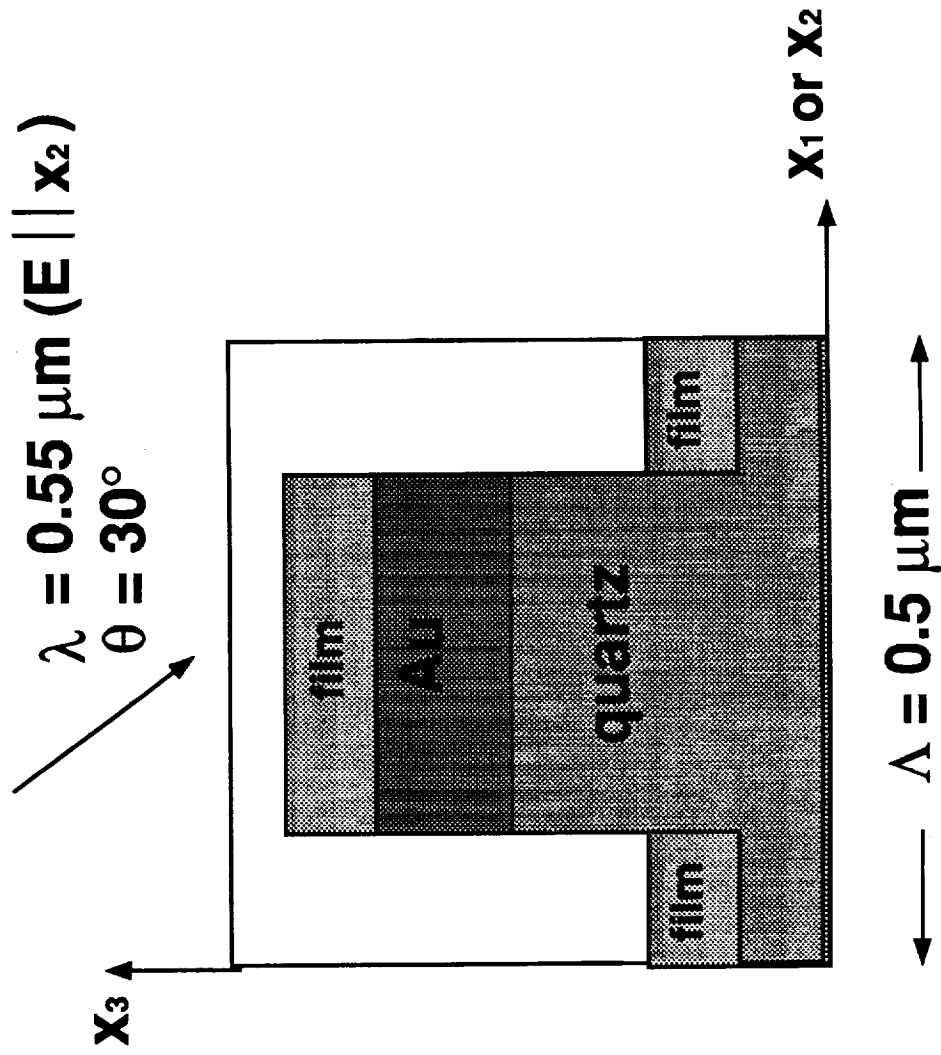
# Variational Method (Maxfelm) Example

## LIGA Grating



# Variational Method (Maxfilm) Example

## Mixed Index Biperiodic Grating



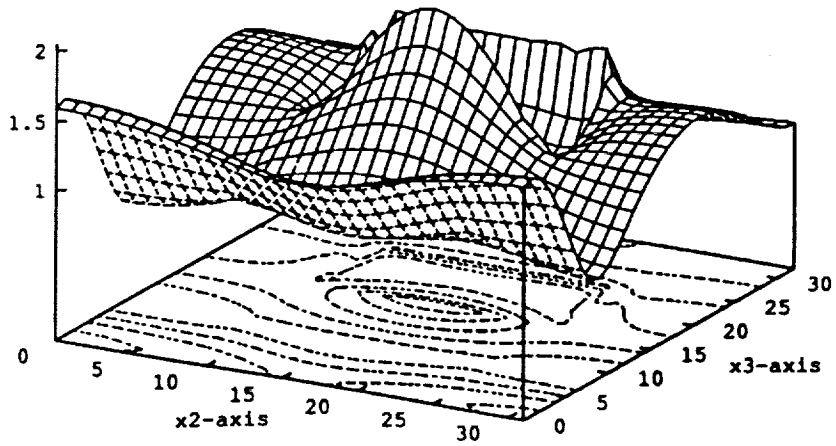


FIG. 2. Cross-section of the amplitude  $|H|$ , taken through the metal region in the  $(x_2, x_3)$  plane.

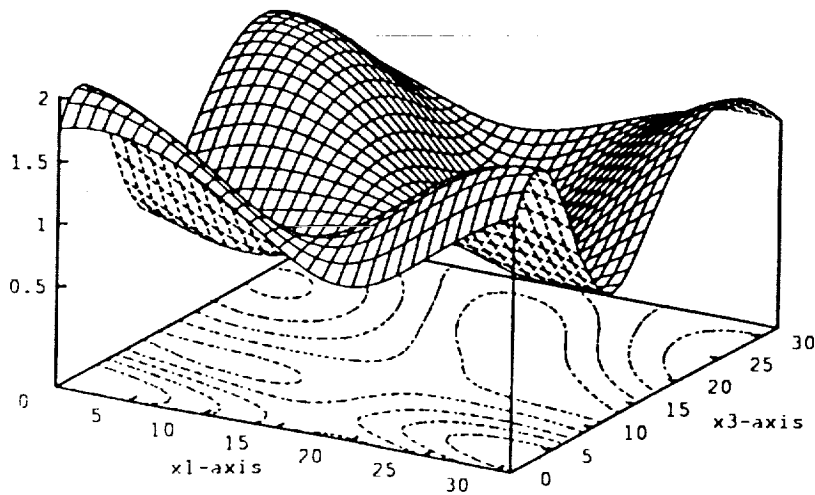


FIG. 3. Cross-section of the amplitude  $|H|$ , taken through the non-absorptive region in the  $(x_1, x_3)$  plane.

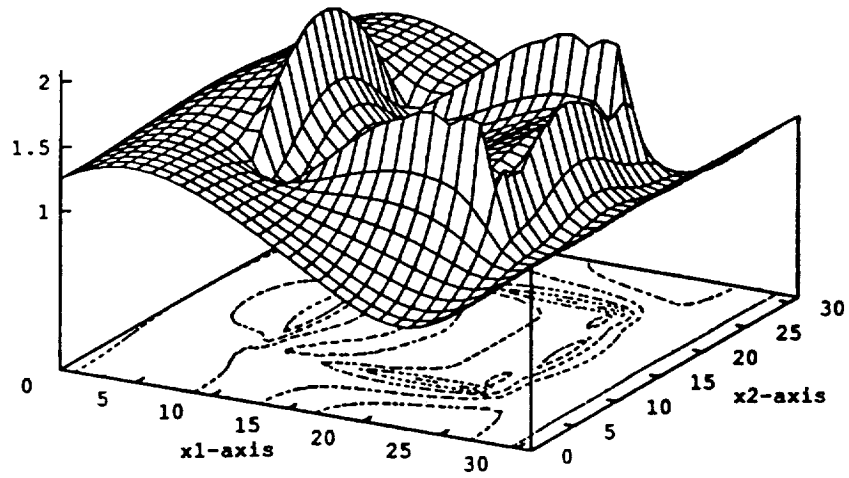


FIG. 4. Cross-section of the amplitude  $|H|$ , taken through the metal region in the  $(x_1, x_2)$  plane.

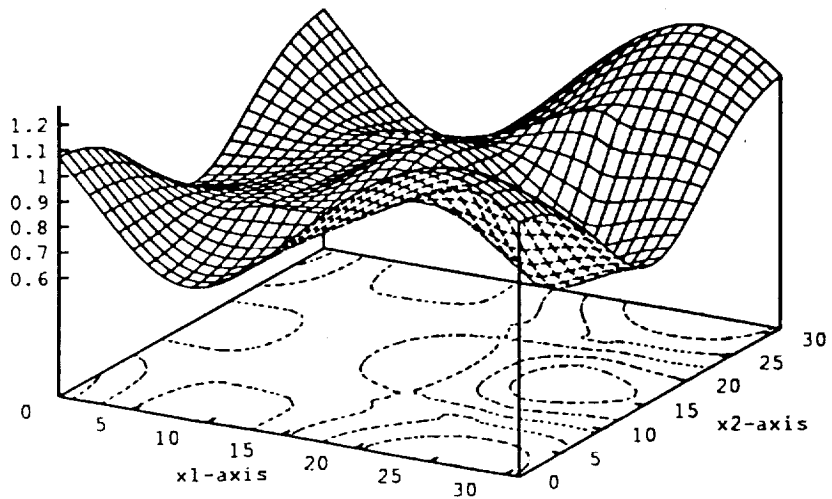
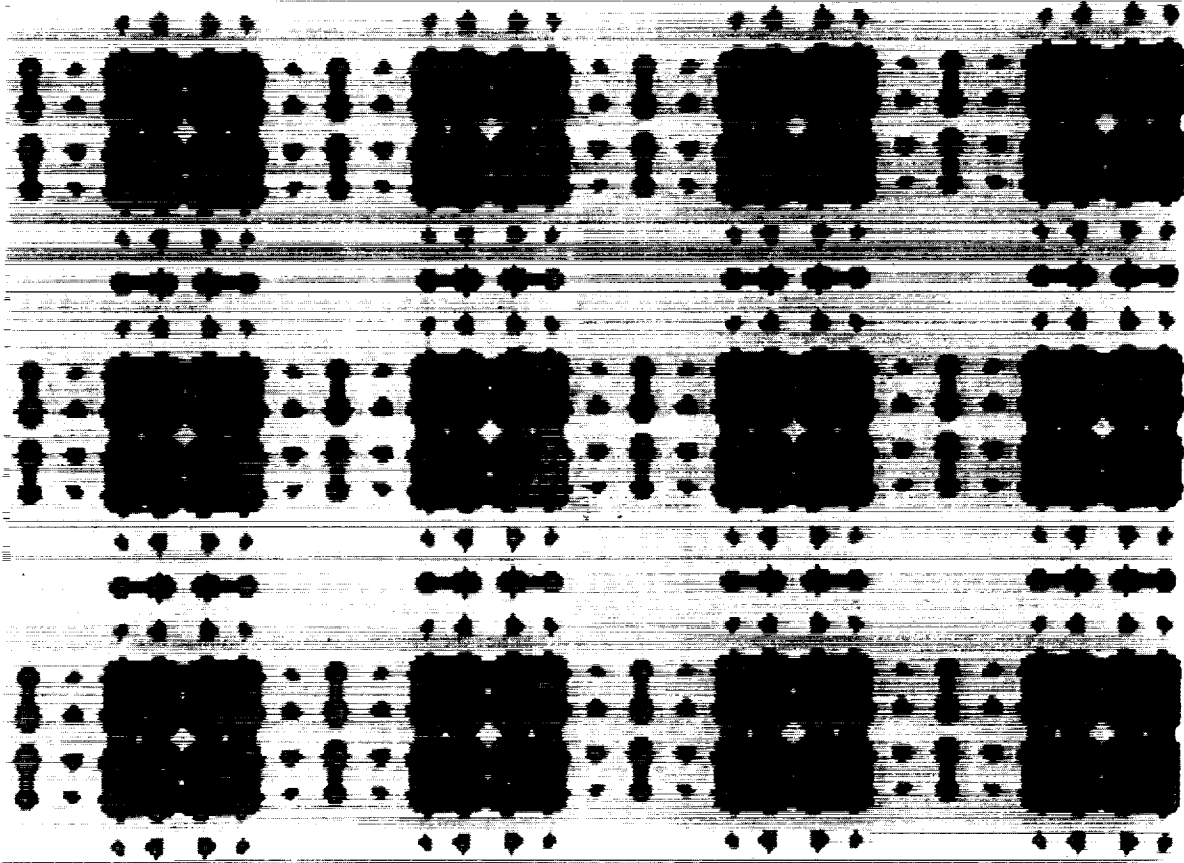
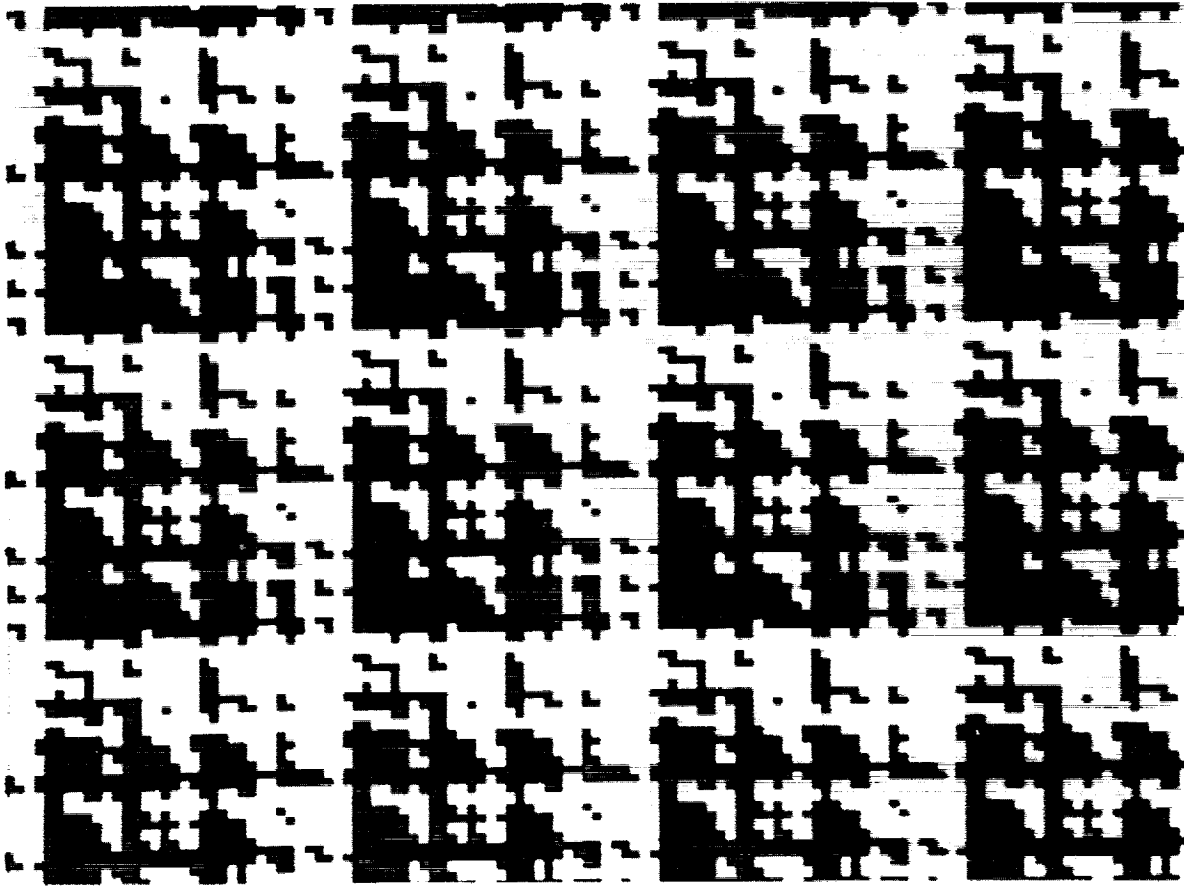


FIG. 5. Cross-section of the amplitude  $|H|$ , taken below the metal region in the  $(x_1, x_2)$  plane.



***Dobson Method***

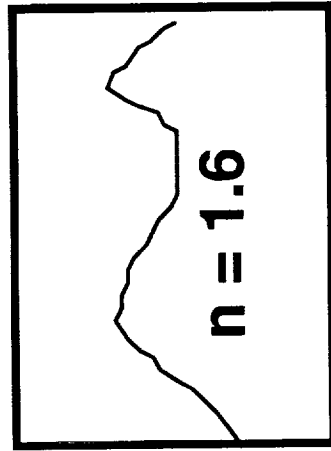
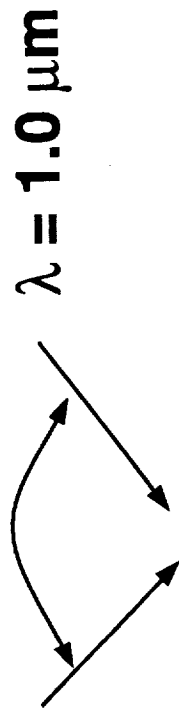


***Gerchberg Saxton Method***

# Relaxed Optimization (Profopt) Example

## Optimized Moth Eye Grating

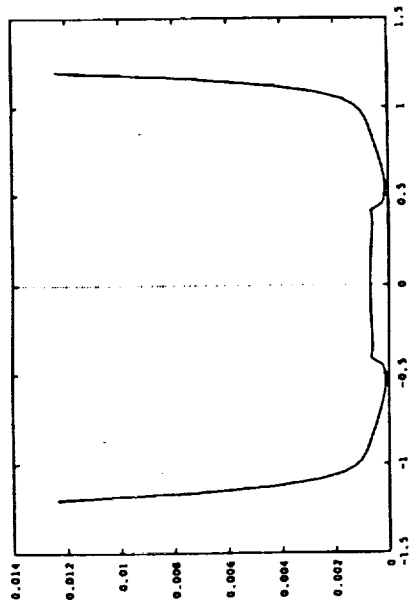
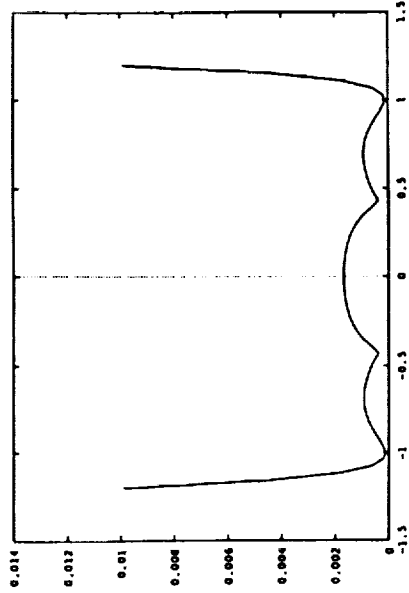
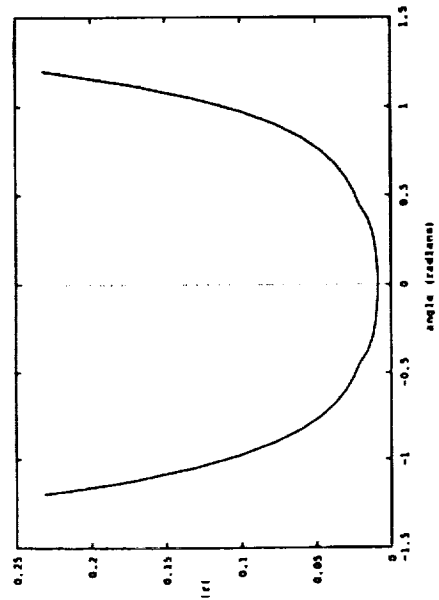
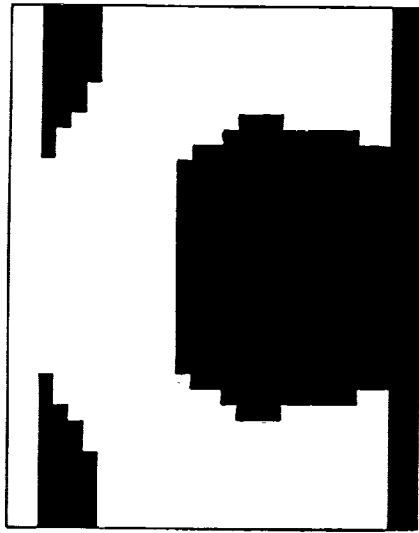
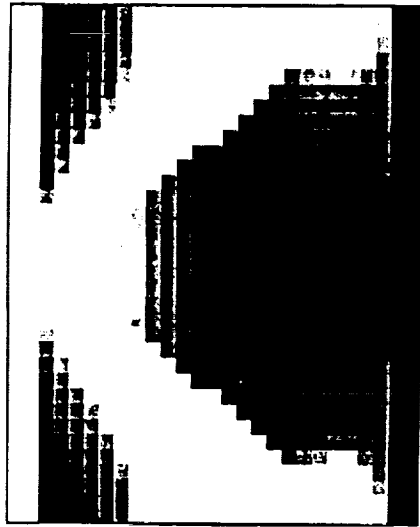
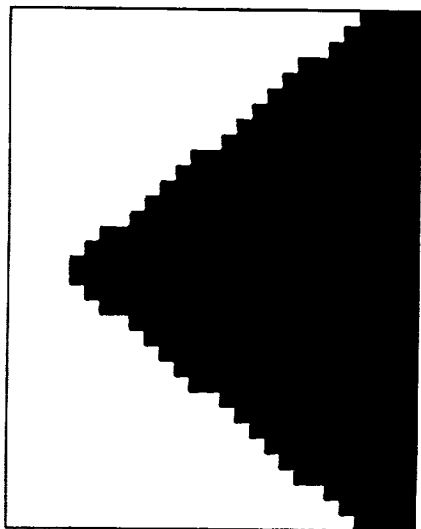
$$\theta = \pm 70^\circ$$



$$\Lambda = 0.5 \mu\text{m}$$

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

# 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

