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INVERSE ELECTROMAGNETIC SCATTERING PROBLEMS BY A DOUBLY PERIODIC STRUCTURE*

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Abstract. Consider the problem of scattering of electromagnetic waves by a doubly periodic structure. The medium above the structure is assumed to be inhomogeneous characterized completely by an index of refraction. Below the structure is a perfect conductor or an imperfect conductor partially coated with a dielectric. Having established the well-posedness of the direct problem by the variational approach, we prove the uniqueness of the inverse problem, that is, the unique determination of the doubly periodic grating with its physical property and the index of refraction from a knowledge of the scattered near field by a countably infinite number of incident quasi-periodic electromagnetic waves. A key ingredient in our proofs is a novel mixed reciprocity relation derived in this paper.

Key words. Uniqueness, Maxwell's equations, inhomogeneous medium, doubly periodic structure, mixed boundary conditions, mixed reciprocity relation, inverse problem.

AMS subject classifications. 32P25, 35R30.

1. Introduction. Scattering theory in periodic structures has many applications in micro-optics, radar imaging and non-destructive testing. We refer to [20] for historical remarks and details of these applications. This paper is concerned with direct and inverse problems of electromagnetic scattering by a doubly periodic structure. The medium above the structure is assumed to be inhomogeneous. Below the structure is a perfect conductor which may be partially coated with a dielectric.

Let the doubly periodic structure be described by the doubly periodic surface

$$\Gamma_1 := \{x \in \mathbb{R}^3 \,|\, x_3 = f(x_1, x_2)\},$$

where $f \in C^2(\mathbb{R}^2)$ is a 2π-periodic function of x_1 and x_2:

$$f(x_1 + 2n_1\pi, x_2 + 2n_2\pi) = f(x_1, x_2) \quad \forall n = (n_1, n_2) \in \mathbb{Z}^2.$$

Assume that the medium above the structure Γ_1 is filled with an inhomogeneous, isotropic, conducting or dielectric medium of electric permittivity $\epsilon > 0$, magnetic permeability $\mu > 0$ and electric conductivity $\sigma \geq 0$. Suppose the medium is non-magnetic, that is, the magnetic permeability μ is a fixed constant in the region above Γ_1 and the field is source free. Then the electromagnetic wave propagation is governed by the time-harmonic Maxwell equations (with the time variation of the form $e^{-i\omega t}$, $\omega > 0$)

$$\operatorname{curl} E - i\omega\mu H = 0, \qquad \operatorname{curl} H + i\omega(\epsilon + i\sigma/\omega)E = 0,$$

where E and H are the electric and magnetic fields, respectively. Suppose the inhomogeneous medium is 2π-periodic with respect to the x_1 and x_2 directions, that is, for all $n = (n_1, n_2) \in \mathbb{Z}^2$,

$$\epsilon(x_1 + 2\pi n_1, x_2 + 2\pi n_2, x_3) = \epsilon(x_1, x_2, x_3), \quad \sigma(x_1 + 2\pi n_1, x_2 + 2\pi n_2, x_3) = \sigma(x_1, x_2, x_3).$$

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Suppose above the structure Γ_1 is another doubly periodic surface defined by

$$\Gamma_0 := \{x \in \mathbb{R}^3 \,|\, x_3 = g(x_1, x_2)\},$$

where $g \in C^2(\mathbb{R}^2)$ is a 2π-periodic function of x_1 and x_2:

$$g(x_1 + 2n_1\pi, x_2 + 2n_2\pi) = g(x_1, x_2) \quad \forall n = (n_1, n_2) \in \mathbb{Z}^2,$$

which separates the region above Γ_1 into two parts:

$$\Omega_0 := \{x \in \mathbb{R}^3 \,|\, x_3 > g(x_1, x_2)\},$$
$$\Omega_1 := \{x \in \mathbb{R}^3 \,|\, f(x_1, x_2) < x_3 < g(x_1, x_2)\}.$$

Assume further that $\epsilon(x) = \epsilon_0$, $\sigma = 0$ for $x \in \Omega_0$ (which means that the medium above the layer is lossless) and that the doubly periodic surface Γ_1 is a perfectly conductor coated partially with a dielectric.

Consider the scattering of the electromagnetic plane wave

$$E^i(x) = pe^{ik_0 x\cdot d}, \quad H^i(x) = re^{ik_0 x\cdot d}$$

incident on the doubly periodic structure Γ_0 from the top region Ω_0, where $k_0 = \sqrt{\epsilon_0\mu}\omega$ is the wave number, $d = (\alpha_1, \alpha_2, -\beta) = (\cos\theta_1\cos\theta_2, \cos\theta_1\sin\theta_2, -\sin\theta_1)$ is the incident wave vector whose direction is specified by θ_1 and θ_2 with $0 < \theta_1 \le \pi$, $0 < \theta_2 \le 2\pi$ and the vectors p and r are polarization directions satisfying that $p = \sqrt{\mu/\varepsilon_0}(r \times d)$ and $r \perp d$. The problem of scattering of time-harmonic electromagnetic waves in this model leads to the following problem (the magnetic field H is eliminated):

$$\operatorname{curl}\operatorname{curl} E - k_0^2 E = 0 \text{in } \Omega_0, \tag{1.1}$$

$$\operatorname{curl}\operatorname{curl} E - k_0^2 q(x) E = 0 \text{in } \Omega_1, \tag{1.2}$$

$$\nu \times E|_+ = \nu \times E|_-, \quad \nu \times \operatorname{curl} E|_+ = \lambda_0 \nu \times \operatorname{curl} E|_- \text{on } \Gamma_0, \tag{1.3}$$

$$\nu \times E = 0 \text{on } \Gamma_{1,D}, \tag{1.4}$$

$$\nu \times \operatorname{curl} E - i\rho(\nu \times E) \times \nu = 0 \text{on } \Gamma_{1,I} \tag{1.5}$$

where $q(x) = (\epsilon(x) + i\sigma(x)/\omega)/\epsilon_0$ is the refractive index, ν is the unit normal at the boundary, $E = E^i + E^s$ is the total field in Ω_0 with E^s being the scattered electric field, $\Gamma_1 = \overline{\Gamma}_{1,D} \cup \overline{\Gamma}_{1,I}$, λ_0 and ρ are two positive constants.

We require the scattered field E to be *α-quasi-periodic* with respect to x_1 and x_2 in the sense that $E(x_1, x_2, x_3)e^{-i\alpha\cdot x}$ is 2π periodic with respect to x_1 and x_2, where $\alpha = (\alpha_1, \alpha_2, 0) \in \mathbb{R}^3$. It is further required that the scattered field E satisfies the following Rayleigh expansion radiation condition as $x_3 \to +\infty$:

$$E^s(x) = \sum_{n\in\mathbb{Z}^2} E_n e^{i(\alpha_n\cdot x + \beta_n x_3)}, \quad x_3 > g_+ := \max_{x_1,x_2} g(x_1, x_2), \tag{1.6}$$

where $\alpha_n = (\alpha_1 + n_1, \alpha_2 + n_2, 0) \in \mathbb{R}^3$, $E_n = (E_n^{(1)}, E_n^{(2)}, E_n^{(3)}) \in \mathbb{C}^3$ are the Rayleigh coefficients and

$$\beta_n = \begin{cases} (k_0^2 - |\alpha_n|^2)^{1/2} & \text{if } |\alpha_n|^2 \le k_0^2, \\ i(|\alpha_n|^2 - k_0^2)^{1/2} & \text{if } |\alpha_n|^2 > k_0^2 \end{cases}$$

with $i^2 = -1$. From the fact that $\operatorname{div} E^s(x) = 0$ it is clear that

$$\alpha_n \cdot E_n + \beta_n E_n^{(3)} = 0.$$

Throughout this paper we assume that $\beta_n \neq 0$ for all $n \in \mathbb{Z}^2$.

The direct problem is to compute the scattered field E^s in Ω_0 and E in Ω_1 given the incident wave E^i, the diffraction grating profiles Γ_0 and Γ_1 with the corresponding boundary conditions and the refractive index $q(x)$. Our inverse problem is to determine the grating profile Γ_1 together with the impedance coefficient ρ in the case when the interface grating profile Γ_0 is known and the refractive index q in the case when the grating surfaces Γ_0 and Γ_1 are known and flat, utilizing the knowledge of the incident wave E^i and the total tangential electric field $\nu \times E$ on a plane $\Gamma_h = \{x \in \mathbb{R}^3 \,|\, x_3 = h\}$ above the inhomogeneous layer.

Problems of scattering of electromagnetic waves by a doubly periodic structure have been studied by many authors using both integral and variational methods. The reader is referred to, e.g. [1, 3, 4, 5, 11, 12, 18, 21] for results on existence, uniqueness, and numerical approximations of solutions to the direct problems. Compared with the direct problem, not much attention has been paid to inverse problems from doubly periodic structures although they are not only mathematically interesting but have many important applications. For the case when $\Gamma_{1,I} = \emptyset$ and the medium above the periodic structure $\Gamma_1 = \Gamma_{1,D}$ is homogeneous, the inverse scattering problem has been considered in [2, 7, 6]. If the medium is lossy above the perfectly reflecting periodic structure, Ammari [2] proved a global uniqueness result for the inverse problem with one incident plane wave. If the medium is lossless above the perfectly reflecting periodic structure, a local uniqueness result was obtained in [7] for the inverse problem with one incident plane wave by establishing a lower bound of the first eigenvalue of the curl curl operator with the boundary condition (1.4) in a bounded, smooth convex domain in $\mathbb{R}^3$. The stability of the inverse problem was also studied in [7]. Recently in [6], for the class of perfectly reflecting doubly periodic polyhedral structures global uniqueness results have been established in [6] for the inverse problem in the case of lossless medium above the structure, using only a minimal number (though unknown) of incident plane waves. Further, for a general Lipschitz, bi-periodic, partly coated structure Γ_1 a global uniqueness result was proved in [13] for the inverse problem in the case of a lossless, homogeneous medium above the structure, using infinitely many incident dipole sources.

On the other hand, for the case when $\Gamma_{1,I} = \emptyset$ (i.e. $\Gamma_1 = \Gamma_{1,D}$), $\lambda_0 = 1$ and the grating surfaces Γ_0 and Γ_1 are known and flat, a global uniqueness result was obtained in [14] for reconstructing the refractive index q, using all electric dipole incident waves (see [15] for the corresponding result in the 2D case).

In this paper, we prove global uniqueness results for the inverse problem of recovering a general smooth bi-periodic profile with a mixed boundary condition and a known bi-periodic interface from a knowledge of near field measurements above the known interface with a countably infinite number of quasi-periodic incident waves $E^i(x;m) = (1/k_0^2)\mathrm{curl}\,\mathrm{curl}\,[p\exp(i\alpha_m \cdot x - i\beta_m x_3)]$, $m = (m_1, m_2) \in \mathbb{Z}^2$. Further, we also establish a global uniqueness result for the inverse problem of determining the refractive index q which depends on only one direction (x_1 or x_2) for the case when $\Gamma_{1,I} = \emptyset$ (i.e. $\Gamma_1 = \Gamma_{1,D}$) and the grating surfaces Γ_0 and Γ_1 are known and flat, using a countably infinite number of quasi-periodic incident waves $E^i(x;m)$. This is an improvement to the result of [14]. A key ingredient in our proofs is a novel mixed reciprocity relation derived in this paper for bi-periodic structures.

The rest of the paper is organized as follows. In Section 2, we introduce some suitable quasi-periodic function spaces and the Dirichlet-to-Neumann map on an artificial boundary above the structure. The problem (1.1)-(1.6) is then reduced to a boundary value problem in a truncated domain. In Section 3, we establish the well-posedness of the scattering problem (1.1)-(1.6), employing a variational approach. Section 4 is devoted to the inverse problems. In Subsection 4.1 novel mixed reciprocity relations are established for doubly periodic structures, which play a key role in the proofs of the uniqueness results for our inverse problems. Subsection 4.2 is devoted to the unique determination of the doubly periodic grating profile Γ_1 with its physical property, where it is assumed that the interface Γ_0 is known and the refractive index q is a known constant. Subsection 4.3 is concerned with the unique reconstruction of the refractive index q, where we only consider the case when the shape of the two grating profiles is known and flat, which improves the result in [14].

2. Quasi-periodic function spaces. In this section we introduce some function spaces needed in the study of our problems. Due to the periodicity of the problem, the original problem can be reduced to a problem in a single periodic cell of the grating profiles. To this end and for the subsequent analysis, we use Γ_j, Ω_j $(j = 0, 1)$, $\Gamma_{1,D}, \Gamma_{1,I}$ and Γ_h for $h \in \mathbb{R}$ again to denote the single periodic part (i.e. in the range $0 < x_1, x_2 < 2\pi$) of the corresponding notations defined in the last section. We also need the notation

$$\Omega_h = \{x \in \mathbb{R}^3 \,|\, 0 < x_1, x_2 < 2\pi,\ f(x_1, x_2) < x_3 < h\}$$

for $h > \max\{f(x') \,|\, x' \in \mathbb{R}^2\}$.

We now introduce some vector quasi-periodic Sobolev spaces. Let

$$H(\mathrm{curl}\,, \Omega_h) = \{E(x) = \sum_{n\in\mathbb{Z}^2} E_n(x_3) \exp(i\alpha_n \cdot x) \,|\, E \in (L^2(\Omega_h))^3,\ \mathrm{curl}\, E \in (L^2(\Omega_h))^3\}$$

with the norm

$$||E||^2_{H(\mathrm{curl}\,,\Omega_h)} = ||E||^2_{L^2(\Omega_h)} + ||\mathrm{curl}\, E||^2_{L^2(\Omega_h)}.$$

Note that the α-quasi-periodic space $H(\mathrm{curl}\,, \Omega_b)$ is a subset of the classical vector space $\mathbb{H}(\mathrm{curl}\,, \Omega_b)$ defined by

$$\mathbb{H}(\mathrm{curl}\,, \Omega_b) = \{E \in (L^2(\Omega_b))^3 \,|\, \mathrm{curl}\, E \in (L^2(\Omega_b))^3\}$$

with the norm $||E||^2_{\mathbb{H}(\mathrm{curl}\,,\Omega_b)} = ||E||^2_{L^2(\Omega_b)} + ||\mathrm{curl}\, E||^2_{L^2(\Omega_b)}$. Further, it was shown in [5] that $H(\mathrm{curl}\,, \Omega_b)$ can be characterized as

$$\begin{aligned} H(\mathrm{curl}\,, \Omega_b) = \{E \in \mathbb{H}(\mathrm{curl}\,, \Omega_b) \,|\, & e^{2\pi i\alpha_1} E(0, x_2, x_3) \times e_1 = E(2\pi, x_2, x_3) \times e_1, \\ & e^{2\pi i\alpha_2} E(x_1, 0, x_3) \times e_2 = E(x_1, 2\pi, x_3) \times e_2\}, \end{aligned}$$

where $e_1 = (1, 0, 0)$ and $e_2 = (0, 1, 0)$.

To deal with the mixed boundary conditions (1.4) and (1.5), we introduce the subspace of $H(\mathrm{curl}\,, \Omega_h)$:

$$X := \{E \in H(\mathrm{curl}\,, \Omega_h) \,|\, \nu \times E|_{\Gamma_{1,D}} = 0,\ \nu \times E|_{\Gamma_{1,I}} \in L^2_t(\Gamma_{1,I})\}$$

with the norm

$$||E||^2_X = ||E||^2_{H(\mathrm{curl}\,,\Omega_h)} + ||\nu \times E||^2_{L^2_t(\Gamma_{1,I})}$$

where $L^2_t(\Gamma_{1,I}) = \{E \in (L^2(\Gamma_{1,I}))^3 \,|\, \nu \cdot E = 0 \text{ on } \Gamma_{1,I}\}$.

For $x' = (x_1, x_2, h) \in \Gamma_h$, $s \in \mathbb{R}$ define

$$H_t^s(\Gamma_h) = \{E(x') = \sum_{n\in\mathbb{Z}^2} E_n \exp(i\alpha_n \cdot x') \,|\, E_n \in \mathbb{C}^3,\ e_3 \cdot E = 0,$$
$$\|E\|^2_{H^s(\Gamma_h)} = \sum_{n\in\mathbb{Z}^2} (1+|\alpha_n|^2)^s |E_n|^2 < +\infty\}$$
$$H_t^s(\mathrm{div}\,,\Gamma_h) = \{E(x') = \sum_{n\in\mathbb{Z}^2} E_n \exp(i\alpha_n \cdot x') \,|\, E_n \in \mathbb{C}^3,\ e_3 \cdot E = 0,$$
$$||E||^2_{H^s(\mathrm{div}\,,\Gamma_h)} = \sum_{n\in\mathbb{Z}^2} (1+|\alpha_n|^2)^s (|E_n|^2 + |E_n \cdot \alpha_n|^2) < +\infty\}$$
$$H_t^s(\mathrm{curl}\,,\Gamma_h) = \{E(x') = \sum_{n\in\mathbb{Z}^2} E_n \exp(i\alpha_n \cdot x') \,|\, E_n \in \mathbb{C}^3,\ e_3 \cdot E = 0,$$
$$||E||^2_{H^s(\mathrm{curl}\,,\Gamma_h)} = \sum_{n\in\mathbb{Z}^2} (1+|\alpha_n|^2)^s (|E_n|^2 + |E_n \times \alpha_n|^2) < +\infty\}$$

and write $L_t^2(\Gamma_h) = H_t^0(\Gamma_h)$. We have the duality result:

$$(H_t^s(\mathrm{div}\,,\Gamma_h))' = H_t^{-s-1}(\mathrm{curl}\,,\Gamma_h).$$

Recalling the trace theorem on $\mathbb{H}(\mathrm{curl}\,,\Omega_h)$, we have

$$H_t^{-1/2}(\mathrm{div}\,,\Gamma_h) = \{e_3 \times E|_{\Gamma_h} \,|\, E \in H(\mathrm{curl}\,,\Omega_h)\}$$

and that the trace mapping from $H(\mathrm{curl}\,,\Omega_h)$ to $H_t^{-1/2}(\mathrm{div}\,,\Gamma_h)$ is continuous and surjective (see [8] and the references there). We also need the trace space $Y(\Gamma_0)$ and its duality space $Y(\Gamma_0)'$:

$$Y(\Gamma_0) = \{f \in H_t^{-1/2}(\Gamma_0) \,|\, \nabla_{\Gamma_0} \cdot f \in H^{-1/2}(\Gamma_0)\}$$
$$Y(\Gamma_0)' = \{f \in H_t^{-1/2}(\Gamma_0) \,|\, \nabla_{\Gamma_0} \times f \in H^{-1/2}(\Gamma_0)\},$$

where ∇_{Γ_0} denotes the surface gradient on Γ_0. Note that the trace space $Y(\Gamma_0)$ can also be defined as follows (see [10] and [17, p. 58-59]):

$$Y(\Gamma_0) = \{f \in (H^{-1/2}(\Gamma_0))^3 \mid \text{there exists}\, E \in H(\mathrm{curl}\,,\Omega_h\backslash\overline{\Omega}_1)$$
$$\text{with}\, \nu \times E = f \text{ on } \Gamma_0,\ \nu \times E = 0 \text{ on } \Gamma_h\}$$

for $h > g_+$, with norm

$$\|f\|_{Y(\Gamma_0)} = \inf\{\|E\|_{H(\mathrm{curl}\,,\Omega_h\backslash\overline{\Omega}_1)} \mid E \in H(\mathrm{curl}\,,\Omega_h\backslash\overline{\Omega}_1),\ \nu \times E\big|_{\Gamma_0} = f,\ \nu \times E\big|_{\Gamma_h} = 0\}.$$

We assume throughout this paper that q satisfies the following conditions:

(**A1**) $q \in C^1(\overline{\Omega}_1)$ and $q(x) = 1$ for $x \in \Omega_0$;

(**A2**) $\mathrm{Im}\,[q(x)] \geq 0$ for all $x \in \overline{\Omega}_1$ if $\Gamma_{1,I} \neq \emptyset$ and $\mathrm{Im}\,[q(x_0)] > 0$ for some $x_0 \in \overline{\Omega}_1$ if $\Gamma_{1,I} = \emptyset$;

(**A3**) $\mathrm{Re}\,[q(x)] \geq \gamma$ for all $x \in \overline{\Omega}_1$ for some positive constant γ.

3. The direct scattering problem. In this section we will establish the solvability of the scattering problem (1.1)-(1.6), employing the variational method. To this end, we propose a variational formulation of the scattering problem in a truncated domain by introducing a transparent boundary condition on Γ_h for $h > g_+$.

Let $x' = (x_1, x_2, h) \in \Gamma_h$ for $h > g_+$. For $\widehat{E} \in H_t^{-1/2}(\mathrm{div}\,, \Gamma_h)$ with

$$\widehat{E}(x') = \sum_{n \in \mathbb{Z}^2} \widehat{E}_n \exp(i\alpha_n \cdot x')$$

define the Dirichlt-to-Neumann map $\mathcal{R}:\ H_t^{-1/2}(\mathrm{div}\,, \Gamma_h) \to H_t^{-1/2}(\mathrm{curl}\,, \Gamma_h)$ by

$$(\mathcal{R}\widetilde{E})(x') = (e_3 \times \mathrm{curl}\, E) \times e_3 \quad \text{on } \Gamma_h,$$

where E satisfying the Rayleigh expansion condition (1.6) is the unique quasi-periodic solution to the problem

$$\mathrm{curl}\,\mathrm{curl}\, E - k^2 E = 0 \quad \text{for } x_3 > h, \qquad \nu \times E = \widetilde{E}(x') \quad \text{on } \Gamma_h.$$

The map $\mathcal{R}$ is well-defined and can be used to replace the radiation condition (1.6) on Γ_h. The scattering problem (1.1)-(1.6) can then be transformed into the following boundary value problem in the truncated domain Ω_h:

$$\mathrm{curl}\,\mathrm{curl}\, E - k_0^2 E = 0 \text{in } \Omega_0, \tag{3.1}$$

$$\mathrm{curl}\,\mathrm{curl}\, E - k_0^2 qE = 0 \text{in } \Omega_1, \tag{3.2}$$

$$\nu \times E|_+ - \nu \times E|_- = f_1, \ \ \nu \times \mathrm{curl}\, E|_+ - \lambda_0 \nu \times \mathrm{curl}\, E|_- = f_2 \text{on } \Gamma_0, \tag{3.3}$$

$$\nu \times E = f_3 \quad \text{on} \quad \Gamma_{1,D}, \quad \nu \times \mathrm{curl}\, E - i\rho(\nu \times E) \times \nu = f_4 \text{on } \Gamma_{1,I}, \tag{3.4}$$

$$(\mathrm{curl}\, E)_T - \mathcal{R}(e_3 \times E) = 0 \text{on } \Gamma_h, \tag{3.5}$$

where $f_1 = -\nu \times E^i|_{\Gamma_0} \in Y(\Gamma_0)$, $f_2 = -\nu \times \mathrm{curl}\, E^i|_{\Gamma_0} \in Y(\Gamma_0)'$, $f_3 = f_4 = 0$ and, for any vector F, $(F)_T = (\nu \times F) \times \nu$ denotes its tangential component on a surface.

Remark 3.1. In the case when $k_0^2 q(x) \equiv k_1^2$ is a constant and the incident field is given by the electric dipole source $E^i(x) = \widehat{\mathbb{G}}_1(x, y_0)r$ for $y_0 \in \Omega_1$ and $r \in \mathbb{R}^3$ (e.g. in the problem (4.2)-(4.8) of Lemma 4.1), we have $f_1 = \nu \times E^i|_{\Gamma_0} \in Y(\Gamma_0)$, $f_2 = \lambda_0 \nu \times \mathrm{curl}\, E^i|_{\Gamma_0} \in Y(\Gamma_0)'$, $f_3 = -\nu \times E^i|_{\Gamma_{1,D}} \in Y(\Gamma_{1,D})$, $f_4 = -\nu \times \mathrm{curl}\, E^i|_{\Gamma_{1,I}} + i\rho(\nu \times E^i) \times \nu|_{\Gamma_{1,I}} \in L_t^2(\Gamma_{1,I})$ in the problem (3.1)-(3.5), where $Y(\Gamma_{1,D})$ is defined in the same way as $Y(\Gamma_0)$ with Γ_0 replaced by $\Gamma_{1,D}$ (see [13]).

Define

$$\begin{aligned} Y := \{ & E \in H(\mathrm{curl}\,, \Omega_1) \cap H(\mathrm{curl}\,, \Omega_h \backslash \overline{\Omega}_1) \,|\, \nu \times E|_{\Gamma_{1,D}} = f_3, \\ & \nu \times E|_{\Gamma_{1,I}} \in L_t^2(\Gamma_{1,I}),\ \nu \times E|_+ - \nu \times E|_- = f_1 \text{ on } \Gamma_0 \} \end{aligned}$$

with the norm

$$\|E\|_Y^2 = \|E\|^2_{H(\mathrm{curl}\,, \Omega_1)} + \|E\|^2_{H(\mathrm{curl}\,, \Omega_h \backslash \overline{\Omega}_1)} + ||\nu \times E||^2_{L_t^2(\Gamma_{1,I})}.$$

Then the variational formulation for the problem (3.1)-(3.5) is given as follows: find $E \in Y$ such that

$$A(E, F) = B(F) \qquad \forall\, F \in X, \tag{3.6}$$

where

$$\begin{aligned}A(E,F) := &\lambda_0\int_{\Omega_1}(\operatorname{curl}E\cdot\operatorname{curl}\overline{F}-k_0^2qE\cdot\overline{F})dx\\&+\int_{\Omega_h\backslash\overline{\Omega}_1}(\operatorname{curl}E\cdot\operatorname{curl}\overline{F}-k_0^2E\cdot\overline{F})dx\\&-i\lambda_0\rho\int_{\Gamma_{1,I}}E_T\cdot\overline{F}_Tds-\int_{\Gamma_h}\mathcal{R}(\nu\times E)\cdot(\nu\times\overline{F})ds,\\B(F) := &\int_{\Gamma_0}f_2\cdot\overline{F}_Tds+\lambda_0\int_{\Gamma_{1,I}}f_4\cdot\overline{F}_Tds.\end{aligned}$$

If $f_1\in Y(\Gamma_0)$, then there exits $\widetilde{E}_0\in H(\operatorname{curl},\Omega_h\backslash\overline{\Omega}_1)$ such that $\nu\times\widetilde{E}_0|_{\Gamma_0}=f_1$, $\nu\times\widetilde{E}_0|_{\Gamma_h}=0$. Similarly, for $f_3\in Y(\Gamma_{1,D})$ there exists a function $E_1\in H(\operatorname{curl},\Omega_h)$ such that $\nu\times E_1|_{\Gamma_{1,D}}=f_3$, $\nu\times E_1|_{\Gamma_h}=0$ and $\nu\times E_1|_{\Gamma_{1,I}}\in L_t^2(\Gamma_{1,I})$. Let $\widetilde{E}=E-E_0-E_1$, where E_0 is a function in Ω_h satisfying that $E_0|_{\Omega_h\backslash\overline{\Omega}_1}=\widetilde{E}_0$ and $E_0|_{\Omega_1}=0$. Then $\widetilde{E}\in X$ and the variational problem (3.6) is equivalent to the problem: find $\widetilde{E}\in X$ such that

$$A(\widetilde{E},F)=\widetilde{B}(F)\qquad\forall\,F\in X,\tag{3.7}$$

where $\widetilde{B}(F)=B(F)-A(E_0,F)-A(E_1,F)$.

Theorem 3.2. *Assume that the conditions* ***(A1)**-**(A3)*** *are satisfied. Then the problem* (3.1) – (3.5) *has a unique solution* $E\in Y$ *for any* $f_1\in Y(\Gamma_0)$, $f_2\in Y(\Gamma_0)'$, $f_3\in Y(\Gamma_{1,D})$ *and* $f_4\in L_t^2(\Gamma_{1,I})$. *Furthermore, we have*

$$||E||_Y\le C(||f_1||_{Y(\Gamma_0)}+||f_2||_{Y(\Gamma_0)'}+||f_3||_{Y(\Gamma_{1,D})}+||f_4||_{L_t^2(\Gamma_{1,I})}),$$

where C *is a positive constant depending only on* Ω_h.

Proof. It is enough to prove that the problem (3.7) has a unique solution $\widetilde{E}\in X$ with the required estimate.

We first prove the uniqueness of solutions. To this end, let $f_j=0$, $j=1,2,3,4$ and let $F=\widetilde{E}$ in (3.7). Then $A(\widetilde{E},\widetilde{E})=0$, that is,

$$\begin{aligned}\lambda_0\int_{\Omega_1}(|\operatorname{curl}\widetilde{E}|^2-k_0^2q|\widetilde{E}|^2)dx+\int_{\Omega_h\backslash\overline{\Omega}_1}(|\operatorname{curl}\widetilde{E}|^2-k_0^2|\widetilde{E}|^2)dx\\-i\lambda_0\rho\int_{\Gamma_{1,I}}|\widetilde{E}_T|^2ds-\int_{\Gamma_h}\mathcal{R}(\nu\times\widetilde{E})\cdot(\nu\times\overline{\widetilde{E}})ds=0.\end{aligned}$$

Taking the imaginary part of the above equation and noting that the imaginary part of the last integral in the above equation is non-negative (see [13, Equation (16)]), we deduce that

$$k_0^2\int_{\Omega_1}\operatorname{Im}(q)|\widetilde{E}|^2dx+\rho\int_{\Gamma_{1,I}}|\widetilde{E}_T|^2ds\le 0.\tag{3.8}$$

If $\Gamma_{1,I}=\emptyset$, then by (3.8) and the condition (**A2**) we have $\widetilde{E}\equiv 0$ in a small ball $B(x_0;\delta)\subset\Omega_1$. By [9, Theorem 6] we have $\widetilde{E}\in(H^1(\Omega_1))^3$. Thus, by the unique continuation principle (see [19, Theorem 2.3]) we have $\widetilde{E}\equiv 0$ in Ω_1. This, together with the transmission condition (3.3) and Holmgren's uniqueness theorem, implies that $\widetilde{E} \equiv 0$ in $\Omega_h \backslash \overline{\Omega}_1$. If $\Gamma_{1,I} \neq \emptyset$, then (3.8) and the boundary condition (3.4) yield that $\nu \times \widetilde{E}|_{\Gamma_{1,I}} = 0$ and $\nu \times \operatorname{curl} \widetilde{E}|_{\Gamma_{1,I}} = 0$. By unique continuation principle again we have $\widetilde{E} \equiv 0$ in Ω_1. Again, from the transmission condition (3.3) and Holmgren's uniqueness theorem it follows that $\widetilde{E} \equiv 0$ in $\Omega_h \backslash \overline{\Omega}_1$. The uniqueness of solutions is thus proved for both cases.

Now, arguing similarly as in the proof of Theorem 4.1 in [14] or Theorem 3.1 in [13] (see [14, 13] for details) we can prove that the problem (3.7) has a solution $\widetilde{E} \in X$ satisfying the estimate

$$\|\widetilde{E}\|_X \le C(\|f_2\|_{Y(\Gamma_0)'} + \|f_4\|_{L^2_t(\Gamma_{1,I})} + \|\widetilde{E}_0\|_{H(\operatorname{curl}, \Omega_h \backslash \overline{\Omega}_1)} + \|E_1\|_X)$$

with C depending only on Ω_h. Since $\widetilde{E} = E - E_0 - E_1$, and by taking the infimum over all $\widetilde{E}_0 \in H(\operatorname{curl}, \Omega_h \backslash \overline{\Omega}_1)$ such that $\nu \times \widetilde{E}_0|_{\Gamma_0} = f_1$ and $\nu \times \widetilde{E}_0|_{\Gamma_h} = 0$ and over all $E_1 \in H(\operatorname{curl}, \Omega_h)$ such that $\nu \times E_1|_{\Gamma_{1,D}} = f_3$, $\nu \times E_1|_{\Gamma_h} = 0$ and $\nu \times E_1|_{\Gamma_{1,I}} \in L^2_t(\Gamma_{1,I})$ the desired estimate follows (on taking into account the definition of the norm on $Y(\Gamma_0)$ and $Y(\Gamma_{1,D})$). $\square$

4. The inverse problems. In this section we consider the inverse problems of determining the doubly periodic grating profile f with its physical property and the refractive index q from a knowledge of the incident and scattered fields. To this end, we need the free-space quasi-periodic Green's function

$$G_0(x,y) = \frac{1}{8\pi^2} \sum_{n \in \mathbb{Z}^2} \frac{1}{i\beta_n} \exp(i\alpha_n \cdot (x-y) + i\beta_n |x_3 - y_3|)$$

provided $\beta_n \neq 0$ for all $n \in \mathbb{Z}^2$ (see [18]). In the neighborhood of $x = y$, G_0 can be represented in the form $G_0(x,y) = \Phi(x,y) + a(x-y)$, where $\Phi(x,y) = \exp(ik_0|x-y|)/(4\pi|x-y|)$ is the fundamental solution to the three-dimensional Helmholtz equation $(\Delta + k_0^2)u = 0$ and $a(x-y)$ is a C^∞ function (see [16] for the 2D case). We now introduce the quasi-periodic Green's tensor $\mathbb{G}_0 \in \mathbb{C}^{3\times 3}$ for the time-harmonic Maxwell equations:

$$\mathbb{G}_0(x,y) = G_0(x,y)\mathbb{I} + \frac{1}{k_0^2} \nabla_x \operatorname{div}_x (G_0(x,y)\mathbb{I}), \qquad x \neq y, \tag{4.1}$$

where $\mathbb{I}$ is a 3×3 identity matrix. Consider the following incident dipole source located at $z \in \mathbb{R}^3$ with polarization p ($|p| = 1$):

$$E^i(x) = \mathbb{G}_0(x,z)p, \qquad x \neq z.$$

Clearly, we have

$$\operatorname{curl}\operatorname{curl} E^i(x) - k_0^2 E^i(x) = 0, \qquad x \neq z.$$

4.1. Mixed reciprocity relations. We establish two mixed reciprocity relations for the doubly periodic structure, which play a key role in the proofs of uniqueness results for the inverse problems.

LEMMA 4.1. *Assume that $k_0^2 q(x) \equiv k_1^2$ is a constant. For $m = (m_1, m_2) \in \mathbb{Z}^2$ let $E^i(x;m) = (1/k_0^2)\operatorname{curl}\operatorname{curl}[p\exp(i\alpha_m \cdot x - i\beta_m x_3)]$ and let $E(x;m)$ (which is the sum $E^i(x;m) + E^s(x;m)$ in Ω_0) be the solution to the the scattering problem* (1.1) – (1.6) *with* $E^i(x) = E^i(x;m)$. *On the other hand, define* $\widehat{\alpha} := -\alpha$ *and for* $y_0 \in \Omega_1$ *and* $r \in \mathbb{R}^3$ *let* $E^i(x;y_0) = \widehat{\mathbb{G}}_1(x,y_0)r$ *and let* $\widehat{E}(x;y_0)$ *solve the scattering problem:*

$$\operatorname{curl}\operatorname{curl}\widehat{E} - k_0^2\widehat{E} = 0 \text{ in } \Omega_0, \tag{4.2}$$

$$\operatorname{curl}\operatorname{curl}\widehat{E} - k_1^2\widehat{E} = 0 \text{ in } \Omega_1\backslash\{y_0\}, \tag{4.3}$$

$$\nu\times\widehat{E}|_+ = \nu\times\widehat{E}|_-, \quad \nu\times\operatorname{curl}\widehat{E}|_+ = \lambda_0\nu\times\operatorname{curl}\widehat{E}|_- \text{ on } \Gamma_0, \tag{4.4}$$

$$\nu\times\widehat{E} = 0 \quad \text{on } \Gamma_{1,D}, \qquad \nu\times\operatorname{curl}\widehat{E} - i\rho(\nu\times\widehat{E})\times\nu = 0 \text{ on } \Gamma_{1,I}, \tag{4.5}$$

$$\widehat{E}(x;y_0) = E^i(x;y_0) + \widehat{E}^s(x;y_0) \text{ in } \Omega_1\backslash\{y_0\}, \tag{4.6}$$

$$\widehat{E}(x;y_0) = \sum_{n\in\mathbb{Z}^2}\widehat{E}_n(y_0)\exp(i\widehat{\alpha}_n\cdot x + \widehat{\beta}_n x_3) \text{ in } x_3 > g_+, \tag{4.7}$$

$$\widehat{\alpha}_n\cdot\widehat{E}_n + \widehat{\beta}_n\cdot\widehat{E}_n^{(3)} = 0. \tag{4.8}$$

Here, $\widehat{\alpha}_n$ *and* $\widehat{\beta}_n$ *are defined by*

$$\widehat{\alpha}_n = (-\alpha_1 + n_1, -\alpha_2 + n_2, 0) \quad \textit{and} \quad \widehat{\beta}_n = \begin{cases} \sqrt{k_0^2 - |\widehat{\alpha}_n|^2} & \textit{for } |\widehat{\alpha}_n|^2 \le k_0^2, \\ i\sqrt{|\widehat{\alpha}_n|^2 - k_0^2} & \textit{for } |\widehat{\alpha}_n|^2 > k_0^2 \end{cases}$$

and $\widehat{\mathbb{G}}_1(x,y_0)$ *is defined by* (4.1) *with* α_n *and* k_0^2 *replaced by* $\widehat{\alpha}_n$ *and* k_1^2, *respectively. Then we have*

$$r\cdot E(y_0;m) = \frac{8\pi^2 i}{\lambda_0}\widehat{\beta}_{-m}\widehat{E}_{-m}(y_0)\cdot p. \tag{4.9}$$

Proof. Note first that $E(x;m)$ and $\widehat{E}(x;y_0)$ are well-defined by the well-posedness of the direct scattering problem. Applying Green's theorem in $\Omega_1\setminus B(y_0,\delta)$ and using the fact that contributions of the vertical line integrals cancel out due to the periodicity, we have

$$\begin{aligned} 0 &= \int_{\Omega_1\backslash B(y_0,\delta)}\Big\{\operatorname{curl}\operatorname{curl}E(x;m)\cdot[\widehat{\mathbb{G}}_1(x,y_0)r] \\ &\qquad\qquad -E(x;m)\cdot\operatorname{curl}\operatorname{curl}[\widehat{\mathbb{G}}_1(x,y_0)r]\Big\}\,dx \\ &= \left[\int_{\Gamma_0} - \int_{\Gamma_1} + \int_{\partial B_\delta(y_0)}\right]\Big\{\nu\times\operatorname{curl}E(x)\cdot[\widehat{\mathbb{G}}_1(x,y_0)r] \\ &\qquad\qquad -\nu\times\operatorname{curl}[\widehat{\mathbb{G}}_1(x,y_0)r]\cdot E(x)\Big\}\,ds \\ &:= I_1 + I_2 + I_3, \end{aligned} \tag{4.10}$$

where $B(y_0,\delta)$ is a small ball centered at y_0 with the radius δ such that $B(y_0,\delta)\subset\Omega_1$.

We now analyze the asymptotic behavior of I_3 as $\delta\to 0$. From the definition that $\widehat{\mathbb{G}}_1(x,y_0) = \widehat{G}_1(x,y_0)\mathbb{I} + k_1^{-2}\nabla_x\operatorname{div}_x(\widehat{G}_1(x,y_0)\mathbb{I})$ it follows that

$$\begin{aligned} I_3 &= \int_{\partial B(y_0,\delta)}\Big[\nu\times\operatorname{curl}E(x;m)\cdot k_1^{-2}\nabla\operatorname{div}[\widehat{G}_1(x,y_0)r] \\ &\quad -\nu\times\operatorname{curl}[\widehat{G}_1(x,y_0)r]\cdot E(x;m)\Big]\,ds \\ &\quad +\int_{\partial B(y_0,\delta)}\nu\times\operatorname{curl}E(x;m)\cdot r\widehat{G}_1(x,y_0)ds \\ &:= I_4 + I_5. \end{aligned} \tag{4.11}$$

The regularity of $E(x;m)$ and the singularity of $\widehat{G}_1(x,y_0)$ at $x=y_0$ imply that $I_5\to 0$ as $\delta\to 0$. On the other hand, by the divergence theorem on $\partial B(y_0,\delta)$ it can be seen that

$$
\begin{aligned}
& I_4 \\
&= \int_{\partial B_\delta(y_0)} \Big[\nu\times\operatorname{curl} E(x;m)\cdot\frac{1}{k_1^2}\operatorname{Grad}\operatorname{div}[\widehat{G}_1(x,y_0)r] - \nu\times\operatorname{curl}[\widehat{G}_1(x,y_0)r]\cdot E(x;m)\Big]\,ds \\
&= \int_{\partial B_\delta(y_0)} \Big[\operatorname{Div}(-\nu\times\operatorname{curl} E(x;m))\frac{1}{k_1^2}\operatorname{div}[\widehat{G}_1(x,y_0)r] - \nu\times\operatorname{curl}[\widehat{G}_1(x,y_0)r]\cdot E(x;m)\Big]\,ds \\
&= \int_{\partial B_\delta(y_0)} \Big[(\nu\cdot\operatorname{curl}\operatorname{curl} E(x;m))\frac{1}{k_1^2}\operatorname{div}[\widehat{G}_1(x,y_0)r] - \nu\times\operatorname{curl}[\widehat{G}_1(x,y_0)r]\cdot E(x;m)\Big]\,ds \\
&= \int_{\partial B_\delta(y_0)} \Big[(\nu\cdot E(x;m))\operatorname{div}[\widehat{G}_1(x,y_0)r] + \nu\times E(x;m)\cdot\operatorname{curl}[\widehat{G}_1(x,y_0)r]\Big]\,ds \\
&= \int_{\partial B_\delta(y_0)} \Big[(\nu\cdot E(x;m))\nabla\widehat{G}_1(x,y_0) - \nabla\widehat{G}_1(x,y_0)\times(\nu\times E(x;m))\Big]\,ds\cdot r \\
&\to -r\cdot E(y_0;m)
\end{aligned}
$$

as $\delta\to 0$. This combined with (4.10) and (4.11) implies that

$$
\begin{aligned}
& r\cdot E(y_0;m) \\
&= \Big(\int_{\Gamma_0} - \int_{\Gamma_1}\Big)\Big[\nu\times\operatorname{curl} E(x)\cdot[\widehat{\mathbb{G}}_1(x,y_0)r] - \nu\times\operatorname{curl}[\widehat{\mathbb{G}}_1(x,y_0)r]\cdot E(x)\Big]\,ds.
\end{aligned} \tag{4.12}
$$

Similarly, we have on noting the regularity of $\widehat{E}^s(x;y_0)$ that

$$
\Big(\int_{\Gamma_0} - \int_{\Gamma_1}\Big)\Big[\nu\times\operatorname{curl} E(x;m)\cdot\widehat{E}^s(x;y_0) - \nu\times\operatorname{curl}\widehat{E}^s(x;y_0)\cdot E(x;m)\Big]\,ds = 0 \tag{4.13}
$$

Combine (4.12) with (4.13) to conclude that

$$
\begin{aligned}
& r\cdot E(y_0;m) \\
&= \Big(\int_{\Gamma_0} - \int_{\Gamma_1}\Big)\Big[\nu\times\operatorname{curl} E(x;m)\cdot\widehat{E}(x;y_0) - \nu\times\operatorname{curl}\widehat{E}(x;y_0)\cdot E(x;m)\Big]\,ds.
\end{aligned}
$$

Making use of the boundary conditions on Γ_j $(j=0,1)$ and Green's theorem in $\Omega_h\backslash\overline{\Omega}_1$ we obtain that

$$
\begin{aligned}
& r\cdot E(y_0;m) \\
&= \int_{\Gamma_0}\Big[\nu\times\operatorname{curl} E(x;m)|_-\cdot\widehat{E}(x;y_0)|_- - \nu\times\operatorname{curl}\widehat{E}(x;y_0)|_-\cdot E(x;m)|_-\Big]\,ds \\
&= \frac{1}{\lambda_0}\int_{\Gamma_0}\Big[\nu\times\operatorname{curl} E(x;m)|_+\cdot\widehat{E}(x;y_0)|_+ - \nu\times\operatorname{curl}\widehat{E}(x;y_0)|_+\cdot E(x;m)|_+\Big]\,ds \\
&= \frac{1}{\lambda_0}\int_{\Gamma_h}\Big[\nu\times\operatorname{curl} E(x;m)\cdot\widehat{E}(x;y_0) - \nu\times\operatorname{curl}\widehat{E}(x;y_0)\cdot E(x;m)\Big]\,ds
\end{aligned}
$$

Now, by the Rayleigh expansion radiation condition and the divergence-free property for $E^s(x;m)$ and $\widehat{E}(x;y_0)$ we have, on noting that $\beta_n(\alpha)=\widehat{\beta}_{-n}(\widehat{\alpha})$, that

$$
\int_{\Gamma_h}\Big[\nu\times\operatorname{curl} E^s(x;m)\cdot\widehat{E}(x;y_0) - \nu\times\operatorname{curl}\widehat{E}(x;y_0)\cdot E^s(x;m)\Big]\,ds = 0.
$$

This implies that

$$r\cdot E(y_0;m)=\frac{1}{\lambda_0}\int_{\Gamma_h}\Big[\nu\times\operatorname{curl}E^i(x;m)\cdot\widehat{E}(x;y_0)-\nu\times\operatorname{curl}\widehat{E}(x;y_0)\cdot E^i(x;m)\Big]\,ds.$$

Insert $E^i(x;m) = k_0^{-2}\operatorname{curl}\operatorname{curl}[p\exp(i\alpha_m\cdot x-i\beta_m x_3)]$ and $\widehat{E}(x;y_0) = \sum_{n\in\mathbb{Z}^2}\widehat{E}_n\exp\{i\widehat{\alpha}_n\cdot x+i\widehat{\beta}_n x_3\}$ into the above equation to get

$$r\cdot E(y_0;m)=\frac{i}{\lambda_0}\sum_{n\in\mathbb{Z}^2}\Big\{[\widehat{E}_n(y_0)\times e_3]\times(\alpha_m;-\beta_m)-e_3\times[(\widehat{\alpha}_n;\widehat{\beta}_n)\times\widehat{E}_n(y_0)]\Big\}\,e^{i(\widehat{\beta}_n-\beta_m)h}$$
$$\cdot p_m\int_0^{2\pi}\int_0^{2\pi}e^{i(\widehat{\alpha}_n+\alpha_m)\cdot x}dx_1dx_2,$$

where $(\vec{a};b)$ is defined as $(\vec{a};b):=\vec{a}+(0,0,b)$ and $p_m = p-[(\alpha_m;-\beta_m)\cdot p/k_0^2](\alpha_m;-\beta_m)$.

Finally, use the fact that $\widehat{\alpha}_n+\alpha_m=(n+m,0)$, $\widehat{\beta}_{-l}(\widehat{\alpha})=\beta_{-l}(\alpha)$ for all $l\in\mathbb{Z}^2$ and $\int_0^{2\pi}\int_0^{2\pi}e^{i(n+m,0)\cdot x}dx_1dx_2=0$ for $n+m\neq(0,0)$ to conclude that

$$\begin{aligned}
&r\cdot E(y_0;m)\\
&=\frac{4\pi^2 i}{\lambda_0}\Big\{[\widehat{E}_{-m}(y_0)\times e_3]\times(\alpha_m;-\beta_m)-e_3\times[(\widehat{\alpha}_{-m};\widehat{\beta}_{-m})\times\widehat{E}_{-m}(y_0)]\Big\}\cdot p_m\\
&=-\frac{4\pi^2 i}{\lambda_0}\Big\{(\alpha_m;-\beta_m)\times[\widehat{E}_{-m}(y_0)\times e_3]+e_3\times[(\widehat{\alpha}_{-m};\widehat{\beta}_{-m})\times\widehat{E}_{-m}(y_0)]\Big\}\cdot p_m\\
&=-\frac{4\pi^2 i}{\lambda_0}\Big\{-\beta_m\widehat{E}_{-m}-[(\alpha_m;-\beta_m)\cdot\widehat{E}_{-m}]e_3+\widehat{E}^{(3)}_{-m}(\widehat{\alpha}_{-m};\widehat{\beta}_{-m})-\widehat{\beta}_{-m}\widehat{E}_{-m}\Big\}\cdot p_m\\
&=-\frac{4\pi^2 i}{\lambda_0}\Big\{\widehat{E}^{(3)}_{-m}(y_0)(\widehat{\alpha}_{-m};\widehat{\beta}_{-m})-2\widehat{\beta}_{-m}\widehat{E}_{-m}(y_0)\Big\}\cdot p_m\\
&=\frac{8\pi^2 i}{\lambda_0}\widehat{\beta}_{-m}\widehat{E}_{-m}(y_0)\cdot p,
\end{aligned}$$

where we have used the fact that

$$(\widehat{\alpha}_{-m};\widehat{\beta}_{-m})\cdot p_m=(\alpha_m;-\beta_m)\cdot p_m=0,$$
$$(\alpha_m;-\beta_m)\cdot\widehat{E}_{-m}=(-\widehat{\alpha}_{-m};-\widehat{\beta}_{-m})\cdot\widehat{E}_{-m}=0.$$

This completes the proof. □

If $y_0\in\Omega_0$, define the total field $\widehat{E}(x;y_0)=\widehat{E}^s(x;y_0)+\widehat{\mathbb{G}}_0(x,y_0)s$ in Ω_0, where $\widehat{\mathbb{G}}_0(x,y_0)$ is an $\widehat{\alpha}$-quasi-periodic Green tensor defined in (4.1) with α replaced with $\widehat{\alpha}$. Then arguing similarly as in the proof of Lemma 4.1 we can prove the following result.

Lemma 4.2. *For $m=(m_1,m_2)\in\mathbb{Z}^2$ let $E^i(x;m) = (1/k_0^2)\operatorname{curl}\operatorname{curl}[p\exp(i\alpha_m\cdot x-i\beta_m x_3)]$ and let $E(x;m)$ (which is the sum $E^i(x;m)+E^s(x;m)$ in Ω_0) be the solution to the the scattering problem* (1.1) – (1.6) *with $E^i(x)=E^i(x;m)$. For $y_0\in\Omega_0$, $\widehat{\alpha}=-\alpha$ and $r\in\mathbb{R}^3$ let $E^i(x;y_0)=\widehat{\mathbb{G}}_0(x,y_0)r$ and let $\widehat{E}(x;y_0)$ (which equals to the sum $E^i(x;y_0)+\widehat{E}^s(x;y_0)$ in $\Omega_0\backslash\{y_0\}$) satisfy the Maxwell equations* $\operatorname{curl}\operatorname{curl}\widehat{E}-k_0^2\widehat{E}=0$ *in $\Omega_0\backslash\{y_0\}$ and* $\operatorname{curl}\operatorname{curl}\widehat{E}-k_0^2q\widehat{E}=0$ *in Ω_1 together with the transmission condition*

$$\nu\times\widehat{E}|_+=\nu\times\widehat{E}|_-,\quad \nu\times\operatorname{curl}\widehat{E}|_+=\lambda_0\nu\times\operatorname{curl}\widehat{E}|_-\ \ \textit{on}\ \Gamma_0,$$

the boundary condition

$$\nu \times \widehat{E} = 0 \quad on \ \Gamma_{1,D}, \qquad \nu \times \operatorname{curl} \widehat{E} - i\rho(\nu \times \widehat{E}) \times \nu = 0 \ \ on \ \Gamma_{1,I}$$

and the Rayleigh expansion radiation condition

$$\widehat{E}^s(x; y_0) = \sum_{n \in \mathbb{Z}^2} \widehat{E}_n(y_0) \exp(i\widehat{\alpha}_n \cdot x + \widehat{\beta}_n x_3) \qquad for \ x_3 > g_+,$$

where

$$\widehat{\alpha}_n \cdot \widehat{E}_n + \widehat{\beta}_n \cdot \widehat{E}_n^{(3)} = 0.$$

Then we have

$$r \cdot E(y_0; m) = 8\pi^2 i \widehat{\beta}_{-m} \widehat{E}_{-m}(y_0) \cdot p. \tag{4.14}$$

4.2. Unique determination of the impenetrable profile f. We now consider the unique determination of the impenetrable grating profile f, assuming that the interface profile g is known and $k_0^2 q(x) \equiv k_1^2$ is a constant. A key ingredient in our proof is the mixed reciprocity relation for the doubly periodic structure (see Lemma 4.1).

THEOREM 4.3. *Assume that $\beta_n \neq 0$ for all $n \in \mathbb{Z}^2$, the interface profile g is known and $k_0^2 q(x) \equiv k_1^2$ is a constant. Let f_1, $f_2 \in C^2(\mathbb{R}^2)$ be 2π-periodic, let ρ_1, ρ_2 be two constants and let $h > \max_{x \in \mathbb{R}^2}\{f_1(x), f_2(x)\}$. If $\nu \times E^s_{1,m}|_{\Gamma_h} = \nu \times E^s_{2,m}|_{\Gamma_h}$ for all incident waves $E^i_m(x) = (1/k_0^2)\operatorname{curl}\operatorname{curl}[e_l \exp(i\alpha_m \cdot x - i\beta_m x_3)]$ with $m \in \mathbb{Z}^2$ and $l = 1, 2, 3$, then*

$$f_1 = f_2, \quad \Gamma_{f_1,D} = \Gamma_{f_2,D}, \ \ \Gamma_{f_1,I} = \Gamma_{f_2,I}, \ \ \rho_1 = \rho_2,$$

where e_l is the unit vector in the direction x_l, $l = 1, 2, 3$. Here, $E_{j,m} = E^i_m + E^s_{j,m}$ in Ω_0 and $E_{j,m}$ in Ω_{1f_j} are the unique quasi-periodic solution of the scattering problem (1.1) – (1.6) with $E^i = E^i_m$, $\rho = \rho_j$ and $f = f_j$, where $\Omega_{f_j} = \{x \in \mathbb{R}^3 \,|\, f_j(x_1, x_2) < x_3 < g(x_1, x_2)\}$, $j = 1, 2$.

Proof. We assume without loss of generality that $f_1 \neq f_2$ and there exists a $z^* = (z_1^*, z_2^*, z_3^*) \in \Gamma_{f_1}$ with $f_1(z_1^*, z_2^*) > f_2(z_1^*, z_2^*)$, where $\Gamma_{f_j} = \{x \in \mathbb{R}^3 \,|\, x_3 = f_j(x_1, x_2)\}$. We choose $\epsilon > 0$ such that $z_\epsilon := z^* + \epsilon e_3 \in \Omega_{f_1} \cap \Omega_{f_2}$.

Let $\widehat{E}_{\epsilon,j}$ be the unique quasi-periodic solution to the scattered problem (4.2)-(4.8) with $y_0 = z_\epsilon$, $\rho = \rho_j$, $f = f_j$. By Lemma 4.1 we have

$$r \cdot E_{1,m}(z_\epsilon) = \frac{8\pi^2 i}{\lambda_0} \widehat{\beta}_{-m} \widehat{E}_{1,-m}(z_\epsilon) \cdot e_l, \tag{4.15}$$

$$r \cdot E_{2,m}(z_\epsilon) = \frac{8\pi^2 i}{\lambda_0} \widehat{\beta}_{-m} \widehat{E}_{2,-m}(z_\epsilon) \cdot e_l, \tag{4.16}$$

where $\widehat{E}_{j,n}(z_\epsilon)$ are the Rayleigh coefficients for $\widehat{E}_{\epsilon,j}$.

On the other hand, from the Rayleigh expansion radiation condition and the assumption that $\nu \times E^s_{1,m}|_{\Gamma_h} = \nu \times E^s_{2,m}|_{\Gamma_h}$ we conclude by the unique continuation principle that $E^s_{1,m} = E^s_{2,m}$ in Ω_0. This, together with the transmission condition on

Γ_0 and Holmgren's uniqueness theorem, implies that $E_{1,m} = E_{2,m}$ in $\Omega_{f_1} \cap \Omega_{f_2}$, so $E_{1,m}(z_\epsilon) = E_{2,m}(z_\epsilon)$. It then follows from (4.15) and (4.16) that

$$\frac{8\pi^2 i}{\lambda_0}\widehat{\beta}_{-m}\widehat{E}_{1,-m}(z_\epsilon)\cdot e_l = \frac{8\pi^2 i}{\lambda_0}\widehat{\beta}_{-m}\widehat{E}_{2,-m}(z_\epsilon)\cdot e_l \qquad \text{or} \quad \widehat{E}_{1,-m}(z_\epsilon) = \widehat{E}_{2,-m}(z_\epsilon).$$

Thus, by the Rayleigh expansion radiation condition we have $\widehat{E}_{\epsilon,1}(x) = \widehat{E}_{\epsilon,2}(x)$ for $x_3 > g_+$. By the unique continuation principle, the transmission condition on Γ_0 and Holmgren's uniqueness theorem again we obtain that

$$\widehat{E}_{\epsilon,1}(x) = \widehat{E}_{\epsilon,2}(x) \quad \text{in} \quad \overline{\Omega}_0 \quad \text{and} \quad \widehat{E}^s_{\epsilon,1}(x) = \widehat{E}^s_{\epsilon,2}(x) \quad \text{in} \quad \overline{\Omega_{f_1} \cap \Omega_{f_2}}.$$

Without loss of generality we may assume that z^* lies on the coated part of Γ_{f_1}. Since z^* has a positive distance from Γ_{f_2}, then the well-posedness of the direct problem implies that there exists $C > 0$ (independent of ϵ) such that

$$|(\nu \times \operatorname{curl} \widehat{E}^s_{\epsilon,1} - i\rho_1 \nu \times \widehat{E}^s_{\epsilon,1} \times \nu)(z^*)| = |(\nu \times \operatorname{curl} \widehat{E}^s_{\epsilon,2} - i\rho_1 \nu \times \widehat{E}^s_{\epsilon,2} \times \nu)(z^*)| \le C.$$

However, from the boundary condition on Γ_{f_1} it is seen that

$$\begin{aligned}&|(\nu \times \operatorname{curl} \widehat{E}^s_{\epsilon,1} - i\rho_1 \nu \times \widehat{E}^s_{\epsilon,1} \times \nu)(z^*)| \\ &\qquad = |(\nu \times \operatorname{curl} [\widehat{\mathbb{G}}_1(\cdot, z_\epsilon) r] - i\rho_1 \nu \times [\widehat{\mathbb{G}}_1(\cdot, z_\epsilon) r] \times \nu)(z^*)| \to +\infty\end{aligned}$$

as $\epsilon \to 0$. This is a contradiction, which implies that $f_1 = f_2$, that is, $\Omega_{f_1} = \Omega_{f_2}$ and $\Gamma_{f_1} = \Gamma_{f_2}$. Hence, we have $E_{1,m} = E_{2,m}$ in Ω_{f_1}. We claim that $\Gamma_{f_1,D} \cap \Gamma_{f_2,I}$ must be empty (so $\Gamma_{f_1,D} = \Gamma_{f_2,D}$ and $\Gamma_{f_1,I} = \Gamma_{f_2,I}$) since, otherwise, a similar argument as below deduces that the total field $E_{1,m}$ vanishes in Ω_{f_1}, which is impossible.

Now let $f = f_1 = f_2$. Then by the boundary condition we deduce that

$$i(\rho_1 - \rho_2)(\nu \times E_{1,m}) \times \nu = 0 \quad \text{on} \quad \Gamma_{1,I}.$$

If $\rho_1 \ne \rho_2$, then the above equation implies that $\nu \times E_{1,m} = 0$ on $\Gamma_{1,I}$, so by the boundary condition again $\nu \times \operatorname{curl} E_{1,m} = 0$ on $\Gamma_{1,I}$. Thus, by Holmgren's uniqueness theorem, $E_{1,m} = 0$ in Ω_1. By the transmission condition on Γ_0 and Holmgren's uniqueness theorem again it follows that $E_{1,m} = E^i_m + E^s_{1,m} = 0$ in Ω_0, which is a contradiction. The proof is thus completed. ▯

4.3. Unique determination of the refractive index. We now consider the inverse problem of recovering the refractive index q. We only consider the case that $\Gamma_{1,I} = \emptyset$, that is, the grating surface Γ_1 is a perfect conductor. However, we expect the result to hold in a more general case by constructing special solutions of the Maxwell equations. Throughout this section we assume that the transmission constant λ_0 is known and the shape of the grating surfaces Γ_0 and Γ_1 is also known and flat, that is, for two known constants $b > c$, $g(x') \equiv b$ and $f(x') \equiv c$ for all $x' \in \mathbb{R}^2$.

We have the following global uniqueness result for the inverse problem.

THEOREM 4.4. *Assume that $q = q_j$ satisfies the conditions (**A1**)$-$(**A3**) and that q_j depends only on x_1 or x_2, $j = 1, 2$. Let $h > b$. If*

$$\nu \times E^s_{1,m}|_{\Gamma_h} = \nu \times E^s_{2,m}|_{\Gamma_h}$$

for all incident waves $E^i_m(x) = (1/k_0^2)\operatorname{curl}\operatorname{curl}[e_l \exp(i\alpha_m \cdot x - i\beta_m x_3)]$ with $m \in \mathbb{Z}^2$ and $l = 1, 2, 3$, then we have $q_1 = q_2$. Here, $E_{j,m} = E^i_m + E^s_{j,m}$ in Ω_0 and $E_{j,m}$ in

Ω_1 *are the unique quasi-periodic solution of the scattering problem* (1.1) − (1.6) *with* $E^i = E^i_m$ *and* $q = q_j$, $j = 1, 2$.

REMARK 4.5. Theorem 4.4 improves the result in [14, Theorem 5.4], where only the special case $\lambda_0 = 1$ is considered and incident waves of the form (4.17) below are used for all $r \in L^2_t(\Gamma_h)$.

To prove Theorem 4.4 we need the following denseness result which is related to the incident waves of the form

$$E^i(x; r) = \int_{\Gamma_h} \widehat{\mathbb{G}}_0(x, y)r(y)ds(y), \qquad x_3 < h, \tag{4.17}$$

where $r \in L^2_t(\Gamma_h)$. This result was proved in [14, Lemma 5.2] for the case $\lambda_0 = 1$, and the general case can be proved similarly (see the proof of Lemma 5.2 in [14]).

LEMMA 4.6. *The operator* F *has a dense range in* $H_t^{-1/2}(\mathrm{div}\,, \Gamma_0)$. *Here,* $F : L^2_t(\Gamma_h) \to H_t^{-1/2}(\mathrm{div}\,, \Gamma_0)$ *is defined by* $(Fr)(x) = e_3 \times \widehat{E}(x; r)|_-$ *on* Γ_0, *where* $\widehat{E}(x; r)$ *is the solution of the scattering problem* (1.1) − 1.6) *with the incident wave* $E^i(x) = E^i(x; r)$ *given by* (4.17).

Proof of Theorem 4.4. For any $r \in L^2_t(\Gamma_h)$ and $y \in \Gamma_h$ we have by Lemma 4.2 that

$$r(y) \cdot E^s_j(y; m) = 8\pi^2 i\widehat{\beta}_{-m}\widehat{E}_{j,-m}(y) \cdot e_l, \qquad j = 1, 2,\ l = 1, 2, 3, \tag{4.18}$$

where $\widehat{E}_{j,-m}(y)$ are the Rayleigh coefficients of the scattered field $\widehat{E}^s_j(\cdot; y)$ corresponding to $q = q_j$ and the incident wave $E^i(x) = \widehat{\mathbb{G}}_0(x, y)r(y)$. It follows from (4.18) that

$$\int_{\Gamma_h} r(y) \cdot E^s_j(y; m)ds(y) = 8\pi^2 i\widehat{\beta}_{-m} \int_{\Gamma_h} \widehat{E}_{j,-m}(y)ds(y) \cdot e_l. \tag{4.19}$$

Denote by $\widehat{E}^s_j(x; r)$ and $\widehat{E}_j(x; r)$ the scattered and total electric fields, respectively, corresponding to $q = q_j$ and the incident wave $E^i(x) = E^i(x; r)$, $j = 1, 2$. Then from the definition (4.17) of $E^i(x; r)$ it is seen that

$$\int_{\Gamma_h} \widehat{E}_{j,-m}(y)ds(y) \ \text{ are the Rayleigh coefficients of } \ \widehat{E}^s_j(x; r). \tag{4.20}$$

On the other hand, from the Rayleigh expansion radiation condition and the assumption that $\nu \times E^s_1(x; m) = \nu \times E^s_2(x; m)$ on Γ_h we conclude on using the unique continuation principle that $E^s_1(x; m) = E^s_2(x; m)$ in $\overline{\Omega}_0$. This, together with (4.19) and (4.20), implies that

$$\int_{\Gamma_h} \widehat{E}_{1,-m}(y)ds(y) = \int_{\Gamma_h} \widehat{E}_{2,-m}(y)ds(y).$$

From this, the Rayleigh expansion radiation condition and the unique continuation principle it follows that

$$\widehat{E}^s_1(x; r) = \widehat{E}^s_2(x; r) \quad \text{or} \quad \widehat{E}_1(x; r) = \widehat{E}_2(x; r) \quad \text{in } \Omega_h \backslash \Omega_1.$$

With the help of the transmission conditions on Γ_0, we get

$$\begin{aligned} \nu \times \widehat{E}_1(x;r)|_- &= \nu \times \widehat{E}_2(x;r)|_- \qquad \text{on } \Gamma_0, \\ \nu \times \operatorname{curl} \widehat{E}_1(x;r)|_- &= \nu \times \operatorname{curl} \widehat{E}_2(x;r)|_- \qquad \text{on } \Gamma_0. \end{aligned}$$

Now define $E(x) := \widehat{E}_1(x;r) - \widehat{E}_2(x;r)$ in $\overline{\Omega}_1$. Then E satisfies the equation

$$\operatorname{curl}\operatorname{curl} E - k_0^2 q_2 E = k_0^2(q_1 - q_2)\widehat{E}_1(x;r) \quad \text{in } \Omega_1$$

and the boundary conditions

$$\begin{aligned} \nu \times E = 0, \ \ \nu \times \operatorname{curl} E &= 0 \qquad \text{on } \Gamma_0, \\ \nu \times E &= 0 \qquad \text{on } \Gamma_1. \end{aligned}$$

Thus it follows from Green's vector formula that

$$\begin{aligned} & k_0^2 \int_{\Omega_1} (q_1 - q_2)\widehat{E}_1(x;r) \cdot \overline{E}_2(x) dx \\ &= \int_{\Omega_1} (\operatorname{curl}\operatorname{curl} E - k_0^2 q_2 E) \cdot \overline{E}_2(x) dx \\ &= \int_{\Omega_1} (\operatorname{curl}\operatorname{curl} \overline{E}_2(x) - k_0^2 q_2 \overline{E}_2(x)) \cdot E(x) dx \\ &= 0 \end{aligned} \tag{4.21}$$

for any $r \in L_t^2(\Gamma_h)$, where $E_2 \in H(\operatorname{curl}, \Omega_1)$ satisfies the Maxwell equation (1.2) with $q = \overline{q}_2$ and the boundary condition $\nu \times E_2|_{\Gamma_1} = 0$.

Now by Lemma 4.6 and (4.21) we obtain that

$$\int_{\Omega_1} (q_1 - q_2) E_1(x) \cdot \overline{E}_2(x) dx = 0, \tag{4.22}$$

where E_1 satisfies of the Maxwell equation (1.2) with $q = q_1$ and the boundary condition $\nu \times E_1|_{\Gamma_1} = 0$.

Finally, using the orthogonal relation (4.22) and arguing in exactly the same way as in the proof of Theorem 5.4 in [14], we can easily prove that $q_1 = q_2$. The proof is thus completed. ☐

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