

A computational inverse diffraction grating problem

Gang Bao,^{1,2} Peijun Li,^{3,*} and Haijun Wu⁴

¹Department of Mathematics, Zhejiang University, Hangzhou 310027, China

²Department of Mathematics, Michigan State University, East Lansing, Michigan 48824, USA

³Department of Mathematics, Purdue University, West Lafayette, Indiana 47907, USA

⁴Department of Mathematics, Nanjing University, Jiangsu 210093, China

*Corresponding author: lipeijun@math.purdue.edu

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Consider the diffraction of a time-harmonic plane wave incident on a perfectly reflecting periodic surface. A continuation method on the wavenumber is developed for the inverse diffraction grating problem, which reconstructs the grating profile from measured reflected waves a constant distance away from the structure. Numerical examples are presented to show the validity and efficiency of the proposed method. © 2012 Optical Society of America

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1. INTRODUCTION

Consider a time-harmonic electromagnetic plane wave incident on a slab of some optical material, often referred to as grating material, that is periodic in the x -direction. Throughout, we assume that the material is invariant in the z -direction. Thus the model problem of the three-dimensional Maxwell equations can be reduced to a simpler model problem of the two-dimensional Helmholtz equation. The more complicated bi-periodic diffraction problem will be considered in a separate work. The scattering theory in periodic structures has many applications in micro-optics, where periodic structures are often called diffraction gratings. Diffractive optics is an emerging technology with many applications, which include the design and fabrication of optical elements such as corrective lenses, antireflective interfaces, beam splitters, and sensors.

Recently, the scattering of electromagnetic waves in a periodic structure has received considerable attention in the applied mathematics community and has been studied extensively by either integral equation methods (e.g., [1]) or variational approaches (e.g., [2]). We refer to Bao *et al.* [2] and references cited therein for the mathematical studies of the existence and uniqueness of the diffraction grating problem. Numerical methods based on both an integral equation method and a variational (finite element) method have been developed in [3,4]. A good introduction to the problem of electromagnetic diffraction through periodic structures, along with some numerical methods, can be found in Petit [5]. A more recent review on diffractive optics technology and its mathematical modeling can be found in Bao *et al.* [6].

In this work, we are concerned with the numerical solution of the inverse diffraction problem, which may be described as follows: given the incident field, determine the grating structure from a measured reflected field a constant distance away from the structure. Besides the intrinsic motivation and potential applications in the optical sciences, the inverse diffraction problem also arises naturally in the study of optimal design problems in diffractive optics, which is to design a grating structure that gives rise to some specified far-field patterns

(see, e.g., the optimal design of antireflective and blazed diffraction gratings by Dobson [7,8] and the optimal design of binary gratings by Elschner and Schmidt [9,10]).

The mathematical questions on uniqueness and stability for the inverse diffraction problem of both the two-dimensional Helmholtz equation and the three-dimensional Maxwell equations have been studied by Kirsch [11], Bao [12], Ammari [13], Hettlich and Kirsch [14], Bao and Friedman [15], Bao and Zhou [16], Bao *et al.* [17], and Bruckner *et al.* [18]. We refer to [6] for a survey of recent developments in the mathematical modeling of optimal design and inverse problems for diffractive optics. A complete account of the general theory of inverse scattering problems in general (nonperiodic) structures may be found in the book by Colton and Kress [19] and references cited therein.

Computationally, various numerical methods have been proposed for the reconstruction of the grating profile of perfectly conducting gratings, e.g., García and Nieto-Vesperinas [20] (within the validity of Rayleigh's hypothesis [21,22]), Ito and Reitich [23], Arens and Kirsch [24], Hettlich [25], and Bruckner and Elschner [26]. Elschner *et al.* [27] proposed an algorithm for the recovery of a two-dimensional periodic structure based on finite elements and optimization techniques. Our goal in this work is to present an efficient continuation method that solves the nonlinear inverse diffraction grating problem in a one-dimensional perfectly reflecting structure based on a single-layer potential representation [26]. The algorithm requires multifrequency data, and the iterative steps are obtained by a continuation method with respect to the wavenumber: at each step a nonlinear Landweber iteration is applied, with the starting point given by the output from the previous step at a lower wavenumber. Thus, at each stage an approximation to the grating surface filtered at a higher frequency is created. Starting from a reasonable initial guess, the continuation method is shown to converge for a larger class of surfaces than the usual Newton's method using the same initial guess. We refer to Chen [28] and Bao and Li [29–31] for closely related inverse medium scattering

problems in the two-dimensional Helmholtz equation and three-dimensional Maxwell's equations, where recursive linearization methods were proposed through a continuation with respect to either the wavenumber or the spatial frequency. For a nonperiodic perfectly reflecting surface scattering problem, we refer to Coifman *et al.* [32] for discussions on an operator expansion method for the direct and inverse scattering, where a similar continuation method with respect to the wavenumber was proposed to reconstruct the nonperiodic surface. We also refer to Ammari *et al.* [33] for stability and resolution analysis in the presence of measurement noise for a topological derivative based imaging functional.

The plan of this paper is as follows. The mathematical modeling of the diffraction grating is briefly presented in Section 2. In Section 3, a continuation method for solving the inverse diffraction problem is proposed and a nonlinear Landweber iteration is presented. Numerical examples are presented in Section 4, and the paper is concluded with some remarks and directions for future research in Section 5.

2. A MODEL PROBLEM

Let us first specify the problem geometry. Since the grating surface is periodic in the variable x of period Λ , we may then restrict it to a single period in x , as seen in Fig. 1. Let the profile of the diffraction grating in one period be described by the curve

$$S = \{(x, y) \in \mathbb{R}^2 : y = f(x), 0 < x < \Lambda\},$$

which is assumed to be above the x axis. Here f is assumed to be a periodic function of period Λ . Let $\Omega = \{(x, y) \in \mathbb{R}^2 : y > f(x), 0 < x < \Lambda\}$ be filled with a material whose dielectric permittivity and magnetic permeability are ε and μ , respectively. Denote as $\omega > 0$ the angular frequency, and the wavenumber as $\kappa = \omega\sqrt{\varepsilon\mu}$. Assume that a plane wave of the form $u^{\text{inc}} = e^{i(\alpha x - \beta y)}$ is incident on the grating surface S from the top, where $\alpha = \kappa \sin \theta$, $\beta = \kappa \cos \theta$, and $\theta \in (-\pi/2, \pi/2)$ is the angle of incidence. For convenience, ε and μ are assumed to be equal to unity everywhere, i.e., $\kappa = \omega$. For $n \in \mathbb{Z}$, let $\alpha_n = \alpha + 2\pi n/\Lambda$, and denote

$$\beta_n = \begin{cases} \sqrt{\kappa^2 - \alpha_n^2}, & \text{for } \kappa > |\alpha_n|, \\ i\sqrt{\alpha_n^2 - \kappa^2}, & \text{for } \kappa < |\alpha_n|. \end{cases}$$

We exclude ‘‘resonance’’ by assuming that $\kappa \neq |\alpha_n|$ for all $n \in \mathbb{Z}$. The diffraction of time-harmonic electromagnetic waves in the transverse electric mode (TE polarization) by a one-dimensional perfectly reflecting grating can be formulated as follows: to find the diffracted field u such that

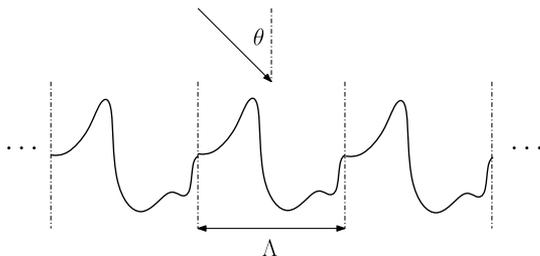


Fig. 1. Problem geometry.

$$\Delta u + \kappa^2 u = 0, \quad \text{in } \Omega, \tag{1}$$

$$u + u^{\text{inc}} = 0, \quad \text{on } S. \tag{2}$$

Motivated by uniqueness, we shall seek the quasiperiodic solution, i.e., solution u , for which $ue^{-i\alpha x}$ is Λ periodic in x . Moreover, the diffracted field u is required to be bounded by outgoing plane waves in Ω . It follows from Rayleigh's expansion that u can be expressed as a sum of plane waves:

$$u = \sum_{n \in \mathbb{Z}} A_n e^{i\alpha_n x + i\beta_n y}, \quad y > \max_{x \in (0, \Lambda)} f(x), \tag{3}$$

where the coefficient A_n is a complex scalar. Each term $n \in \{n: |\alpha_n| < \kappa\}$ of the outgoing wave in Eq. (3) represents a propagating plane wave. If $|n|$ is large $n \in \{n: |\alpha_n| > \kappa\}$, then the corresponding term in Eq. (3) represents an evanescent wave that exponentially decays with respect to y and $|n|$. As pointed out, the direct scattering problem has been well studied and will not be discussed in this paper. This work is to study the inverse problem of grating profile reconstruction: given the incident wave u^{inc} , determine the profile $y = f(x)$ from the measurements of the diffracted field at a straight line:

$$\Gamma = \{(x, y_0) \in \mathbb{R}^2 : x \in (0, \Lambda), y_0 > \max_{x \in (0, \Lambda)} f(x)\},$$

i.e., the near-field data $u(x, y_0)$.

3. RECONSTRUCTION METHOD

Following Bruckner and Elschner [26], we begin with the single-layer potential representation for the diffracted field:

$$u(x, y) = \int_0^\Lambda \phi(s) G(x, y; s, 0) ds, \tag{4}$$

with an unknown periodic density function ϕ in $L^2(0, \Lambda)$, where the free-space quasiperiodic Green function is given explicitly as

$$G(x, y; s, t) = \frac{i}{2\pi} \sum_{n \in \mathbb{Z}} \frac{1}{\beta_n} e^{i\alpha_n(x-s) + i\beta_n|y-t|}, \quad (x, y) \neq (s, t). \tag{5}$$

This function is well-defined, i.e., $\beta_n \neq 0$, since the resonance is excluded by assuming $\kappa \neq |\alpha_n|$. We then have

$$u(x, y_0) = \int_0^\Lambda \phi(s) G(x, y_0; s, 0) ds. \tag{6}$$

Since the unknown density ϕ is assumed to be a periodic function with periodicity Λ , it admits a Fourier series expansion

$$\phi(s) = \sum_{n \in \mathbb{Z}} \phi_n e^{i\alpha_n s}, \tag{7}$$

where ϕ_n is the Fourier coefficient of ϕ . It follows from the quasiperiodicity of $u(x, y_0)$ that

$$u(x, y_0) = \sum_{n \in \mathbb{Z}} u_n e^{i\alpha_n x}, \tag{8}$$

where u_n can be calculated from the measurement

$$u_n = \frac{1}{\Lambda} \int_0^\Lambda u(x, y_0) e^{-i\alpha_n x} dx. \tag{9}$$

Combining the above expansions yields

$$\phi_n = -i\beta_n u_n e^{-i\beta_n y_0}. \tag{10}$$

We define the operator $T_f: L^2(0, \Lambda) \rightarrow L^2(0, \Lambda)$:

$$(T_f \phi)(x) = \int_0^\Lambda \phi(s) G(x, f(x); s, 0) ds. \tag{11}$$

Substituting Eqs. (7) and (10) and the quasiperiodic Green function [Eq. (5)] into Eq. (11) gives

$$(T_f \phi)(x) = \sum_{n \in \mathbb{Z}} \psi_n e^{i\alpha_n x + i\beta_n f(x)},$$

where $\psi_n = u_n e^{-i\beta_n y_0}$. In practice, some regularization should be employed in order to suppress the possible exponential growth of noise [34]:

$$\psi_n = \begin{cases} u_n e^{-i\sqrt{k^2 - \alpha_n^2} y_0}, & \text{for } k > |\alpha_n|, \\ u_n \frac{e^{-\sqrt{\alpha_n^2 - k^2} y_0}}{e^{-2\sqrt{\alpha_n^2 - k^2} y_0 + \gamma}}, & \text{for } k < |\alpha_n|, \end{cases} \tag{12}$$

where γ is some positive regularization parameter. Because of the perfectly conducting condition [Eq. (2)], we may study the nonlinear problem

$$\left\| (T_f \phi)(x) + u^{\text{inc}}(x, f(x)) \right\|_{L^2(0, \Lambda)}^2 = 0,$$

which yields, after substituting the expansion for the operator T_f ,

$$\left\| \sum_{n \in \mathbb{Z}} \psi_n e^{i\alpha_n x + i\beta_n f(x)} + e^{i(\alpha x - \beta f(x))} \right\|_{L^2(0, \Lambda)}^2 = 0.$$

Though the summation has infinitely many terms of evanescent waves, it could be truncated into finite summation with arbitrary accuracy due to its exponential decay with respect to $|n|$. Choosing a sufficiently large N , we consider the numerical solution of the following nonlinear equation:

$$\left\| \sum_{|n| \leq N} \psi_n e^{i\alpha_n x + i\beta_n f(x)} + e^{i(\alpha x - \beta f(x))} \right\|_{L^2(0, \Lambda)}^2 = 0. \tag{13}$$

The profile $f(x)$ is a real Λ -periodic function. Without the loss of generality, the period Λ is taken to be 2π from now on. Since the profile $f(x)$ is a periodic function with periodicity 2π , it has the following Fourier series expansion:

$$f(x) = c_0 + \sum_{m=1}^\infty [c_{2m-1} \cos(mx) + c_{2m} \sin(mx)], \tag{14}$$

where m is exactly the m th Fourier mode for the 2π -periodic function $f(x)$, which may have finitely or infinitely many Fourier modes. In practice, the infinite series [Eq. (14)] needs to be approximated by truncating the expansion into a finite series:

$$f(x) \approx c_0 + \sum_{m=1}^M [c_{2m-1} \cos(mx) + c_{2m} \sin(mx)]. \tag{15}$$

Theoretically, for sufficiently large M , the finite series representation [Eq. (15)] can either fully recover the original grating profile, if f has finitely many Fourier modes, or reasonably approximate the original profile, if f has infinitely many Fourier modes. Therefore, it is necessary to determine all the Fourier coefficients $c_0, c_1, c_2, \dots, c_{2M-1}, c_{2M}$ in order to reconstruct the grating profile.

Because of the nonlinearity of Eq. (13), we propose a continuation method to recursively reconstruct these Fourier coefficients. The method proceeds as follows to solve the nonlinear equation [Eq. (13)].

- Step 1. Set the initial approximation $c_0 = y_0$, with $c_j = 0, j = 1, 2, \dots$
- Step 2. Choose an initial value for the wavenumber κ , and seek an approximation to the function $f(x)$ by a Fourier series with Fourier modes not exceeding the wavenumber κ :

$$f_k(x) = c_0 + \sum_{m=1}^k [c_{2m-1} \cos(mx) + c_{2m} \sin(mx)],$$

where k is taken to be the largest integer that is smaller or equal to the wavenumber κ . Denote $\mathbf{C}_k = [c_0, c_1, \dots, c_{2k-1}, c_{2k}]^\top$, where \top denotes transpose. For incident angle $\theta_l \in (-\pi/2, \pi/2), l = 1, 2, \dots, L$, define

$$g_l(\mathbf{C}_k, x) = \sum_{|n| \leq N} \psi_n e^{i\alpha_n x + i\beta_n f(x)} + e^{i(\alpha x - \beta f(x))},$$

$$H_l(\mathbf{C}_k) = \int_0^{2\pi} |g_l(\mathbf{C}_k, x)|^2 dx.$$

Now we denote $\mathbf{H}(\mathbf{C}_k) = [H_1(\mathbf{C}_k), \dots, H_L(\mathbf{C}_k)]^\top$. Then the nonlinear equation [Eq. (13)] could be reformulated as

$$\mathbf{H}(\mathbf{C}_k) = 0,$$

where $\mathbf{H}: \mathbb{R}^{2k+1} \rightarrow \mathbb{R}^L$. In order to reduce the computational cost and instability, we consider the nonlinear Landweber iteration [34],

$$\mathbf{C}_k^{(i+1)} = \mathbf{C}_k^{(i)} - \tau_k \mathbf{D}\mathbf{H}^\top(\mathbf{C}_k^{(i)}) \mathbf{H}(\mathbf{C}_k^{(i)}), \quad i = 1, 2, \dots,$$

where τ_k is a relaxation parameter and the Jacobi matrix

$$\mathbf{D}\mathbf{H} = \left(\frac{\partial H_l}{\partial c_j} \right)_{l=1, \dots, L, j=0, 1, \dots, 2k}$$

can be computed explicitly. So, we solve for coefficients c_j using the above nonlinear Landweber method with the

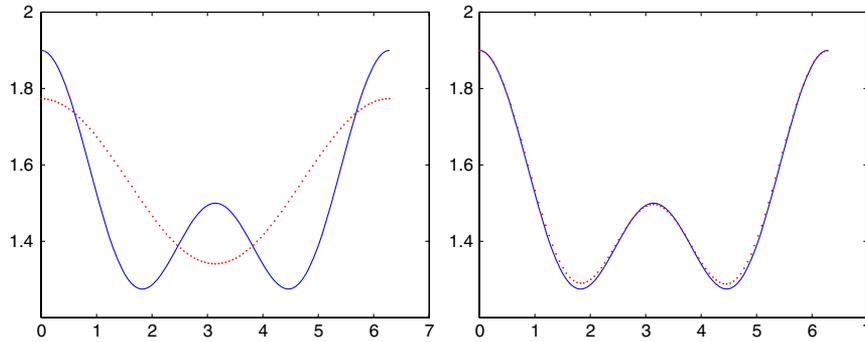


Fig. 2. (Color online) Evolution of the reconstructions in Example 1. Solid curve, test profile; dotted curve, reconstructed profile. Left: reconstruction at $\kappa = 1$. Right: reconstruction at $\kappa = 2$.

previous approximation as the starting point. The resulting solution represents the Fourier coefficients of $f(x)$ corresponding to the frequencies not exceeding k .

- Step 3. Increase k to a new value \tilde{k} , which is again the largest integer smaller than or equal to the wavenumber $\tilde{\kappa} > \kappa$ for the next available data. We repeat Step 2 with the previous approximation to $f(x)$ as our starting point. More precisely, we approximate $f(x)$ by the Fourier series

$$\tilde{c}_0 + \sum_{m=1}^{\tilde{k}} [\tilde{c}_{2m-1} \cos(mx) + \tilde{c}_{2m} \sin(mx)]$$

and determine the coefficients \tilde{c}_j , $j = 0, 1, \dots, \tilde{k}$, by using the nonlinear Landweber method starting from the previous result:

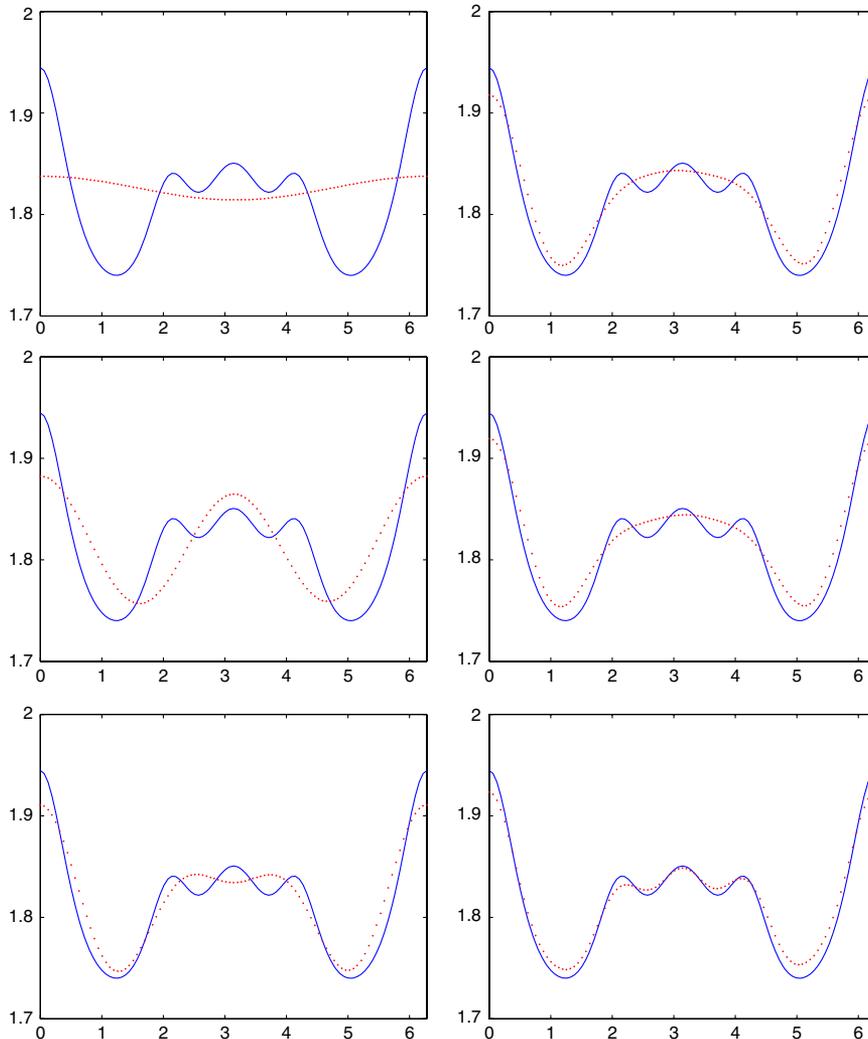


Fig. 3. (Color online) Evolution of the reconstructions in Example 2. Solid curve, test profile; dotted curve, reconstructed profile. Left column from top to bottom: reconstruction at $\kappa = 1$, reconstruction at $\kappa = 2$, reconstruction at $\kappa = 3$. Right column from top to bottom: reconstruction at $\kappa = 4$, reconstruction at $\kappa = 5$, reconstruction at $\kappa = 6$.

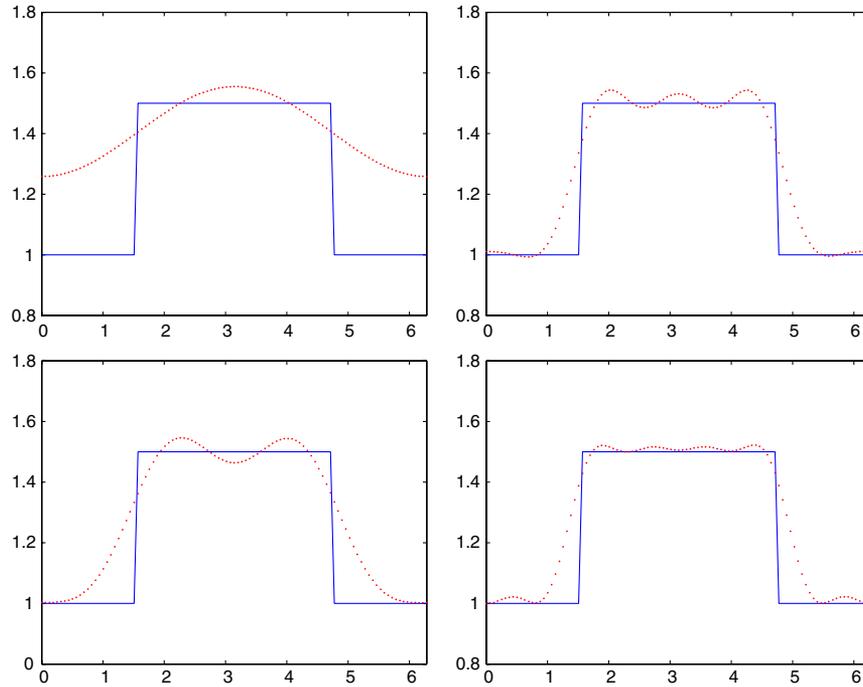


Fig. 4. (Color online) Evolution of the reconstructions in Example 3. Solid curve, test profile; dotted curve, reconstructed profile. Left column from top to bottom: reconstruction at $\kappa = 1$, reconstruction at $\kappa = 3$. Right column from top to bottom: reconstruction at $\kappa = 5$, reconstruction at $\kappa = 7$.

$$\tilde{c}_j = \begin{cases} c_j, & \text{for } j \leq 2k, \\ 0, & \text{for } j > 2k, \end{cases}$$

where the coefficients c_j come from Step 2. The resulting solution in this step represents the Fourier coefficients of $f(x)$ corresponding to the frequencies not exceeding \tilde{k} .

We now repeat Step 3 until a prescribed frequency is reached. For a complete reconstruction we need to choose the prescribed wavenumber larger than the highest Fourier mode of the grating profile. Numerical experiments have shown that the continuation method described above converges for a larger class of surfaces than the usual Newton's method starting at the same initial guess of y_0 .

4. NUMERICAL EXPERIMENTS

Here we present the results of numerical experiments using our method. The near-field measurements $u(x, y_0)$ are simulated by solving the direct problem using an adaptive finite element method with a perfectly matched absorbing layer [4,35]. For a simple stability analysis, some relative random noise is added to the data, i.e., the diffracted field measurement is updated with

$$u(x, y_0) := u(x, y_0)(1 + \sigma \text{rand}),$$

where rand represents normally distributed random numbers in $[-1, 1]$ and σ is the noise level. In the following experiments, The unknown profile will be probed by incoming incident plane waves with incident angle $\theta_l = -\pi/3 + 2\pi l/18$, $l = 0, 1, \dots, 6$. The noise level σ and regularization parameter γ are taken as 0.02 and 10^{-6} , respectively. The truncation of the infinite summation in Eq. (13) is taken as $N = 8$.

Example 1. Reconstruct a finite Fourier grating

$$f(x) = 1.5 + 0.2 \cos x + 0.2 \cos 2x.$$

This is a simple example, since the profile only contains a few Fourier modes. The diffractive field is measured at $y_0 = 2.1$, and the relaxation parameter $\tau_k = 0.002/\kappa$. The graphs of this tested profile and the reconstructed profiles with a different wavenumber κ are shown in Fig. 2. Since the tested profile consists of a couple of low frequencies, only a few iterations are needed to get a good reconstruction.

Example 2. Reconstruct a smooth infinite Fourier grating

$$f(x) = 1.7 + 0.05e^{\cos 2x} + 0.04e^{\cos 3x}.$$

The diffractive field is measured at $y_0 = 2.1$, and the relaxation parameter $\tau_k = 0.002/k$. The graphs of this tested profile and the reconstructed profiles with a different wavenumber k are shown in Fig. 3. As we can see, this grating profile contains more Fourier modes. It is expected that incident waves with higher frequencies are needed in order to recover those Fourier modes for the grating profile and to get a good resolution of the reconstruction.

Example 3. Reconstruct a binary grating

$$f(x) = \begin{cases} 1.5, & \text{for } x \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right), \\ 1.0, & \text{otherwise.} \end{cases}$$

The diffractive field is measured at $y_0 = 2.0$, and the relaxation parameter $\tau_k = 0.0001/k$. The graphs of this tested profile and the reconstructed profiles with a different wavenumber k are shown in Fig. 4. The profile is a piecewise constant function and thus contains infinitely many Fourier modes with slow decay of the Fourier coefficients. Clearly, incident fields

with even higher wavenumbers and more iterations are needed to get a reasonable reconstruction. In addition, the Gibbs phenomenon appears in the reconstructed surface because of the discontinuity.

5. CONCLUSION

We presented an efficient continuation method for reconstructing the diffraction grating profile. The continuation proceeds along the wavenumber, and a nonlinear Landweber iteration is done at each step. Experimentally, the proposed continuation method converges for a larger class of surfaces, starting at a reasonable initial guess $c_0 = y_0$. Although our numerical examples demonstrate the convergence of the method, no rigorous convergence analysis is available. We plan to investigate the convergence properties of the continuation method and the reconstruction of the grating profile from the far-field measurement, i.e., to reconstruct the grating profile from the far-field pattern of the reflected field. It will be interesting and may be more practical to study the inverse diffraction grating problem by using phaseless measurements. We also plan to extend the method to solve the inverse diffraction grating problem for three-dimensional Maxwell's equations.

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