AN ADAPTIVE FINITE ELEMENT METHOD WITH PERFECTLY MATCHED ABSORBING LAYERS FOR THE WAVE SCATTERING BY PERIODIC STRUCTURES

ZHIMING CHEN* AND HAIJUN WU†

Abstract. We develop a finite element adaptive strategy with error control for the wave scattering by periodic structures. The unbounded computational domain is truncated to a bounded one by an extension of the PML technique which attenuates both the outgoing and evanescent waves in the PML region. The PML parameters such as the thickness of the layer and the medium property are determined through sharp a posteriori error estimates. Numerical experiments are included to illustrate the competitive behavior of the proposed adaptive method.

Key words. Adaptivity, perfectly matched layer, a posteriori error analysis, grating optics

AMS subject classifications. 65N30, 78A45, 35Q60

1. Introduction. We consider the prediction of the scattered modes that arise when an electromagnetic wave is incident on some periodic structure. The media are assumed to be nonmagnetic and the magnetic permeability μ is constant everywhere. Then the electromagnetic fields in the whole space are governed by the following time harmonic (time dependence $e^{-\mathbf{i}\omega t}$) Maxwell equations

$$\nabla \times \mathbf{E} - \mathbf{i}\omega\mu\mathbf{H} = 0, \tag{1.1}$$

$$\nabla \times \mathbf{H} + \mathbf{i}\omega\varepsilon\mathbf{E} = 0. \tag{1.2}$$

Here $\mathbf{E}$ and $\mathbf{H}$ are the electric and the magnetic field vectors, respectively. The physical structure is described by the dielectric coefficient $\varepsilon(x), x = (x_1, x_2, x_3)$. In this paper we restrict ourselves to the two-dimensional setting (1D grating problem), the medium and the grating surface are assumed to be constant in x_2 direction, The more complicated biperiodic diffraction (three-dimensional) problems will be considered in a separate work. We assume the dielectric coefficient $\varepsilon(x) = \varepsilon(x_1, x_3)$ is periodic in x_1 direction with period $L > 0$

$$\varepsilon(x_1 + nL, x_3) = \varepsilon(x_1, x_3) \ \ \forall\, x_1, x_3 \in \mathbf{R}, \ \ n \text{ integer}\ .$$

The dielectric coefficient $\varepsilon(x)$ may be complex. We assume $\operatorname{Im}\varepsilon(x) \geq 0$ and $\operatorname{Re}\varepsilon(x) > 0$ whenever $\operatorname{Im}\varepsilon(x) = 0$. It is natural to assume that ε is constant away from a region $\{(x_1, x_3) : b_2 < x_3 < b_1\}$ which includes the structure, that is, there exist constants ε_1 and ε_2 such that

$$\varepsilon(x_1, x_3) = \varepsilon_1 \ \text{ in } \ \Omega_1 = \{(x_1, x_3) : x_3 \geq b_1\},$$
$$\varepsilon(x_1, x_3) = \varepsilon_2 \ \text{ in } \ \Omega_2 = \{(x_1, x_3) : x_3 \leq b_2\}.$$

In practical applications, we have $\varepsilon_1 > 0$ but ε_2 may be complex according to the substrate material used in Ω_2. Depending on the direction and polarization of the incident plane wave, the Maxwell equations can be simplified by considering the two

*LSEC, Institute of Computational Mathematics, Chinese Academy of Sciences, Beijing 100080, PR China. This author was supported in part by China NSF under the grant 10025102 and by China MOS under the grant G1999032802. (zmchen@lsec.cc.ac.cn).

†LSEC, Institute of Computational Mathematics, Chinese Academy of Sciences, Beijing 100080, PR China. (whj@lsec.cc.ac.cn).

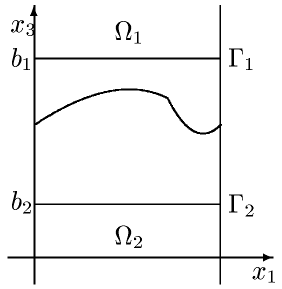

FIG. 1.1. *Geometry of the grating problem*

fundamental polarizations: the transverse electric (TE) polarization and the transverse magnetic (TM) polarization. In the TE case, the electric field $\mathbf{E}$ is parallel to x_2 axis: $\mathbf{E} = (0, u, 0)^T \in \mathbf{R}^3$, where $u = u(x_1, x_3)$ satisfies the Helmholtz equation

$$\Delta u + k^2(x)u = 0 \quad \text{in} \quad \mathbf{R}^2. \tag{1.3}$$

Here $k^2(x) = \omega^2\varepsilon(x)\mu$ is the magnitude of the wave vector. Similarly, in the TM case, the magnetic field $\mathbf{H}$ is parallel to the x_2 axis: $\mathbf{H} = (0, u, 0)^T \in \mathbf{R}^3$, where $u = u(x_1, x_3)$ satisfies the equation:

$$\mathrm{div}\left(\frac{1}{k^2(x)}\nabla u\right) + u = 0 \quad \text{in} \quad \mathbf{R}^2. \tag{1.4}$$

Scattering theory in periodic structures which has many important applications in micro-optics has recently received considerable attention among applied mathematical community. We refer to Dobson and Friedman [14], Abboud [1], Dobson [13], Bao, Dobson and Cox [4], Bao [5], Bao and Yang [7] for the existence, uniqueness and numerical approximations of solutions to grating problems. A good introduction to the problem of electromagnetic diffraction through periodic structures can be found in Petit [19]. More recent review on the diffractive optics technology and its mathematical modeling can be found in Bao, Cowsar and Masters [6].

The purpose of this paper is to develop efficient numerical methods solving the 1D grating problem for both the TE (1.3) and the TM (1.4) polarizations. In doing so, the first difficulty is to truncate the domain into an bounded computational domain. The finite element method studied in [4] and [7] are based on variational formulation on the bounded domain Ω with periodic condition in x_1 direction and the transparent boundary condition on the top and bottom boundaries Γ_1 and Γ_2 (see Fig. 1.1). The transparent boundary condition is obtained by insisting the solution u of (1.3) or (1.4) is composed of bounded outgoing plane waves in Ω_1 and Ω_2, plus the incident wave u_{I} in Ω_1. The derived transparent boundary condition is represented as a quasi-differential operator and is nonlocal. In practical computations, the infinite series in the definition of the quasi-differential operator must be truncated. The second difficulty is the singularity of the solutions. Usually, the grating surface is piecewise smooth and across the surface the dielectric coefficient $\varepsilon(x)$ is discontinuous. Thus the solution of (1.4) will have singularities which slow down the finite element convergence when using uniform mesh refinements. Even in the TE case (1.3), when there are lossy materials beneath the grating surface, the transmitted waves decay exponentially. This makes the uniform mesh refinements uneconomical.

The purpose of this paper is twofolds: First we explore the possibility of applying the recently introduced perfectly matched layer (PML) technique to deal with the first difficulty on truncating the unbounded domain. Secondly we explore the possibility of using a posteriori error analysis to design efficient adaptive method with error control which adaptively determines the finite element meshes and the PML parameters such as the thickness of the PML region and the medium property inside the region. We hope the ideas developed in this paper will be useful to solving other scattering problems on unbounded domains.

A posteriori error estimates are computable quantities in terms of the discrete solution and data that measure the actual discrete errors without the knowledge of limit solutions. They are essential in designing algorithms for mesh modification which equi-distribute the computational effort and optimize the computation. Ever since the pioneering work of Babuška and Rheinboldt [3], the adaptive finite element methods based on a posteriori error estimates have become a central theme in scientific and engineering computations. The ability of error control and the asymptotically optimal approximation property (see e.g. Morin, Nochetto and Siebert [18], Chen and Dai [10]) make the adaptive finite element method attractive for complicated physical and industrial processes (cf. e.g. Chen and Dai [9], Chen, Nochetto and Schmidt [11]). For the efforts to solve scattering problems using adaptive methods based on a posterior error estimate, we refer to the recent work Monk [16], Monk and Süli [17].

Under the assumption that the exterior solution is composed of outgoing waves only, the basic idea of the PML technique is to surround the computational domain by a finite thickness layer of the specially designed model medium that would either slow down or attenuate all the waves that propagate from inside the computational domain. Since the work of Berenger [8] which proposed a PML layer for use with the time dependent Maxwell equations, various constructions of PML absorbing layers have been proposed and studied in the literature. We refer to Turkel and Yefet [22] for a review on various proposed models and Lassas and Somersalo [15] for the study of mathematical properties of the PML equations. In practical applications involving PML method, there is a judicial compromise between a thin layer which requires a rapid variation of the artificial material property and a thick layer which requires more grid points and hence more computer time and more storage (see e.g. Collino and Monk [12]). In this paper, we propose to use a posteriori error estimate to determine the PML parameters. Moreover, the derived a posteriori error estimate has the nice feature of exponentially decay in terms of the distance to the computational domain. This property leads to coarse mesh size away from the computational domain and thus makes the total computational cost insensitive to the thickness of the PML absorbing layer.

The layout of the paper is as follows. In §2 we first recall the transparent boundary condition for 1D grating problems and introduce our PML formulation, which extends the standard PML condition for Helmholtz equation in that our PML condition attenuates both the outgoing plane waves and the evanescent waves. This extension allows us to reduce the computational domain and thus reduce the computational cost. Existence, uniqueness and convergence of the PML formulation are considered. In §3 we introduce the finite element discretization. In §4 we derive sharp a posteriori error estimate which lays down the basis of the adaptive method. In §5, we present parallel results for the case when $\operatorname{Im}\varepsilon_2 > 0$. Finally, in §6 we discuss the implementation of the adaptive method and present several numerical examples to illustrate the competitive behavior of the method.

2. The PML formulation. In this section we shall introduce variational formulations for the 1D grating problem (1.3) and (1.4) using PML technique which are suitable for further finite element approximations. As the discussions for the TE polarization and TM polarization are parallel, we shall concentrate on the TE polarization first and state the corresponding results on the TM polarization without proof. In §2–§4, we consider the case when $\mathrm{Im}\,\varepsilon_2 = 0$, and thus $k_j = \omega\sqrt{\varepsilon_j \mu}$ is real, for $j = 1, 2$. The parallel results for the case when $\mathrm{Im}\,\varepsilon_2 > 0$ will be presented in §5.

2.1. TE polarization. We start by recalling the variational formulation with the transparent boundary condition in [4] which is the basis of the analysis in this paper. Let $u_{\mathrm{I}} = e^{\mathbf{i}\alpha x_1 - \mathbf{i}\beta x_3}$ be the incoming plane wave which is incident upon the grating surface from the top, where $\alpha = k_1 \sin\theta, \beta = k_1 \cos\theta$, and $-\pi/2 < \theta < \pi/2$ is the incident angle. We are interested in quasi-periodic solutions u, that is, solutions u of (1.3) such that $u_\alpha = ue^{-\mathbf{i}\alpha x_1}$ are periodic in x_1 with period $L > 0$.

Denote by $\Gamma_j = \{(x_1, x_3) : 0 < x_1 < L, x_3 = b_j\}, j = 1, 2$. We wish to reduce the problem to the bounded domain

$$\Omega = \{(x_1, x_3) : 0 < x_1 < L \text{ and } b_2 < x_3 < b_1\}.$$

The radiation condition for the diffraction problem insists that u is composed of bounded outgoing plane waves in Ω_1 and Ω_2, plus the incident wave u_{I} in Ω_1.

For each integer n, let $\alpha_n = 2\pi n/L$, since u_α is periodic in x_1 direction with period $L > 0$, it has a Fourier series expansion:

$$u_\alpha(x_1, x_3) = \sum_{n\in Z} u_\alpha^{(n)}(x_3) e^{\mathbf{i}\alpha_n x_1}, \quad u_\alpha^{(n)}(x_3) = \frac{1}{L}\int_0^L u_\alpha e^{-\mathbf{i}\alpha_n x_1} dx_1.$$

Thus we have the expansion

$$u(x_1, x_3) = u_\alpha e^{\mathbf{i}\alpha x_1} = \sum_{n\in Z} u_\alpha^{(n)}(x_3) e^{\mathbf{i}(\alpha_n+\alpha)x_1}. \tag{2.1}$$

Since u satisfies Helmholtz equation $\Delta u + k_1^2 u = 0$ in Ω_1, we deduce that

$$\sum_{n\in Z}\left[\left(k_1^2 - (\alpha_n+\alpha)^2\right) u_\alpha^{(n)}(x_3) + \frac{d^2}{dx_3^2} u_\alpha^{(n)}(x_3)\right] e^{\mathbf{i}(\alpha_n+\alpha)x_1} = 0,$$

which yields

$$\left(k_1^2 - (\alpha_n+\alpha)^2\right) u_\alpha^{(n)}(x_3) + \frac{d^2}{dx_3^2} u_\alpha^{(n)}(x_3) = 0 \quad \text{for} \quad x_3 \geq b_1. \tag{2.2}$$

For any integer $n \in Z$ and $j = 1, 2$, we define

$$\beta_j^n = \beta_j^n(\alpha) = \begin{cases} \left(k_j^2 - (\alpha_n+\alpha)^2\right)^{1/2} & \text{if } k_j^2 \geq (\alpha_n+\alpha)^2 \\ \mathbf{i}\left((\alpha_n+\alpha)^2 - k_j^2\right)^{1/2} & \text{if } k_j^2 < (\alpha_n+\alpha)^2. \end{cases} \tag{2.3}$$

Note that $\beta_1^0 = \beta$ by definition. We assume that $k_j^2 \neq (\alpha_n+\alpha)^2$ for all $n \in Z, j = 1, 2$. This condition excludes "resonance". All the solutions of the ODE (2.2) can then be written as

$$u_\alpha^{(n)}(x_3) = A_1^n e^{\mathbf{i}\beta_1^n x_3} + B_1^n e^{-\mathbf{i}\beta_1^n x_3}$$

with complex constants A_1^n and B_1^n. The assumption that only bounded outgoing plane waves except $u_{\rm I}$ exist in Ω_1 implies $B_1^n = 0$ for $n \neq 0$. Thus we deduce from (2.1) the following Rayleigh expansion in Ω_1:

$$u = u_{\rm I} + \sum_{n \in Z} A_1^n e^{\mathbf{i}(\alpha_n + \alpha)x_1 + \mathbf{i}\beta_1^n x_3} \quad , \quad x \in \Omega_1. \tag{2.4}$$

Similarly, we have the following Rayleigh expansion in Ω_2:

$$u = \sum_{n \in Z} A_2^n e^{\mathbf{i}(\alpha_n + \alpha)x_1 - \mathbf{i}\beta_2^n x_3} \quad , \quad x \in \Omega_2. \tag{2.5}$$

For any quasi-periodic function f which has the expansion $f = \sum_{n \in Z} f^{(n)}\, e^{\mathbf{i}(\alpha_n + \alpha)x_1}$, the following Dirichlet to Neumann Operator T_j is introduced in [4]

$$(T_j f)(x_1) = \sum_{n \in Z} \mathbf{i}\beta_j^n f^{(n)} e^{\mathbf{i}(\alpha_n + \alpha)x_1} \quad , \quad 0 < x_1 < L \ , \ j = 1, 2. \tag{2.6}$$

With this notation in mind, simple calculation shows that the Rayleigh expansion u in $\Omega_j, j = 1, 2$, defined in (2.4) and (2.5) satisfies respectively the following relations

$$\frac{\partial(u - u_{\rm I})}{\partial \nu} - T_1(u - u_{\rm I}) = 0 \quad \text{on} \quad \Gamma_1, \qquad \frac{\partial u}{\partial \nu} - T_2 u = 0 \quad \text{on} \quad \Gamma_2, \tag{2.7}$$

where ν stands for the unit outer normal to $\partial\Omega$. These are the transparent boundary conditions used in [4]. To define a variational formulation for the 1D grating problem (1.3) using the boundary conditions (2.7), we first introduce the following subspace of $H^1(\Omega)$ which includes all the quasi-periodic functions:

$$X(\Omega) = \{w \in H^1(\Omega) : w(0, x_3) = e^{-\mathbf{i}\alpha L} w(L, x_3) \ \text{ for } b_2 < x_3 < b_1\}.$$

Define the sesquilinear form $b : X(\Omega) \times X(\Omega) \to \mathbf{C}$ as follows:

$$b(\varphi, \psi) = \int_\Omega \left(\nabla\varphi\nabla\bar{\psi} - k^2(x)\varphi\bar{\psi}\right) dx - \sum_{j=1}^{2} \int_{\Gamma_j} (T_j\varphi)\bar{\psi} dx_1. \tag{2.8}$$

Note that $\dfrac{\partial u_{\rm I}}{\partial \nu} - T_1 u_{\rm I} = -2\mathbf{i}\beta u_{\rm I}$ on Γ_1, the weak formulation of the 1D grating problem in the TE polarization reads then as follows: Given incoming plane wave $u_{\rm I} = e^{\mathbf{i}\alpha x_1 - \mathbf{i}\beta x_3}$, seek $u \in X(\Omega)$ such that

$$b(u, \psi) = -\int_{\Gamma_1} 2\mathbf{i}\beta u_{\rm I}\bar{\psi} dx_1 \quad , \quad \forall\, \psi \in X(\Omega). \tag{2.9}$$

Recall that $k^2(x) = \omega^2\varepsilon(x)\mu$. The existence of a unique solution u to (2.9) is proved for all but a sequence of countable frequencies ω_j with $|\omega_j| \to +\infty$. Further uniqueness results can be obtained for any frequency ω if the dielectric coefficient $\varepsilon(x)$ has nonzero imaginary part in some subdomains in Ω. In this paper, we shall not elaborate on this issue and assume in the following that the variational problem (2.9) has a unique solution. Then the general theory in Babuška and Aziz [2, Chap. 5] implies that there exists a constant $\gamma > 0$ such that the following inf-sup condition holds

$$\sup_{0 \neq \psi \in H^1(\Omega)} \frac{|b(\varphi, \psi)|}{\|\,\psi\,\|_{H^1(\Omega)}} \geq \gamma\,\|\,\varphi\,\|_{H^1(\Omega)} \quad , \quad \forall\, \varphi \in X(\Omega). \tag{2.10}$$

Now we turn to the introduction of absorbing PML layers. We surround our computational domain Ω with two PML layers of thickness δ_1 and δ_2 in Ω_1 and Ω_2 respectively. The specially designed model medium in the PML layers should basically be so chosen that the wave either never reaches its external boundary or the amplitude of the reflected wave is so small that it does not essentially contaminate the solution in Ω. Let $s(x_3) = s_1(x_3) + \mathbf{i}s_2(x_3)$ be the model medium property which satisfies

$$s_1, s_2 \in C(\mathbf{R}), s_1 \geq 1, s_2 \geq 0, \text{ and } s(x_3) = 1 \text{ for } b_2 \leq x_3 \leq b_1. \tag{2.11}$$

Here we remark that in contrast to the original PML condition which takes $s_1 \equiv 1$ in the PML region, we allow a variable s_1 in order to attenuate both the outgoing and evanescent waves there. The advantage of this extension makes our method insensitive to the distance of the PML region to the structure. Following the general idea in designing PML absorbing layers, we introduce the the PML region

$$\Omega_1^{\mathrm{PML}} = \{(x_1, x_3) : 0 < x_1 < L \text{ and } b_1 < x_3 < b_1 + \delta_1\},$$
$$\Omega_2^{\mathrm{PML}} = \{(x_1, x_3) : 0 < x_1 < L \text{ and } b_2 - \delta_2 < x_3 < b_2\},$$

and the PML differential operator

$$\mathcal{L} := \frac{\partial}{\partial x_1}\left(s(x_3)\frac{\partial}{\partial x_1}\right) + \frac{\partial}{\partial x_3}\left(\frac{1}{s(x_3)}\frac{\partial}{\partial x_3}\right) + k^2(x)s(x_3).$$

The PML equations in the PML region are

$$\mathcal{L}(\hat{u} - u_{\mathrm{I}}) = 0 \quad \text{in } \Omega_1^{\mathrm{PML}}, \tag{2.12}$$
$$\mathcal{L}\hat{u} = 0 \quad \text{in } \Omega_2^{\mathrm{PML}}. \tag{2.13}$$

The equation satisfied by the PML solution $\hat{u}$ in the domain Ω is the original Helmholtz equation $\Delta\hat{u} + k^2(x)\hat{u} = 0$. Let $D = \{(x_1, x_3) : 0 < x_1 < L, b_2 - \delta_2 < x_3 < b_1 + \delta_1\}$. Due to the assumption (2.11) we can now formulate the PML model which we are going to solve in this paper

$$\mathcal{L}\hat{u} = -g \quad \text{in} \quad D \tag{2.14}$$

with the quasi-periodic boundary condition $\hat{u}(0, x_3) = e^{-\mathbf{i}\alpha L}\hat{u}(L, x_3)$ for $b_2 - \delta_2 < x_3 < b_1 + \delta_1$ and the Dirichlet condition $\hat{u} = u_{\mathrm{I}}$ on $\Gamma_1^{\mathrm{PML}} = \{(x_1, x_3) : 0 < x_1 < L, x_3 = b_1 + \delta_1\}$, $\hat{u} = 0$ on $\Gamma_2^{\mathrm{PML}} = \{(x_1, x_3) : 0 < x_1 < L, x_3 = b_2 - \delta_2\}$. Here the source function

$$g = \begin{cases} -\mathcal{L}u_{\mathrm{I}} & \text{in } \Omega_1^{\mathrm{PML}}, \\ 0 & \text{elsewhere} . \end{cases}$$

For any $G \subset D$, define

$$X(G) = \{w \in H^1(G) : w_\alpha = we^{-\mathbf{i}\alpha x_1} \text{ is periodic in } x_1 \text{ with period } L\}$$

and introduce the sesquilinear form $a_G : X(G) \times X(G) \to \mathbf{C}$ as

$$a_G(\varphi, \psi) = \int_G \left(s(x_3)\frac{\partial\varphi}{\partial x_1}\frac{\partial\bar{\psi}}{\partial x_1} + \frac{1}{s(x_3)}\frac{\partial\varphi}{\partial x_3}\frac{\partial\bar{\psi}}{\partial x_3} - k^2(x)s(x_3)\varphi\bar{\psi}\right) dx.$$

Denote by $\overset{\circ}{X}(D) = \{w \in X(D), w = 0 \text{ on } \Gamma_1^{\rm PML} \cup \Gamma_2^{\rm PML}\}$. Then the weak formulation of the PML model reads as follows: Find $\hat{u} \in X(D)$ such that $\hat{u} = u_{\rm I}$ on $\Gamma_1^{\rm PML}, \hat{u} = 0$ on $\Gamma_2^{\rm PML}$ and

$$a_D(\hat{u}, \psi) = \int_D g\bar{\psi}dx \qquad \forall\, \psi \in \overset{\circ}{X}(D). \tag{2.15}$$

Our next objective is to prove the existence and uniqueness of the above problem and derive an error estimate between $\hat{u}$ and u, the solution of the original 1D grating problem (2.9). To achieve the goal, we first find an equivalent formulation of (2.15) in the domain Ω. Similar to the argument leading to the Rayleigh expansion (2.4),we deduce from (2.12) that

$$\hat{u} = u_{\rm I} + \sum_{n\in Z} \left(A_1^n e^{\mathbf{i}\beta_1^n \int_{b_1}^{x_3} s(\tau)d\tau} + B_1^n e^{-\mathbf{i}\beta_1^n \int_{b_1}^{x_3} s(\tau)d\tau} \right) e^{\mathbf{i}(\alpha_n+\alpha)x_1} \text{ in } \Omega_1^{\rm PML}. \tag{2.16}$$

If we write $\hat{u}(x_1, b_1) = u_{\rm I}(x_1, b_1) + \sum_{n\in Z} \hat{u}_\alpha^{(n)}(b_1)e^{\mathbf{i}(\alpha_n+\alpha)x_1}$ on Γ_1, then the constants A_1^n, B_1^n can be uniquely determined by the additional boundary condition $\hat{u} = u_{\rm I}$ on $\Gamma_1^{\rm PML}$ through following equations

$$\begin{aligned} &A_1^n + B_1^n = \hat{u}_\alpha^n(b_1) \\ &A_1^n e^{\mathbf{i}\beta_1^n \int_{b_1}^{b_1+\delta_1} s(\tau)d\tau} + B_1^n e^{-\mathbf{i}\beta_1^n \int_{b_1}^{b_1+\delta_1} s(\tau)d\tau} = 0. \end{aligned}$$

Thus we conclude from (2.16) that

$$\hat{u} = u_{\rm I} + \sum_{n\in Z} \frac{\zeta_1^n(x_3)}{\zeta_1^n(b_1)} \hat{u}_\alpha^{(n)}(b_1)e^{\mathbf{i}(\alpha_n+\alpha)x_1} \quad \text{in} \quad \Omega_1^{\rm PML}, \tag{2.17}$$

where $\zeta_1^n(x_3) = e^{-\mathbf{i}\beta_1^n \int_{x_3}^{b_1+\delta_1} s(\tau)d\tau} - e^{\mathbf{i}\beta_1^n \int_{x_3}^{b_1+\delta_1} s(\tau)d\tau}$. Similarly, we deduce from (2.13) that

$$\hat{u} = \sum_{n\in Z} \frac{\zeta_2^n(x_3)}{\zeta_2^n(b_2)} \hat{u}_\alpha^{(n)}(b_2)e^{\mathbf{i}(\alpha_n+\alpha)x_1} \quad \text{in} \quad \Omega_2^{\rm PML}, \tag{2.18}$$

where $\zeta_2^n(x_3) = e^{-\mathbf{i}\beta_2^n \int_{b_2-\delta_2}^{x_3} s(\tau)d\tau} - e^{\mathbf{i}\beta_2^n \int_{b_2-\delta_2}^{x_3} s(\tau)d\tau}$. Similar to (2.6), for any quasi-periodic function f which has the expansion $f = \sum_{n\in Z} f^{(n)}e^{\mathbf{i}(\alpha_n+\alpha)x_1}$, we define the following Dirichlet to Neumann operator $T_j^{\rm PML}$:

$$\left(T_j^{\rm PML} f\right)(x_1) = \sum_{n\in Z} \mathbf{i}\beta_j^n \coth(-\mathbf{i}\beta_j^n\sigma_j) f^{(n)} e^{\mathbf{i}(\alpha_n+\alpha)x_1}, \tag{2.19}$$

where $\coth(\tau) = \dfrac{e^\tau + e^{-\tau}}{e^\tau - e^{-\tau}}$, and

$$\sigma_1 = \int_{b_1}^{b_1+\delta_1} s(\tau)d\tau, \quad \sigma_2 = \int_{b_2-\delta_2}^{b_2} s(\tau)d\tau. \tag{2.20}$$

Then we know easily from (2.17), (2.18) that

$$\frac{\partial(\hat{u} - u_{\rm I})}{\partial\nu} - T_1^{\rm PML}(\hat{u} - u_{\rm I}) = 0 \quad \text{on} \quad \Gamma_1, \quad \frac{\partial\hat{u}}{\partial\nu} - T_2^{\rm PML}\hat{u} = 0 \quad \text{on} \quad \Gamma_2. \tag{2.21}$$

This motivates us to introduce the sesquilinear form $b^{\text{PML}}: X(\Omega) \times X(\Omega) \to \mathbf{C}$

$$b^{\text{PML}}(\varphi, \psi) = \int_\Omega (\nabla\varphi\nabla\bar{\psi} - k^2(x)\varphi\bar{\psi})dx - \sum_{j=1}^{2} \int_{\Gamma_j} (T_j^{\text{PML}}\varphi)\bar{\psi}dx_1, \tag{2.22}$$

and introduce the following variational problem: Find $\vartheta \in X(\Omega)$ such that

$$b^{\text{PML}}(\vartheta, \psi) = -\int_{\Gamma_1} \mathbf{i}\beta(1 + \coth(-\mathbf{i}\beta\sigma_1))u_{\text{I}}\bar{\psi}dx_1, \ \ \forall\, \psi \in X(\Omega), \tag{2.23}$$

where we have used the fact that $\dfrac{\partial u_{\text{I}}}{\partial\nu} - T_1^{\text{PML}}u_{\text{I}} = -\mathbf{i}\beta(1 + \coth(-\mathbf{i}\beta\sigma_1))u_{\text{I}}$ on Γ_1. The following lemma establishes the relation of this variational problem to the PML model problem (2.15).

LEMMA 2.1. *Any solution $\hat{u}$ of the problem* (2.15) *restrict to Ω is a solution of* (2.23). *Conversely, any solution ϑ of the problem* (2.23) *can be uniquely extended to the whole domain D to be a solution of* (2.15).

Proof. This proof is standard based on the constructions given in (2.17) and (2.18). We omit the details. □

Let $\Delta_j^n = |k_j^2 - (\alpha_n + \alpha)^2|^{1/2}$ and $U_j = \{n : k_j^2 > (\alpha_n + \alpha)^2\}$, $j = 1, 2$. Then we have $\beta_j^n = \Delta_j^n$ for $n \in U_j$ and $\beta_j^n = \mathbf{i}\Delta_j^n$ for $n \notin U_j$. Let

$$\Delta_j^- = \min\{\Delta_j^n : n \in U_j\}, \quad \Delta_j^+ = \min\{\Delta_j^n : n \notin U_j\}. \tag{2.24}$$

The following lemma plays the key role in the subsequent analysis.

LEMMA 2.2. *For any $\varphi, \psi \in X(\Omega)$, we have*

$$\left|\int_{\Gamma_j} (T_j\varphi - T_j^{\text{PML}}\varphi)\bar{\psi}dx_1\right| \le M_j \|\varphi\|_{L^2(\Gamma_j)} \|\psi\|_{L^2(\Gamma_j)},$$

where $M_j = \max\left(\dfrac{2\Delta_j^-}{e^{2\sigma_j^I\Delta_j^-} - 1}, \dfrac{2\Delta_j^+}{e^{2\sigma_j^R\Delta_j^+} - 1}\right)$, σ_j^R, σ_j^I *are the real and imaginary part of σ_j defined in* (2.20), *that is, $\sigma_j = \sigma_j^R + \mathbf{i}\sigma_j^I$.*

Proof. For any $\varphi, \psi \in X(\Omega)$, their traces on Γ_j have the following expansions

$$\varphi(x_1, b_j) = \sum_{n\in Z} \varphi_\alpha^{(n)}(b_j)e^{\mathbf{i}(\alpha_n+\alpha)x_1} \ \ , \ \ \psi(x_1, b_j) = \sum_{n\in Z} \psi_\alpha^{(n)}(b_j)e^{\mathbf{i}(\alpha_n+\alpha)x_1}.$$

The $\varphi_\alpha^{(n)}$ and $\psi_\alpha^{(n)}$ are the Fourier coefficients of periodic functions $\varphi_\alpha(x_1, b_j) = \varphi(x_1, b_j)e^{-\mathbf{i}\alpha x_1}$ and $\psi_\alpha(x_1, b_j) = \psi(x_1, b_j)e^{-\mathbf{i}\alpha x_1}$. The property of Fourier series yields

$$\|\varphi\|^2_{L^2(\Gamma_j)} = \|\varphi_\alpha\|^2_{L^2(\Gamma_j)} = L\sum_{n\in Z} |\varphi_\alpha^{(n)}(b_j)|^2,$$
$$\|\psi\|^2_{L^2(\Gamma_j)} = \|\psi_\alpha\|^2_{L^2(\Gamma_j)} = L\sum_{n\in Z} |\psi_\alpha^{(n)}(b_j)|^2$$

By the orthogonality of Fourier series, we also have

$$\int_{\Gamma_j} (T_j\varphi - T_j^{\text{PML}}\varphi)\bar{\psi}dx = L\sum_{n\in Z} \mathbf{i}\beta_j^n(1 - \coth(-\mathbf{i}\beta_j^n\sigma_j))\varphi_\alpha^{(n)}(b_j)\bar{\psi}_\alpha^{(n)}(b_j). \tag{2.25}$$

For $n \in U_j$, we have $\beta_j^n = \Delta_j^n > 0$, thus

$$|\mathbf{i}\beta_j^n(1-\coth(-\mathbf{i}\beta_j^n\sigma_j))| = \left|\frac{2\beta_j^n}{1-e^{-2\mathbf{i}\beta_j^n\sigma_j}}\right| = \frac{2\Delta_j^n}{|e^{2\mathbf{i}\Delta_j^n\sigma_j^R} - e^{2\Delta_j^n\sigma_j^I}|}$$
$$\leq \frac{2\Delta_j^n}{e^{2\Delta_j^n\sigma_j^I}-1} \leq \frac{2\Delta_j^-}{e^{2\Delta_j^-\sigma_j^I}-1} \leq M_j,$$

where we have used the fact that $\Delta_j^n \geq \Delta_j^-$ for $n \in U_j$ and the function $\xi(\tau) = 2\tau/(e^{2\tau}-1)$ is decreasing for $\tau > 0$. Similar argument shows that for $n \notin U_j$,

$$\left|\mathbf{i}\beta_j^n(1-\coth(-\mathbf{i}\beta_j^n\sigma_j))\right| \leq \frac{2\Delta_j^+}{e^{2\Delta_j^+\sigma_j^R}-1} \leq M_j.$$

This completes proof upon using Cauchy inequality in (2.25). □

Now let us take a closer look at the structure of constant M_j which controls the modeling error of the PML equation towards the original 1D grating problem (see Theorem 2.4 and Theorem 2.5 below). Once the incoming plane wave $u_{\mathrm{I}} = e^{\mathbf{i}\alpha x_1 - \mathbf{i}\beta x_3}$ is fixed, the numbers Δ_j^-, Δ_j^+ are fixed according to (2.24). Thus the constant M_j approaches to zero exponentially as the PML parameters σ_j^R, σ_j^I tend to infinity. From the definition (2.20) we know that σ_j^R, σ_j^I can be calculated by the medium property $s(x_3)$, which is usually taken as power function

$$s(x_3) = \begin{cases} 1+\sigma_1^m\left(\dfrac{x_3-b_1}{\delta_1}\right)^m & \text{if } x_3 \geq b_1 \\ 1+\sigma_2^m\left(\dfrac{b_2-x_3}{\delta_2}\right)^m & \text{if } x_3 \leq b_2 \end{cases}, \quad m \geq 1.$$

Thus we have

$$\sigma_j^R = \left(1+\frac{\operatorname{Re}\sigma_j^m}{m+1}\right)\delta_j, \quad \sigma_j^I = \frac{\operatorname{Im}\sigma_j^m}{m+1}\,\delta_j. \tag{2.26}$$

It is obvious that either enlarge the thichness δ_j of the PML layers or enlarge the medium parameters $\operatorname{Re}\sigma_j^m$ and $\operatorname{Im}\sigma_j^m$ will reduce the PML approximation error.

LEMMA 2.3. *For any $\psi \in X(\Omega)$, we have*

$$\|\,\psi\,\|_{L^2(\Gamma_j)} \leq \|\,\psi\,\|_{H^{1/2}(\Gamma_j)} \leq \hat{C}\|\,\psi\,\|_{H^1(\Omega)}$$

with $\hat{C} = \sqrt{1+(b_2-b_1)^{-1}}$. Here if $\psi(x_1,b_j) = \sum_{n\in Z}\psi_\alpha^{(n)}(b_j)e^{\mathbf{i}(\alpha_n+\alpha)x_1}$ on Γ_j,

$$\|\,\psi\,\|_{H^{1/2}(\Gamma_j)} = \left(L\sum_{n\in Z}(1+|\alpha_n+\alpha|^2)^{1/2}|\psi_\alpha^{(n)}(b_j)|^2\right)^{1/2}.$$

Proof. Since $\psi \in X(\Omega)$, we have the expansion

$$\psi(x_1,x_3) = \sum_{n\in Z}\psi_\alpha^{(n)}(x_3)e^{\mathbf{i}(\alpha_n+\alpha)x_1} \quad \text{in} \quad \Omega.$$

Thus

$$\|\psi\|_{H^1(\Omega)}^2 = L\sum_{n\in Z}\int_{b_2}^{b_1}\left((1+|\alpha_n+\alpha|^2)|\psi_\alpha^{(n)}(x_3)|^2 + \left|\frac{d}{dx_3}\psi_\alpha^{(n)}(x_3)\right|^2\right)dx_3.$$

Now the proof follows from the identity

$$|\psi_\alpha^{(n)}(b_j)|^2 = |\psi_\alpha^{(n)}(x_3)|^2 + \int_{b_j}^{x_3} \frac{d}{dx_3}|\psi_\alpha^{(n)}(\tau)|^2 d\tau, \quad b_2 \le x_3 \le b_1$$

and the Cauchy inequality. This completes the proof. □

THEOREM 2.4. *Let $\gamma > 0$ be the constant in the inf-sup condition* (2.10) *and $(M_1 + M_2)\hat{C}^2 < \gamma$. Then the PML variational problem exists a unique solution $\hat{u}$. Moreover, we have the following error estimate*

$$\begin{aligned} |||u - \hat{u}|||_\Omega &:= \sup_{0 \ne \psi \in H^1(\Omega)} \frac{|b(u - \hat{u}, \psi)|}{\|\psi\|_{H^1(\Omega)}} \\ &\le \hat{C}M_1\|\hat{u} - u_{\mathrm{I}}\|_{L^2(\Gamma_1)} + \hat{C}M_2\|\hat{u}\|_{L^2(\Gamma_2)}. \end{aligned} \tag{2.27}$$

Proof. By Lemma 2.1 we only need to show the variational problem (2.23) has a unique solution. We resort to the general existence and uniqueness result for sesquilinear forms in [2, Chap. 5]. The key point is to show the inf-sup condition for the sesquilinear form $b^{\mathrm{PML}} : X(\Omega) \times X(\Omega) \to \mathbf{C}$ defined in (2.22). Thanks to Lemma 2.2 and Lemma 2.3 and the assumption $(M_1 + M_2)\hat{C}^2 < \gamma$, this is now obvious:

$$\begin{aligned} |b^{\mathrm{PML}}(\varphi, \psi)| &\ge |b(\varphi, \psi)| - \sum_{j=1}^2 \left| \int_{\Gamma_j} (T_j\varphi - T_j^{\mathrm{PML}}\varphi)\bar{\psi} dx_1 \right| \\ &\ge |b(\varphi, \psi)| - (M_1 + M_2)\hat{C}^2\|\varphi\|_{H^1(\Omega)}\|\psi\|_{H^1(\Omega)}, \quad \forall \varphi, \psi \in X(\Omega). \end{aligned}$$

It remains to prove the estimate (2.27). By (2.8), (2.9), (2.22), (2.23) and Lemma 2.1 we conclude that

$$\begin{aligned} b(u - \hat{u}, \psi) &= -\int_{\Gamma_1} 2\mathbf{i}\beta u_{\mathrm{I}}\bar{\psi} dx_1 + \int_{\Gamma_1} \mathbf{i}\beta(1 + \coth(-\mathbf{i}\beta\sigma_1))u_{\mathrm{I}}\bar{\psi} dx_1 \\ &\quad + b^{\mathrm{PML}}(\hat{u}, \psi) - b(\hat{u}, \psi) \\ &= \int_{\Gamma_1} (T_1 - T_1^{\mathrm{PML}})(\hat{u} - u_{\mathrm{I}})\bar{\psi} dx_1 \\ &\quad + \int_{\Gamma_2} (T_2 - T_2^{\mathrm{PML}})\hat{u}\bar{\psi} dx_1, \quad \forall \psi \in X(\Omega). \end{aligned} \tag{2.28}$$

This complete the proof of the theorem upon using Lemma 2.2 and Lemma 2.3. □

To conclude we remark that the error estimate (2.27) is a posteriori in nature as it depends on the PML solution $\hat{u}$. This makes a posterior error control possible (see §3 for details).

2.2. TM polarization. In this subsection we state the parallel results for the grating problem (1.4). First we introduce the sesquilinear form $b_{\mathrm{TM}} : X(\Omega) \times X(\Omega) \to \mathbf{C}$ as follows:

$$b_{\mathrm{TM}}(\varphi, \psi) = \int_\Omega \left(\frac{1}{k^2(x)} \nabla\varphi\nabla\bar{\psi} - \varphi\bar{\psi} \right) dx - \sum_{j=1}^2 \int_{\Gamma_j} \frac{1}{k_j^2}(T_j\varphi)\bar{\psi} dx_1. \tag{2.29}$$

The variational form for the 1D grating problem in the TM polarization then reads as follows: Given incoming plane wave $u_{\mathrm{I}} = e^{\mathbf{i}\alpha x_1 - \mathbf{i}\beta x_3}$, seek $u^{\mathrm{TM}} \in X(\Omega)$ such that

$$b_{\mathrm{TM}}(u^{\mathrm{TM}}, \psi) = -\int_{\Gamma_1} \frac{2\mathbf{i}\beta}{k_1^2} u_{\mathrm{I}}\bar{\psi} dx_1 \ , \ \forall \psi \in X(\Omega). \tag{2.30}$$

We again assume the above variational problem exists a unique solution and thus there exists a constant $\gamma_{\rm TM} > 0$ such that

$$\sup_{0\neq\psi\in H^1(\Omega)} \frac{|b_{\rm TM}(\varphi,\psi)|}{\|\,\psi\,\|_{H^1(\Omega)}} \geq \gamma_{\rm TM}\|\,\varphi\,\|_{H^1(\Omega)} \ , \quad \forall\,\varphi\in X(\Omega). \tag{2.31}$$

The sesquilinear form $a_{\rm TM} : X(D)\times X(D)\to \mathbf{C}$ associated with the PML problem is

$$a_{\rm TM}(\varphi,\psi) = \int_\Omega \left(\frac{1}{k^2(x)} s(x_3) \frac{\partial\varphi}{\partial x_1}\frac{\partial\bar\psi}{\partial x_1} + \frac{1}{k^2(x)}\frac{1}{s(x_3)}\frac{\partial\varphi}{\partial x_3}\frac{\partial\bar\psi}{\partial x_3} - s(x_3)\varphi\bar\psi \right) dx$$

and the weak formulation of the PML problem reads as the following: Find $\hat u^{\rm TM}\in X(D)$ such that $\hat u^{\rm TM} = u_{\rm I}$ on $\Gamma_1^{\rm PML}, \hat u^{\rm TM} = 0$ on $\Gamma_2^{\rm PML}$, and

$$a_{\rm TM}(\hat u^{\rm TM},\psi) = \int_D g_{\rm TM}\bar\psi dx \quad \forall\,\psi\in \overset{\circ}{X}(D), \tag{2.32}$$

where $g_{\rm TM} = g/k_1^2$. The following theorem is an analogue of Theorem 2.4.

THEOREM 2.5. *Assume that $\sum_{j=1}^2 M_j\hat C^2/k_j^2 < \gamma_{\rm TM}$. Then the PML variational problem* (2.32) *exists a unique solution $\hat u^{\rm TM}$. Moreover, we have the following error estimate*

$$\begin{aligned} |||u^{\rm TM} - \hat u^{\rm TM}|||_\Omega^{\rm TM} &= \sup_{0\neq\psi\in H^1(\Omega)} \frac{|b_{\rm TM}(u^{\rm TM}-\hat u^{\rm TM},\psi)|}{\|\,\psi\,\|_{H^1(\Omega)}} \\ &\leq (M_1\hat C/k_1^2)\|\,\hat u^{\rm TM} - u_{\rm I}\,\|_{L^2(\Gamma_1)} + (M_2\hat C/k_2^2)\|\,\hat u^{\rm TM}\,\|_{L^2(\Gamma_2)}. \end{aligned}$$

3. The Discrete problem. In this section we introduce the finite element approximations of the PML problems (2.15) and (2.32). Let $\mathcal{M}_h$ be a regular triangulation of the domain D. Remember that any triangle $T\in\mathcal{M}_h$ is considered as closed. We assume any element T must be completely included in $\overline{\Omega_1^{\rm PML}}$, $\overline{\Omega_2^{\rm PML}}$ or $\overline{\Omega}$. To define finite element space whose functions are quasi-periodic in x_1 direction, we also require that if $(0,z)$ is a node on the left boundary, then (L,z) is also a node on the right boundary, and vice versa. Let $V_h(D)\subset X(D)$ be the conforming linear finite element space and $\overset{\circ}{V}_h(D) = V_h(D)\bigcap \overset{\circ}{X}(D)$. Denote by $I_h : C(\bar D)\to V_h(D)$ the standard finite element interpolation operator.

The finite element approximation to the PML problem (2.15) reads as following: Find $\hat u_h\in V_h(D)$ such that $\hat u_h = I_h u_{\rm I}$ on $\Gamma_1^{\rm PML}, \hat u_h = 0$ on $\Gamma_2^{\rm PML}$ and

$$a_D(\hat u_h,\psi_h) = \int_D g\bar\psi_h dx \qquad \forall\,\psi_h\in \overset{\circ}{V}_h(D). \tag{3.1}$$

Following the general theory in [2, Chap. 5], the existence of unique solution of the discrete problem (3.1) and the finite element convergence analysis depend on the following discrete inf-sup condition

$$\sup_{0\neq\psi_h\in \overset{\circ}{V}_h(D)} \frac{|a_D(\varphi_h,\psi_h)|}{\|\,\psi_h\,\|_{H^1(D)}} \geq \gamma_D\ \|\,\varphi_h\,\|_{H^1(D)} \quad \forall\,\varphi_h\in \overset{\circ}{V}_h(D), \tag{3.2}$$

where the constant $\gamma_D > 0$ is independent of the finite element mesh size. Since the continuous problem (2.15) has a unique solution by Theorem 2.4, the sesquailinear form $a_D : X(D) \times X(D) \to \mathbf{C}$ satisfies the continuous inf-sup condition. Then a general argument of Schatz [20] implies (3.2) is valid for sufficiently small mesh size $h < h^*$. Based on (3.2), appropriate a priori error estimate can also be derived which depends on the regularity of the PML solution $\hat{u}$. In this paper, we are interested in a posterior error estimates and the associated adaptive algorithm. Thus in the following we simply assume the discrete problem (3.1) has a unique solution $\hat{u}_h \in V_h(D)$.

Let

$$A(x) = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} = \begin{pmatrix} s(x_3) & 0 \\ 0 & 1/s(x_3) \end{pmatrix}, \quad B(x) = k^2(x)s(x_3).$$

Then the definitions of $\mathcal{L}$ and a_D can be rewritten as

$$\mathcal{L} = \text{div }(A(x)\nabla) + B(x),$$
$$a_D(\varphi, \psi) = \int_D \left(A(x)\nabla\varphi\nabla\bar{\psi} - B(x)\varphi\bar{\psi}\right) dx.$$

For any $T \in \mathcal{M}_h$, we denote by h_T its diameter. Let $\mathcal{B}_h$ denote the set of all sides that do not lie on Γ_j^{PML}, $j = 1, 2$. For any $e \in \mathcal{B}_h$, h_e stands for its length. For any $T \in \mathcal{M}_h$, we introduce the residual

$$R_T := \mathcal{L}\hat{u}_h|_T + g|_T = \begin{cases} \mathcal{L}(\hat{u}_h|_T - u_{\text{I}}|_T) & \text{if } T \subset \overline{\Omega_1^{\text{PML}}}, \\ \mathcal{L}\hat{u}_h|_T & \text{otherwise .} \end{cases} \tag{3.3}$$

For any interior side $e \in \mathcal{B}_h$ which is the common side of T_1 and $T_2 \in \mathcal{M}_h$, we define the jump residual across e

$$J_e = (A\nabla\hat{u}_h|_{T_1} - A\nabla\hat{u}_h|_{T_2}) \cdot \nu_e, \tag{3.4}$$

using the convention that the unit normal vector ν_e to e points from T_2 to T_1. Denote by $\Gamma_{\text{left}} = \{(x_1, x_3) : x_1 = 0, b_2 - \delta_2 < x_3 < b_1 + \delta_1\}$ and $\Gamma_{\text{right}} = \{(x_1, x_3) : x_1 = L, b_2 - \delta_2 < x_3 < b_1 + \delta_1\}$. If $e = \Gamma_{\text{left}} \cap \partial T$ for some element $T \in \mathcal{M}_h$ and e' the corresponding side on Γ_{right} which is also a side of some element T', then we define the jump residual

$$\begin{aligned} J_e &= A_{11}\left[\frac{\partial}{\partial x_1}(\hat{u}_h|_T) - e^{-\mathrm{i}\alpha L} \cdot \frac{\partial}{\partial x_1}(\hat{u}_h|_{T'})\right], \\ J_{e'} &= A_{11}\left[e^{\mathrm{i}\alpha L} \cdot \frac{\partial}{\partial x_1}(\hat{u}_h|_T) - \frac{\partial}{\partial x_1}(\hat{u}_h|_{T'})\right]. \end{aligned} \tag{3.5}$$

For any $T \in \mathcal{M}_h$, denote by η_T the local error estimator which is defined as follows

$$\eta_T = \max_{x \in \tilde{T}} \rho(x_3) \cdot \left[h_T \|R_T\|_{L^2(T)} + \left(\frac{1}{2}\sum_{e \subset T} h_e \| J_e \|^2_{L^2(e)}\right)^{1/2}\right], \tag{3.6}$$

where $\tilde{T}$ is the union of all elements having non-empety intersection with T, and

$$\rho(x_3) = \begin{cases} |s(x_3)|e^{-R_j(x_3)} & \text{if } x \in \overline{\Omega_j^{\text{PML}}}, \\ 1 & \text{if } x \in \Omega. \end{cases}$$

with $R_j(x_3)$ $(j = 1, 2)$ being defined in (4.5)–(4.6) below.

The following theorem is the main result in this paper.

THEOREM 3.1. *There exists a constant $C > 0$ depending only on the minimum angle of the mesh $\mathcal{M}_h$, such that the following a posterior error estimate is valid*

$$
\begin{aligned}
|||u - \hat{u}_h|||_\Omega \le \hat{C} M_1 \|\hat{u}_h - u_{\rm I}\|_{L^2(\Gamma_1)} + \hat{C} M_2 \|\hat{u}_h\|_{L^2(\Gamma_2)} \\
+ \hat{C} M_3 \|\, I_h u_{\rm I} - u_{\rm I}\,\|_{L^2(\Gamma_1^{\rm PML})} + C(1 + C_1 + C_2) \left(\sum_{T \in \mathcal{M}_h} \eta_T^2 \right)^{1/2},
\end{aligned}
$$

where the constants $M_j (j = 1, 2)$, $\hat{C}$, C_j and M_3 are defined in Lemma 2.2, Lemma 2.3, Lemma 4.3, and Lemma 4.4, respectively.

The proof of this theorem will be given in §4. We notice that when the PML parameters σ_j^R and σ_j^I tend to infinity, the constants M_j decay exponentially and the constants C_j remain bounded. The important exponentially decay factors $e^{-R_j(x_3)}$ in the PML region $\Omega_j^{\rm PML}$ allow us to take thicker PML layers without introducing unnecessary fine meshes away from the computational domain. Recall that thicker PML layers allow smaller PML medium property, which enhances numerical stability.

To conclude this section, we state the parallel results for the TM polarization. The finite element approximation to the TM polarization problem (2.32) reads as following: Find $\hat{u}_h^{\rm TM} \in V_h(D)$ such that $\hat{u}_h^{\rm TM} = I_h u_{\rm I}$ on $\Gamma_1^{\rm PML}$, $\hat{u}_h^{\rm TM} = 0$ on $\Gamma_2^{\rm PML}$, and

$$
a_{\rm TM}(\hat{u}_h^{\rm TM}, \psi_h) = \int_D g_{\rm TM} \bar{\psi}_h dx, \quad \forall\, \psi_h \in \mathring{V}_h(D). \tag{3.7}
$$

Let $A_{\rm TM}(x) = A(x)/k^2(x)$, $B_{\rm TM}(x) = B(x)/k^2(x)$ and $\mathcal{L}_{\rm TM} = {\rm div}\,(A_{\rm TM}(x)\nabla) + B_{\rm TM}(x)$. Then we have the following theorem parallel to Theorem 3.1 whose proof is omitted.

THEOREM 3.2. *There exists a constant $C > 0$ depending only on the minimum angle of the mesh $\mathcal{M}_h$, such that the following a posterior error estimate is valid*

$$
\begin{aligned}
|||u^{\rm TM} - \hat{u}_h^{\rm TM}|||_\Omega^{\rm TM} \le (\hat{C} M_1/k_1^2) \|\hat{u}_h^{\rm TM} - u_{\rm I}\|_{L^2(\Gamma_1)} + (\hat{C} M_2/k_2^2) \|\hat{u}_h^{\rm TM}\|_{L^2(\Gamma_2)} \\
+ (\hat{C} M_3/k_1^2) \|\, I_h u_{\rm I} - u_{\rm I}\,\|_{L^2(\Gamma_1^{\rm PML})} + C(1 + C_1 + C_2) \left(\sum_{T \in \mathcal{M}_h} \eta_T^2 \right)^{1/2},
\end{aligned}
$$

where the constants $M_j (j = 1, 2)$, $\hat{C}$, C_j and M_3 are defined in Lemma 2.2, Lemma 2.3, Lemma 4.3, and Lemma 4.4, respectively. η_T is defined as in (3.6) *with $A, \mathcal{L}, g$ and $\hat{u}_h$ being replaced by $A_{\rm TM}, \mathcal{L}_{\rm TM}, g_{\rm TM}$ and $\hat{u}_h^{\rm TM}$, respectively.*

4. A posteriori error analysis. In this section we prove the a posterior error estimates in Theorem 3.1.

4.1. Error representation formula. For any $\psi \in X(\Omega)$, we extend it to be function in $X(D)$ denoted by $\tilde{\psi}$ as follows:

$$
\tilde{\psi}(x_1, x_3) = \sum_{n \in Z} \frac{\bar{\zeta}_j^n(x_3)}{\bar{\zeta}_j^n(b_j)} \psi_\alpha^{(n)}(b_j) e^{{\bf i}(\alpha_n + \alpha)x_1} \quad \text{in } \Omega_j^{\rm PML},\ j = 1, 2, \tag{4.1}
$$

where $\zeta_j^n(x_3)$ are defined in (2.17) and (2.18), and $\psi_\alpha^{(n)}(b_j)$ are the Fourier coefficients of the function $\psi_\alpha = \psi e^{-{\bf i}\alpha x_1}$ on Γ_j, that is,

$$
\psi(x_1, b_j) = \sum_{n \in Z} \psi_\alpha^{(n)}(b_j) e^{{\bf i}(\alpha_n + \alpha)x_1}. \tag{4.2}
$$

It is easy to see that $\tilde{\psi} = \psi$ on Γ_j and $\mathcal{L}\bar{\tilde{\psi}} = 0$ in $\Omega_j^{\rm PML}$.

LEMMA 4.1. *Let ν_j be the unit outer normal to $\Omega_j^{\rm PML}$. Then for any $\varphi, \psi \in X(\Omega)$, we have*

$$\int_{\Gamma_j} T_j^{\rm PML}\varphi\bar{\psi}dx_1 = -\int_{\Gamma_j}\varphi\frac{\partial\bar{\tilde{\psi}}}{\partial\nu_j}dx_1. \tag{4.3}$$

Proof. Denote by

$$\varphi(x_1, b_j) = \sum_{n\in Z}\varphi_\alpha^{(n)}(b_j)e^{\mathbf{i}(\alpha_n+\alpha)x_1}.$$

Then by the definition of $T_j^{\rm PML}$ in (2.19) and the property of Fourier series, we have

$$\int_{\Gamma_j} T_j^{\rm PML}\varphi\bar{\psi}dx_j = L\sum_{n\in Z}\mathbf{i}\beta_j^n\coth(-\mathbf{i}\beta_j^n\sigma_j)\varphi_\alpha^{(n)}(b_j)\bar{\psi}_\alpha^{(n)}(b_j).$$

On the other hand, by direct calculation from (4.1), we have

$$\begin{aligned}
-\int_{\Gamma_j}\varphi\frac{\partial\bar{\tilde{\psi}}}{\partial\nu_j}dx_1 &= (-1)^{j-1}\int_{\Gamma_j}\varphi\frac{\partial\bar{\tilde{\psi}}}{\partial x_3}dx_1\\
&= (-1)^{j-1}L\sum_{n\in Z}\frac{d}{dx_3}\left(\frac{\zeta_j^n(x_3)}{\zeta_j^n(b_j)}\right)\bigg|_{x_3=b_j}\varphi_\alpha^{(n)}(b_j)\bar{\psi}_\alpha^{(n)}(b_j)\\
&= L\sum_{n\in Z}\mathbf{i}\beta_j^n\coth(-\mathbf{i}\beta_j^n\sigma_j)\varphi_\alpha^{(n)}(b_j)\bar{\psi}_\alpha^{(n)}(b_j).
\end{aligned}$$

This completes the proof. □

Whenever no confusion of the notation incurred, we shall write in the following $\tilde{\psi}$ as ψ in $\Omega_j^{\rm PML}$.

LEMMA 4.2 (Error representational formula). *For any $\psi \in X(\Omega)$, which is extended to be a function in $X(D)$ according to* (4.1), *and $\psi_h \in \overset{\circ}{V}_h(D)$, we have*

$$\begin{aligned}
b(u-\hat{u}_h,\psi) &= \int_D g(\overline{\psi-\psi_h})dx - a_D(\hat{u}_h,\psi-\psi_h)\\
&\quad+\int_{\Gamma_1}(T_1-T_1^{\rm PML})(\hat{u}_h-u_{\rm I})\bar{\psi}dx_1+\int_{\Gamma_2}(T_2-T_2^{\rm PML})\hat{u}_h\bar{\psi}dx_1\\
&\quad+\int_{\Gamma_1^{\rm PML}}\frac{1}{s(x_3)}\frac{\partial\bar{\psi}}{\partial x_3}(I_hu_{\rm I}-u_{\rm I})dx_1.
\end{aligned}\tag{4.4}$$

Proof. First by (2.28), (2.22) and (2.8) we have

$$\begin{aligned}
b(u-\hat{u}_h,\psi) &= b(u-\hat{u},\psi)+b(\hat{u}-\hat{u}_h,\psi)\\
&= \int_{\Gamma_1}(T_1-T_1^{\rm PML})(\hat{u}-u_{\rm I})\bar{\psi}dx_1+\int_{\Gamma_2}(T_2-T_2^{\rm PML})\hat{u}\bar{\psi}dx_1\\
&\quad+b^{\rm PML}(\hat{u}-\hat{u}_h,\psi)-\sum_{j=1}^2\int_{\Gamma_j}(T_j-T_j^{\rm PML})(\hat{u}-\hat{u}_h)\bar{\psi}dx_1\\
&= \int_{\Gamma_1}(T_1-T_1^{\rm PML})(\hat{u}_h-u_{\rm I})\bar{\psi}dx_1+\int_{\Gamma_2}(T_2-T_2^{\rm PML})\hat{u}_h\bar{\psi}dx_1\\
&\quad+b^{\rm PML}(\hat{u}-\hat{u}_h,\psi).
\end{aligned}$$

Next, by (2.22) and Lemma 4.1, we obtain

$$b^{\rm PML}(\hat u-\hat u_h,\psi)=a_\Omega(\hat u-\hat u_h,\psi)-\sum_{j=1}^2\int_{\Gamma_j}T_j^{\rm PML}(\hat u-\hat u_h)\bar\psi dx_1$$
$$=a_\Omega(\hat u-\hat u_h,\psi)+\sum_{j=1}^2\int_{\Gamma_j}(\hat u-\hat u_h)\frac{\partial\bar\psi}{\partial\nu_j}dx_1.$$

Recall that ν_j is the unit outer normal to $\partial\Omega_j^{\rm PML}$. Since $\mathcal{L}\bar\psi=0$ in $\Omega_j^{\rm PML}$, we deduce by Green formula that

$$a_{\Omega_j^{\rm PML}}(\hat u-\hat u_h,\psi)=\int_{\Gamma_j}(\hat u-\hat u_h)\frac{\partial\bar\psi}{\partial\nu_j}dx_1+\int_{\Gamma_j^{\rm PML}}\frac{1}{s(x_3)}\frac{\partial\bar\psi}{\partial\nu_j}(\hat u-\hat u_h)dx_1.$$

Thus, by using (2.15) and (3.1), we conclude that

$$b^{\rm PML}(\hat u-\hat u_h,\psi)=a_D(\hat u-\hat u_h,\psi)-\int_{\Gamma_j^{\rm PML}}\frac{1}{s(x_3)}\frac{\partial\bar\psi}{\partial\nu_j}(\hat u-\hat u_h)dx_1$$
$$=\int_D g(\overline{\psi-\psi_h})dx-a_D(\hat u_h,\psi-\psi_h)-\int_{\Gamma_1^{\rm PML}}\frac{1}{s(x_3)}\frac{\partial\bar\psi}{\partial x_3}(\hat u-\hat u_h)dx_1,$$

where we have used the fact that $\hat u=\hat u_h=0$ on $\Gamma_2^{\rm PML}$. This completes the proof. ☐

We remark that evaluating the various terms in the error representation formula in suitable Sobolev norms would yield the desired a posterior error estimate in Theorem 3.1. To achieve the goal, we need to prove stability estimates for the extension (4.1) of the function ψ in $\Omega_j^{\rm PML}$.

4.2. Estimates for the extension. We begin with introducing the notation

$$R_1(x_3)=\min\left(\Delta_1^-\int_{b_1}^{x_3}s_2(\tau)d\tau,\Delta_1^+\int_{b_1}^{x_3}s_1(\tau)d\tau\right),\quad x_3\ge b_1,\tag{4.5}$$
$$R_2(x_3)=\min\left(\Delta_2^-\int_{x_3}^{b_2}s_2(\tau)d\tau,\Delta_2^+\int_{x_3}^{b_2}s_1(\tau)d\tau\right),\quad x_3\le b_2.\tag{4.6}$$

The objective of this section is to prove the following two lemmas.

LEMMA 4.3. *For any $\psi\in X(\Omega)$, let ψ be extended to the whole domain D according to* (4.1). *Then we have the following estimates, for $j=1,2$,*

$$\|\, s^{-1}e^{R_j}\nabla\psi\,\|_{L^2(\Omega_j^{\rm PML})}\le C_j\|\,\psi\,\|_{H^1(\Omega)},$$

where

$$C_j=\hat C\max\left(\frac{2k_j\delta_j^{1/2}}{1-e^{-2\Delta_j^-\sigma_j^I}},\ \frac{2(1+2\delta_j(\Delta_j^++k_j))^{1/2}}{1-e^{-2\Delta_j^+\sigma_j^R}}\right)$$

Proof. We denote by

$$r_1(x_3)=\int_{x_3}^{b_1+\delta_1}s(\tau)d\tau,\quad r_2(x_3)=\int_{b_2-\delta_2}^{x_3}s(\tau)d\tau.$$

Then we have $\zeta_j^n(x_3) = e^{-\mathbf{i}\beta_j^n r_j(x_3)} - e^{\mathbf{i}\beta_j^n r_j(x_3)}$ and consequently

$$\frac{d\bar{\zeta}_j^n}{dx_3} = \mathbf{i}\bar{\beta}_j^n(-1)^j \bar{s}(x_3)\left[e^{\mathbf{i}\bar{\beta}_j^n \bar{r}_j(x_3)} + e^{-\mathbf{i}\bar{\beta}_j^n \bar{r}_j(x_3)}\right].$$

By direct calculation, we deduce from (4.1) that

$$\int_0^L |\nabla\psi|^2 dx_1 = L\sum_{n\in Z}|\alpha_n+\alpha|^2|e^{-\mathbf{i}\beta_j^n r_j(x_3)} - e^{\mathbf{i}\beta_j^n r_j(x_3)}|^2|\zeta_j^n(b_j)|^{-2}|\psi_\alpha^{(n)}(b_j)|^2$$
$$+ L\sum_{n\in Z}|\beta_j^n|^2|s(x_3)|^2|e^{-\mathbf{i}\beta_j^n r_j(x_3)} + e^{\mathbf{i}\beta_j^n r_j(x_3)}|^2|\zeta_j^n(b_j)|^{-2}|\psi_\alpha^{(n)}(b_j)|^2. \qquad (4.7)$$

Since $\mathrm{Re}\,\beta_j^n \ge 0$ and $\mathrm{Im}\,\beta_j^n \ge 0$, we have

$$\mathrm{Re}\,(-\mathbf{i}\beta_j^n r_j(x_3)) = \mathrm{Im}\,(\beta_j^n) r_j^R(x_3) + \mathrm{Re}\,(\beta_j^n) r_j^I(x_3) \ge 0.$$

Thus

$$\begin{aligned}&|e^{-\mathbf{i}\beta_j^n r_j(x_3)} \pm e^{\mathbf{i}\beta_j^n r_j(x_3)}|^2\\ =\ &|e^{2\mathbf{i}\mathrm{Im}\,(-\mathbf{i}\beta_j^n r_j(x_3))} \pm e^{-2\mathrm{Re}\,(-\mathbf{i}\beta_j^n r_j(x_3))}|^2 e^{2\mathrm{Re}\,(-\mathbf{i}\beta_j^n r_j(x_3))}\\ \le\ &4e^{2(\mathrm{Im}\,(\beta_j^n) r_j^R(x_3) + \mathrm{Re}\,(\beta_j^n) r_j^I(s_3))}.\end{aligned}$$

Similarly, we have

$$\begin{aligned}|\zeta_j^n(b_j)|^2 &= |e^{-\mathbf{i}\beta_j^n\sigma_j} - e^{\mathbf{i}\beta_j^n\sigma_j}|^2\\ &= |e^{2\mathbf{i}\mathrm{Im}\,(-\mathbf{i}\beta_j^n\sigma_j)} - e^{-2\mathrm{Re}\,(-\mathbf{i}\beta_j^n\sigma_j)}|^2 e^{2\mathrm{Re}\,(-\mathbf{i}\beta_j^n\sigma_j)}\\ &\ge e^{2(\sigma_j^R\mathrm{Im}\,\beta_j^n + \sigma_j^I\mathrm{Re}\,\beta_j^n)}|1 - e^{-2(\sigma_j^R\mathrm{Im}\,\beta_j^n + \sigma_j^I\mathrm{Re}\,\beta_j^n)}|^2.\end{aligned}$$

Therefore, by $r_j(b_j) = \sigma_j$, we have

$$\begin{aligned}&|e^{-\mathbf{i}\beta_j^n r_j(x_3)} \pm e^{\mathbf{i}\beta_j^n r_j(x_3)}|^2|\zeta_j^n(b_j)|^{-2}\\ \le\ &4e^{-2(\mathrm{Im}\,\beta_j^n|\int_{b_j}^{x_3}s_1(\tau)d\tau| + \mathrm{Re}\,\beta_j^n|\int_{b_j}^{x_3}s_2(\tau)d\tau|)}(1 - e^{-2(\sigma_j^R\mathrm{Im}\,\beta_j^n + \sigma_j^I\mathrm{Re}\,\beta_j^n)})^{-2}. \qquad (4.8)\end{aligned}$$

For $n \in U_j$, we have $\mathrm{Re}\,\beta_j^n = \Delta_j^n \ge \Delta_j^-$, $\mathrm{Im}\,\beta_j^n = 0$, and thus

$$|e^{-\mathbf{i}\beta_j^n r_j(x_3)} \pm e^{\mathbf{i}\beta_j^n r_j(x_3)}|^2|\zeta_j^n(b_j)|^{-2} \le 4e^{-2R_j(x)}(1 - e^{-2\Delta_j^-\sigma_j^I})^{-2}.$$

Similarly, for $n \notin U_j$, we have $\mathrm{Re}\,\beta_j^n = 0, \mathrm{Im}\,\beta_j^n = \Delta_j^n \ge \Delta_j^+$, and thus

$$\begin{aligned}&|e^{-\mathbf{i}\beta_j^n r_j(x_3)} \pm e^{\mathbf{i}\beta_j^n r_j(x_3)}|^2|\zeta_j^n(b_j)|^{-2}\\ \le\ &4e^{-2(\Delta_j^n - \Delta_j^+)|\int_{b_j}^{x_3}s_1(\tau)d\tau|}e^{-2R_j(x_3)}(1 - e^{-2\Delta_j^+\sigma_j^R})^{-2}\\ \le\ &4e^{-2R_j(x_3)}e^{-2(\Delta_j^n - \Delta_j^+)|x_3 - b_j|}(1 - e^{-2\Delta_j^+\sigma_j^R})^{-2},\end{aligned}$$

where we have used the fact $s_1(\tau) \ge 1$ (see (2.11)). Denote by $I_1 = (b_1, b_1+\delta_1)$ and $I_2 = (b_2 - \delta_2, b_2)$. It is easy to see that

$$\int_{I_j} e^{-2(\Delta_j^n - \Delta_j^+)|x_3 - b_j|}dx_3 \le \min\left(\delta_j, \frac{1}{2(\Delta_j^n - \Delta_j^+)}\right).$$

Then, by substituting above estimates into (4.7), we obtain that

$$\|s^{-1}e^{R_j}\nabla\psi\|^2_{L^2(\Omega_j^{\rm PML})} = \int_{I_j} |s(x_3)|^{-2}e^{2R_j(x_3)} \int_0^L |\nabla\psi(x_1,x_3)|^2 dx_1 dx_3$$
$$\le 4L\delta_j \sum_{n\in U_j} \frac{|\alpha_n+\alpha|^2+|\beta_j^n|^2}{(1-e^{-2\Delta_j^-\sigma_j^I})^2} |\psi_\alpha^{(n)}(b_j)|^2$$
$$+4L\sum_{n\notin U_j} \frac{|\alpha_n+\alpha|^2+|\beta_j^n|^2}{(1-e^{-2\Delta_j^+\sigma_j^R})^2} |\psi_\alpha^{(n)}(b_j)|^2 \min\left(\delta_j, \frac{1}{2(\Delta_j^n-\Delta_j^+)}\right) := \mathrm{I}+\mathrm{II},$$

If $n\in U_j$, then $|\alpha_n+\alpha|^2+|\beta_j^n|^2 = k_j^2$, we get

$$\mathrm{I} \le C_j^2 \hat{C}^{-2} L \sum_{n\in U_j} |\psi_\alpha^{(n)}(b_j)|^2.$$

If $n\notin U_j$, then $|\alpha_n+\alpha|^2-k_j^2 = |\beta_j^n|^2 = |\Delta_j^n|^2$, we have $|\alpha_n+\alpha|^2+|\beta_j^n|^2 \le k_j^2+2|\Delta_j^n|^2 \le 2(k_j+\Delta_j^n)^2$ and $|\alpha_n+\alpha|^2+|\beta_j^n|^2 \le 2|\alpha_n+\alpha|^2$. Hence

$$|\alpha_n+\alpha|^2+|\beta_j^n|^2 \le 2|\alpha_n+\alpha|(k_j+\Delta_j^n).$$

Therefore

$$(|\alpha_n+\alpha|^2+|\beta_j^n|^2)\min\left(\delta_j, \frac{1}{2(\Delta_j^n-\Delta_j^+)}\right) \le |\alpha_n+\alpha|(1+2\delta_j(\Delta_j^+ + k_j)),$$

which yields

$$\mathrm{II} \le C_j^2\hat{C}^{-2}L\sum_{n\notin U_j} |\alpha_n+\alpha||\psi_\alpha^{(n)}(b_j)|^2.$$

This completes the proof upon using Lemma 2.3. ☐

LEMMA 4.4. *For any $\psi\in X(\Omega)$, let ψ be extended to the whole domain D according to* (4.1). *Then we have the following estimate*

$$\| s^{-1}\partial\psi/\partial x_3 \|_{L^2(\Gamma_1^{\rm PML})} \le \hat{C}M_3 \|\psi\|_{H^1(\Omega)},$$

where

$$M_3 = \max\left(\frac{2\Delta_1^- e^{-\Delta_1^-\sigma_1^I}}{1-e^{-2\Delta_1^-\sigma_1^I}}, \quad \frac{2\Delta_1^+ e^{-\Delta_1^+\sigma_1^R}}{1-e^{-2\Delta_1^+\sigma_1^R}}\right).$$

Proof. From (4.1) we deduce easily that

$$\frac{\partial\psi}{\partial x_3}(x_1, b_1+\delta_1) = -2\sum_{n\in Z} \mathbf{i}\bar{\beta}_1^n \bar{s}(b_1+\delta_1)\bar{\zeta}_1^n(b_1)^{-1}\psi_\alpha^{(n)}(b_1)e^{\mathbf{i}(\alpha_n+\alpha)x_1}.$$

Thus

$$\| s^{-1}\partial\psi/\partial x_3 \|_{L^2(\Gamma_1^{\rm PML})} = 2\left(\sum_{n\in Z} |\beta_1^n|^2 |\zeta_1^n(b_1)|^{-2} |\psi_\alpha^{(n)}(b_1)|^2\right)^{1/2}.$$

Moreover,

$$|\beta_1^n||\zeta_1^n(b_1)|^{-1} = \left|\frac{\beta_1^n e^{\mathbf{i}\beta_1^n\sigma_1}}{1-e^{2\mathbf{i}\beta_1^n\sigma_1}}\right|.$$

The proof now follows by using the similar argument in Lemma 2.2 and using Lemma 2.3. □

4.3. Proof of Theorem 3.1. Since we are going to interpolate nonsmooth functions satisfying quasi-perodic boundary condition, we resort to an interpolation operator $\Pi_h : \overset{\circ}{X}(D) \to \overset{\circ}{V}_h(D)$ of Scott-Zhang [21]. Let $N_h = \{a_i\}_{i=1}^N$ be the set of all nodes of $\mathcal{M}_h$ and $\{\phi_i\}_{i=1}^N$ be the corresponding nodal basis of $V_h(D)$. For any node a_i which is interior to D, we take $\sigma_i = e$, any side in $\mathcal{B}_h$ having a_i as one of its vertex. For any node a_i which is in the interior of the left boundary, that is, $a_i = (0, z_i)$ for some $z_i \in (b_2 - \delta_2, b_1 + \delta_1)$, we take σ_i as any side on the left boundary with one vertex a_i. Now for the corresponding node $a_k = (L, z_i)$ on the right boundary, we choose σ_k as the corresponding side of σ_i on the right boundary. For the nodes a_i lying on $\overline{\Gamma_1^{\rm PML} \cup \Gamma_2^{\rm PML}}$, we can choose σ_i as any side on $\overline{\Gamma_1^{\rm PML}}$ or $\overline{\Gamma_2^{\rm PML}}$ which has a_i as one vertex. Let $a_{i,1} = a_i$, and let $\{a_{i,j}\}_{j=1}^2$ the set of nodal points in σ_i with nodal basis $\{\phi_{i,j}\}_{j=1}^2$. Define $\{\psi_{i,j}\}_{j=1}^2$ as the $L^2(\sigma_i)$ dual basis:

$$\int_{\sigma_i} \psi_{i,j}(x)\phi_{i,k}(x)ds = \delta_{jk}, \quad j,k = 1,2,$$

where δ_{jk} is the Kronecker delta. We let $\psi_i = \psi_{i,1}$. Then the interpolation operator $\Pi_h : H^1(D) \to W_h(D)$, the conforming linear finite element space, is defined by

$$\Pi_h v(x) = \sum_{i=1}^N \phi_i(x) \int_{\sigma_i} \psi_i(x) v(x) ds.$$

This operator enjoys the following interpolation estimates [21]

$$\| v - \Pi_h v \|_{L^2(T)} \le C h_T \| \nabla v \|_{L^2(\tilde{T})}, \| v - \Pi_h v \|_{L^2(e)} \le C h_e^{1/2} \| \nabla v \|_{L^2(\tilde{e})}, \quad (4.9)$$

where $\tilde{T}$ and $\tilde{e}$ are the union of all elements in $\mathcal{M}_h$ having non-empty intersection with $T \in \mathcal{M}_h$ and the side e, respectively.

It remains to check Π_h keeps the boundary condition. It is clear that $\Pi_h v = 0$ on $\Gamma_1^{\rm PML} \cup \Gamma_2^{\rm PML}$ since for any $a_i \in \overline{\Gamma_1^{\rm PML} \cup \Gamma_2^{\rm PML}}, \sigma_i \subset \overline{\Gamma_1^{\rm PML}}$ or $\overline{\Gamma_2^{\rm PML}}$ and $v = 0$ on $\Gamma_1^{\rm PML} \cup \Gamma_2^{\rm PML}$. Now let $a_i = (0, z_i) \in \Gamma_{\rm left}$ and $a_k = (L, z_i) \in \Gamma_{\rm right}$. Without lost of generality, we assume $\sigma_i = \{x \in \mathbf{R}^2 : x_1 = 0, z_i \le x_3 \le z_{i+1}\}$. Then by construction we have $\sigma_k = \{x \in \mathbf{R}^2 : x_1 = L, z_i \le x_3 \le z_{i+1}\}$. The nodal basis $\phi_{i,1} = (z_{i+1} - x_3)/(z_{i+1} - z_i), \phi_{i,2} = (x_3 - z_i)/(z_{i+1} - z_i)$ in σ_i and simple calculation yields the dual basis:

$$\psi_{i,1} = \frac{4}{d_i}\phi_{i,1} - \frac{2}{d_i}\phi_{i,2}, \quad \psi_{i,2} = -\frac{2}{d_i}\phi_{i,1} + \frac{4}{d_i}\phi_{i,2} \quad \text{in} \quad \sigma_i,$$

where $d_i = z_{i+1} - z_i$. Similar computation implies that

$$\psi_k(L, x_3) = \psi_i(0, x_3) = \frac{4}{d_i}\phi_{i,1}(x_3) - \frac{2}{d_i}\phi_{i,2}(x_3).$$

Thus for any $v \in X(D)$, that is, $v(0,x_3) = e^{-\mathbf{i}\alpha L} v(L,x_3)$, we have

$$\Pi_h v(a_i) = \int_{\sigma_i} \psi_i(0,x_3)v(0,x_3)dx_3 = e^{-\mathbf{i}\alpha L}\int_{\sigma_k} \psi_k(L,x_3)v(L,x_3)dx_3 = e^{-\mathbf{i}\alpha L}\Pi_h v(a_k).$$

This shows that $\Pi_h v \in \overset{\circ}{V}_h(D)$ if $v \in \overset{\circ}{X}(D)$.

Now we take $\psi_h = \Pi_h \psi \in \overset{\circ}{V}_h(D)$ in the error representation formula (4.4) to get

$$\begin{aligned} b(u-\hat{u}_h,\psi) \;=\; & \int_D g(\overline{\psi - \Pi_h\psi})dx - a_{_D}(\hat{u}_h, \psi - \Pi_h\psi) \\ & + \int_{\Gamma_1} (T_1 - T_1^{\mathrm{PML}})(\hat{u}_h - u_{\mathrm{I}})\bar{\psi}dx_1 + \int_{\Gamma_2} (T_2 - T_2^{\mathrm{PML}})\hat{u}_h\bar{\psi}dx_1 \\ & + \int_{\Gamma_1^{\mathrm{PML}}} \frac{1}{s(x_3)}\frac{\partial\bar{\psi}}{\partial x_3}(I_h u_{\mathrm{I}} - u_{\mathrm{I}})dx_1 \\ := {} & \mathrm{III} + \cdots + \mathrm{VII} \end{aligned} \tag{4.10}$$

We observe that by integration by parts and using (3.3)– (3.5),

$$\mathrm{III} + \mathrm{IV} = \sum_{T\in\mathcal{M}_h} \left(\int_T R_T(\overline{\psi - \Pi_h\psi})dx + \sum_{e\subset\partial T} \frac{1}{2}\int_e J_e(\overline{\psi - \Pi_h\psi})ds \right).$$

Standard argument in the a posterior error analysis using (4.9) and Lemma 4.3 implies

$$\begin{aligned} |\mathrm{III}+\mathrm{IV}| &\le C\sum_{T\in\mathcal{M}_h} \eta_{_T} \|\, \rho^{-1}\nabla\psi\,\|_{L^2(\tilde{T})} \\ &\le C(1+C_1+C_2)\left(\sum_{T\in\mathcal{M}_h}\eta_{_T}^2\right)^{1/2} \|\,\psi\,\|_{H^1(\Omega)}. \end{aligned} \tag{4.11}$$

By Lemma 2.2 and Lemma 2.3, we obtain

$$\begin{aligned} |\mathrm{V}+\mathrm{VI}| &\le M_1\|\,\hat{u}_h - u_{\mathrm{I}}\,\|_{L^2(\Gamma_1)}\|\,\psi\,\|_{L^2(\Gamma_1)} + M_2\|\,\hat{u}_h\,\|_{L^2(\Gamma_2)}\|\,\psi\,\|_{L^2(\Gamma_2)} \\ &\le \left(\hat{C}M_1\|\,\hat{u}_h - u_{\mathrm{I}}\,\|_{L^2(\Gamma_1)} + \hat{C}M_2\|\,\hat{u}_h\,\|_{L^2(\Gamma_2)}\right)\|\,\psi\,\|_{H^1(\Omega)}. \end{aligned} \tag{4.12}$$

Finally, by Lemma 4.4 and Lemma 2.3, we get

$$\begin{aligned} |\mathrm{VII}| &\le M_3\|\,I_h u_{\mathrm{I}} - u_{\mathrm{I}}\,\|_{L^2(\Gamma_1^{\mathrm{PML}})}\|\,\psi\,\|_{L^2(\Gamma_1)} \\ &\le \hat{C}M_3\|\,I_h u_{\mathrm{I}} - u_{\mathrm{I}}\,\|_{L^2(\Gamma_1^{\mathrm{PML}})}\|\,\psi\,\|_{H^1(\Omega)}. \end{aligned} \tag{4.13}$$

Combining (4.10)-(4.13) we obtain the desired estimate. □

5. The $\mathbf{Im}\,\varepsilon_2 > 0$ case. In this section we consider briefly the case when $\mathrm{Im}\,\varepsilon_2 > 0$. Let $k_2^2 = \omega^2\varepsilon_2\mu$ satisfy $\mathrm{Im}\,k_2 > 0$. The constants β_2^n in the Rayleigh expansion (2.5) in Ω_2 satisfy

$$(\beta_2^n)^2 = k_2^2 - (\alpha_n+\alpha)^2, \quad \mathrm{Im}\,\beta_2^n \ge 0.$$

Denote by

$$\xi_n = \frac{1}{2}(\mathrm{Re}\,(k_2^2) - (\alpha_n+\alpha)^2), \quad \eta = \frac{1}{2}\mathrm{Im}\,(k_2^2),$$

then $(\beta_2^n)^2 = 2(\xi_n + \mathbf{i}\eta)$. Since $\mathrm{Im}\,(k_2^2) = \omega^2 \mathrm{Im}\,(\varepsilon_2)\mu > 0$, we obtain that

$$\mathrm{Re}\,\beta_2^n = (\sqrt{\xi_n^2 + \eta^2} + \xi_n)^{1/2}, \qquad \mathrm{Im}\,\beta_2^n = (\sqrt{\xi_n^2 + \eta^2} - \xi_n)^{1/2}. \tag{5.1}$$

Thus $\mathrm{Re}\,(-2\mathbf{i}\beta_2^n\sigma_2) = 2(\sigma_2^R \mathrm{Im}\,\beta_2^n + \sigma_2^I \mathrm{Re}\,\beta_2^n) \geq 2\sigma_2^R \mathrm{Im}\,\beta_2^n$, which yields

$$\begin{aligned}|\mathbf{i}\beta_2^n(1 - \coth(-\mathbf{i}\beta_2^n\sigma_2))| = \left|\frac{2\beta_2^n}{e^{-2\mathbf{i}\beta_2^n\sigma_2} - 1}\right| &\leq \frac{2|\beta_2^n|}{e^{2\sigma_2^R \mathrm{Im}\,\beta_2^n} - 1} \\ &= \frac{2\sqrt{2}(\xi_n^2 + \eta^2)^{1/4}}{e^{2\sigma_2^R(\sqrt{\xi_n^2+\eta^2}-\xi_n)^{1/2}} - 1}.\end{aligned}$$

Simple but tedious calculation shows that the function at the right-hand side is increasing with respect to $\xi_n \in \mathbf{R}$. Since $\xi_n \leq \frac{1}{2}\mathrm{Re}\,(k_2^2)$, we deduce after some algebraic manipulations that

$$|\mathbf{i}\beta_2^n(1 - \coth(-\mathbf{i}\beta_2^n\sigma_2))| \leq \mathcal{M}_2 := \frac{2|k_2|}{e^{2\sigma_2^R \mathrm{Im}\,k_2} - 1}.$$

Therefore, we conclude that Lemma 2.2 and thus Theorem 2.4 and Theorem 2.5 are also valid in the case $\mathrm{Im}\,\varepsilon_2 > 0$ with the definition of M_2 being replaced by $M_2 = \mathcal{M}_2$.

Moreover, we deduce from (4.8) that

$$|e^{-\mathbf{i}\beta_2^n r_2(x_3)} \pm e^{\mathbf{i}\beta_2^n r_2(x_3)}|^2 |\zeta_2^n(b_2)|^{-2} \leq 4e^{-2\mathrm{Im}\,\beta_2^n \int_{x_3}^{b_2} s_1(\tau)d\tau}(1 - e^{-2\sigma_2^R \mathrm{Im}\,\beta_2^n})^{-2}.$$

Since $\xi_n \leq \frac{1}{2}\mathrm{Re}\,(k_2^2)$, we see easily from (5.1) that $\mathrm{Im}\,\beta_2^n \geq \mathrm{Im}\,k_2$. Now the argument in the proof of Lemma 4.3 implies that

$$\| s^{-1} e^{\mathcal{R}_2} \nabla\psi \|_{L^2(\Omega_2^{\mathrm{PML}})} \leq \mathcal{C}_2 \| \psi \|_{H^1(\Omega)}$$

with $\mathcal{R}_2(x_3) = \mathrm{Im}\,(k_2) \int_{x_3}^{b_2} s_1(\tau)d\tau$ and

$$\mathcal{C}_2 = \hat{C}\frac{2[\max(1, |k_2|)(1 + 2\delta_2(\mathrm{Im}\,k_2 + |k_2|))]^{1/2}}{1 - e^{-2\sigma_2^R \mathrm{Im}\,k_2}}.$$

Therefore, we know that Theorem 3.1 and Theorem 3.2 are also valid with the definitions of $R_2(x_3), C_2$ and M_2 being replaced by $R_2 = \mathcal{R}_2(x_3), C_2 = \mathcal{C}_2$ and $M_2 = \mathcal{M}_2$, respectively.

6. Implementation and numerical examples. The implementation of the adaptive algorithm in this section is based on the PDE toolbox of MATLAB. We use the a posteriori error estimate in Theorem 3.1 in the TE case and Thorem 3.2 in the TM case to determine the PML parameters. According to the discussion in §2, we choose the PML medium property as the power function and thus we need only to specify the thickness δ_j of the layers and the medium parameters σ_j^m (see (2.26)). Recall from Theorem 3.1 that the a posteriori error estimate consists of two parts: the PML error $\mathcal{E}_{\mathrm{PML}}$ and the finite element discretization error $\mathcal{E}_{\mathrm{FEM}}$, where

$$\mathcal{E}_{\mathrm{PML}} = M_1 \| \hat{u}_h - u_{\mathrm{I}} \|_{L^2(\Gamma_1)} + M_2 \| \hat{u}_h \|_{L^2(\Gamma_2)}, \tag{6.1}$$

$$\mathcal{E}_{\mathrm{FEM}} = M_3 \| \hat{u}_h - u_{\mathrm{I}} \|_{L^2(\Gamma_1^{\mathrm{PML}})} + \Big(\sum_{T \in \mathcal{M}_h} \eta_T^2 \Big)^{1/2}. \tag{6.2}$$

$\mathcal{E}_{\rm PML}$ and $\mathcal{E}_{\rm FEM}$ should be changed accordingly in the TM case. In our implementation we first choose δ_j and σ_j^m such that $M_j L^{1/2} \le 10^{-8}$, which makes the PML error negligible compared with the finite element discretization errors. Once the PML region and the medium property are fixed, we use the standard finite element adaptive strategy to modify the mesh according to the a posteriori error estimate (6.2). For any $T \in \mathcal{M}_h$, we define the local a posteriori error estimator as follows:

$$\tilde{\eta}_T = \eta_T + M_3 \| I_h u_{\rm I} - u_{\rm I} \|_{L^2(\Gamma_1^{\rm PML} \cap \partial T)}.$$

Now we describe the adaptive algorithm we used in the paper.

Algorithm 5.1. Given tolerance `TOL` > 0. Let $m = 2, \delta_1 = \delta_2 = \delta$.

- Choose δ and σ_j^m such that $M_j L^{1/2} \le 10^{-8}$ for $j = 1, 2$;
- Set the computational domain $D = \Omega_2^{\rm PML} \cup \Gamma_2 \cup \Omega \cup \Gamma_1 \cup \Omega_1^{\rm PML}$ and generate an initial mesh $\mathcal{M}_h$ over D;
- While $\mathcal{E}_{\rm FEM} >$ `TOL` do
  - refine the mesh $\mathcal{M}_h$ according to the following strategy

    if $\tilde{\eta}_T > \frac{1}{2} \max_{T \in \mathcal{M}_h} \tilde{\eta}_T$, refine the element $T \in \mathcal{M}_h$

  - solve the discrete problem (3.1) or (3.7) on $\mathcal{M}_h$
  - compute error estimators on $\mathcal{M}_h$

  end while

In the following we report several numerical examples to demonstrate the competitive behavior of the proposed algorithm. In all the experiments we only document the value δ of the thickness of the PML layers. The medium parameters σ_j^m are determined accordingly through the relation $M_j L^{1/2} \le 10^{-8}$ for $j = 1, 2$. We normalize the space variables so that $\mu = 1$. We also scale the error estimator by a factor 0.15 as in PDE toolbox of MATLAB.

Example 1. We consider the simplest grating structure, a straight line. Assume that a plane wave $u_{\rm I} = e^{\mathbf{i}\alpha x_1 - \mathbf{i}\beta x_3}$ is incident on the straight line $\{x_3 = 0\}$ which separates two homogeneous media whose dielectric coefficients are ε_1 and ε_2, respectively. The exact solution is known [7]:

$$u = \begin{cases} u_{\rm I} + r e^{\mathbf{i}\alpha x_1 + \mathbf{i}\beta x_3} & \text{if } x_3 > 0 \\ t e^{\mathbf{i}\alpha x_1 - \mathbf{i}\hat{\beta} x_3} & \text{if } x_3 < 0. \end{cases}$$

where $\hat{\beta} = (k_2^2 - \alpha^2)^{1/2}, t = 2\beta/(\beta + \hat{\beta})$, and $r = (\beta - \hat{\beta})/(\beta + \hat{\beta})$. The domain $\Omega = (0, L) \times (-b, b)$, $b > 0$.

In our experiment, the parameter are chosen as $\varepsilon_1 = 1, \varepsilon_2 = (0.22 + 6.71\mathbf{i})^2$, $\theta = \pi/6, \omega = \pi$ and $L = 2$. Table 6.1 compares the results using adaptive and uniform mesh refinements when $b = \delta = 1$. It clearly shows the advantage of using adaptive mesh refinements. Moreover, our a posteriori error estimate $\mathcal{E}_k = (\sum_{T \in \mathcal{M}_k} \tilde{\eta}_T^2)^{1/2}$ provides a rather good estimate of the interested error $e_k = \| \nabla(u - \hat{u}_k) \|_{L^2(\Omega)}$.

Fig. 6.1 shows the curves of $\log N_k$ versus $\log \| \nabla(u - \hat{u}_k) \|_{L^2(\Omega)}$, where N_k is the number of nodes of the mesh $\mathcal{M}_k$. It indicates that for the proposed method, the meshes and the associated numerical complexity are quasi-optimal: $\| \nabla(u - \hat{u}_k) \|_{L^2(\Omega)} = C N_k^{-1/2}$ is valid asymptotically.

Fig. 6.2 shows the robustness of the proposed method with respect to the choice of the thickness of PML layers: the error of the grating efficiency is insensitive to the thickness δ. The definition of the grating efficiency can be found, for example, in [7]. The reason for this robustness is the exponential decay factor in our a posteriori error estimator in the PML region. Our experiences indicate that the choice of δ in the range of $0.5L$ to $1.5L$ usually produces satisfactory results.

The parameter b determines the position of the PML layers which, in the traditional PML technique, should be sufficiently far away from the grating surface to allow the evanescent waves being sufficiently decayed. Fig. 6.3 shows the robustness of our method with respect to the position of the PML layers, which is the purpose of our extended PML technique to attenuate both the out-going and evanescent waves.

Adaptive mesh				Uniform mesh			
k	N_k	e_k	$\mathcal{E}_k/e_k$	k	N_k	e_k	$\mathcal{E}_k/e_k$
0	29	8.7043	0.7830	0	29	8.7043	0.7830
2	62	3.4572	0.9866	1	71	3.7531	1.0117
4	133	2.1563	1.1251	2	143	2.6595	1.1021
5	195	1.6772	1.1143	3	283	1.7305	1.2505
6	302	1.3618	1.1088	4	575	1.3448	1.1709
7	477	0.9488	1.2212	5	1145	0.9556	1.2237
9	1135	0.5874	1.2348	6	2321	0.6984	1.1734
10	1838	0.4592	1.2371	7	4639	0.5065	1.1982
11	3379	0.3503	1.1864	8	9359	0.3549	1.1812

TABLE 6.1

Comparison of numerical results using adaptive and uniform mesh refinements. N_k *is the number of nodal points of mesh* $\mathcal{M}_k$. $\mathcal{E}_k = (\sum_{T\in\mathcal{M}_k} \tilde{\eta}_T^2)^{1/2}$ *and* $e_k = \|\nabla(u-\hat{u}_k)\|_{L^2(\Omega)}$.

Example 2. This example concerns the TM polarization on a grating surface with a sharp angle indicated in Fig. 6.4. The parameters are the same as those in Example 1. There are two reflected out-going waves. The grating efficiency of the reflected waves as well as the total grating efficiency are displayed in Fig. 6.5. Fig. 6.6 shows the mesh and the amplitude of the associated solution after 10 adaptive iterations when the grating efficiency is stabilized. The mesh has 3585 nodes and the a posteriori error estimate over which is 0.6468. The initial a posteriori error estimate is 3.7838. This example shows clearly the ability of the proposed method to capture the singularities of the problem. The meshes near the upper PML boundary is rather coarse, as a result of the exponential decay factor in our a posteriori error estimator.

Example 3. The final example is taken from [7] for TE polarization. The grating structure consists of multiple interfaces as shown in Fig. 6.7. This type of grating structures has applications in optical filters and guided mode resonance devices. The parameters are taken as follows: $\varepsilon_1 = 1, \varepsilon_2 = 2.31, \varepsilon_3 = 4.4, \varepsilon_4 = 3.6, \theta = \pi/4, L = 0.3$ and $\omega = 2\pi/0.526$. The thickness of the PML layers $\delta = 0.4$. There are two transmitted waves and one reflected out-going wave. The grating efficiency of the reflected and transmitted waves as well as the total grating efficiency are displayed in Fig. 6.8. Fig. 6.9 shows the mesh and the amplitude of the associated solution after 7 adaptive iterations when the grating efficiency is stabilized. The mesh has 1480 nodes

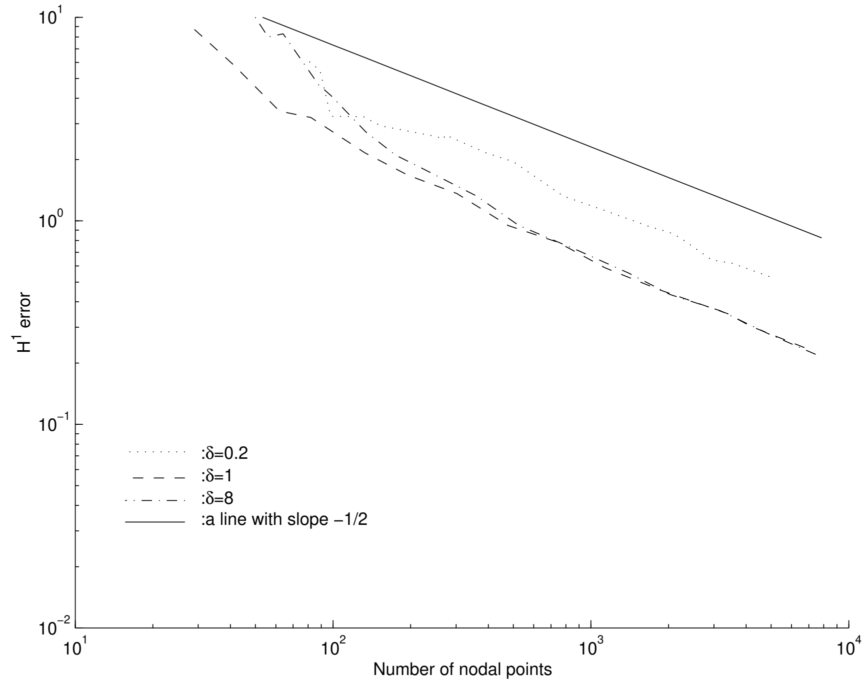

FIG. 6.1. *Quasi-optimality of the adaptive mesh refinements.*

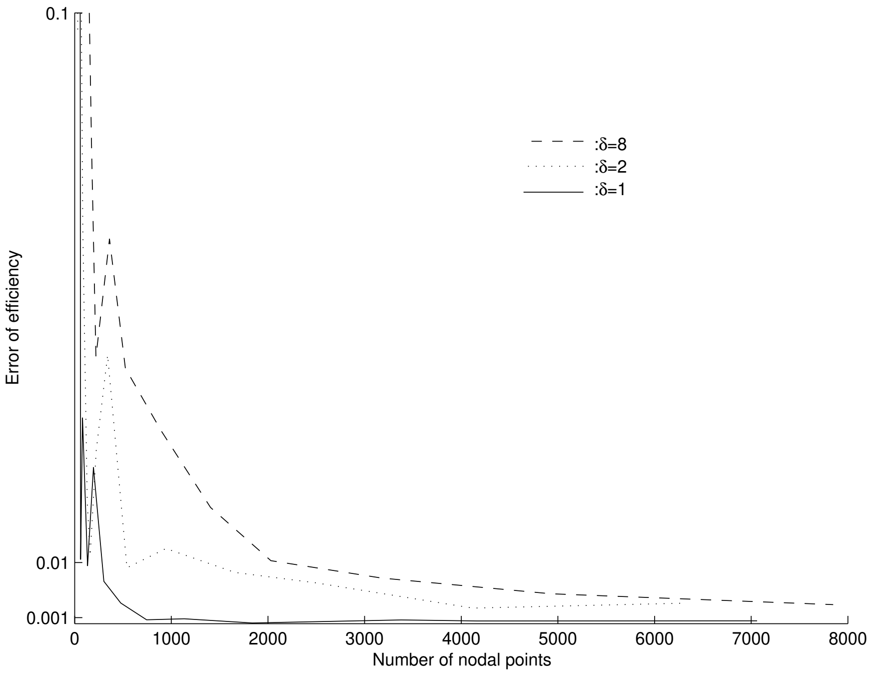

FIG. 6.2. *Robustness of the grating efficiency with respect to the thickness of PML layers.*

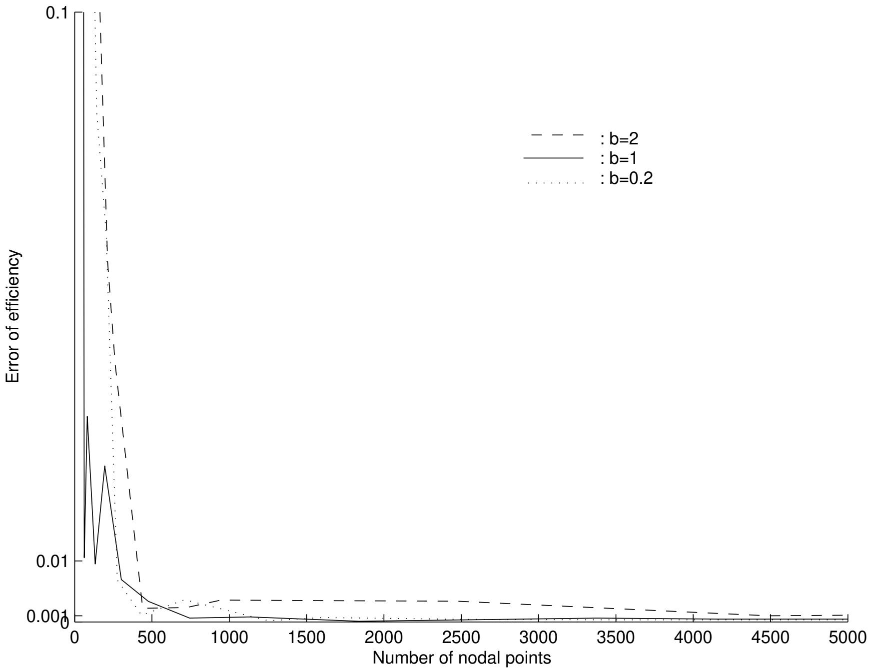

FIG. 6.3. *Robustness of the grating efficiency with respect to the position of PML layers.*

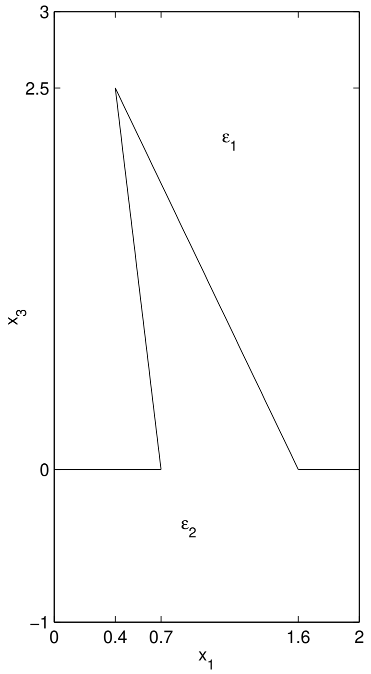

FIG. 6.4. *Geometry of the domain in Example 2.*

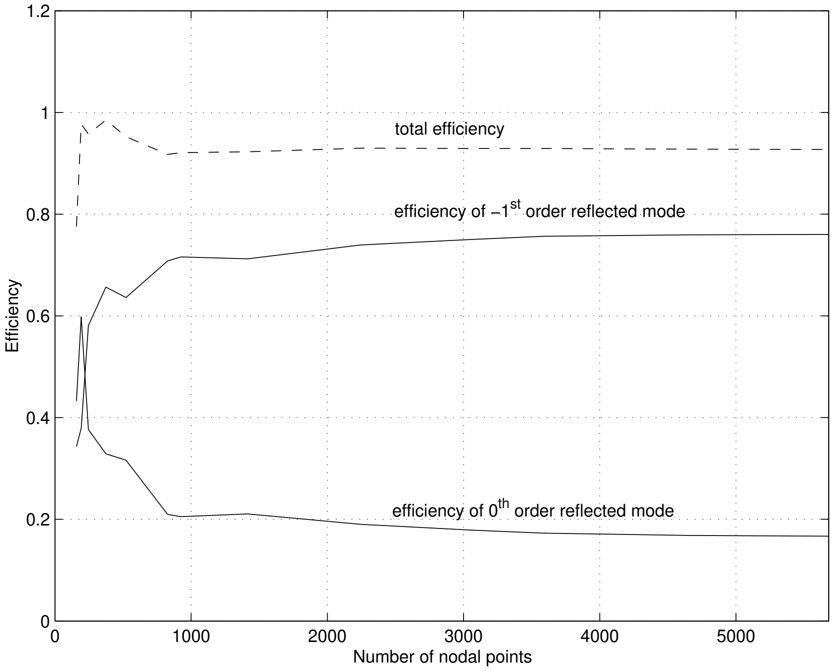

FIG. 6.5. *Grating efficiency of Example 2.*

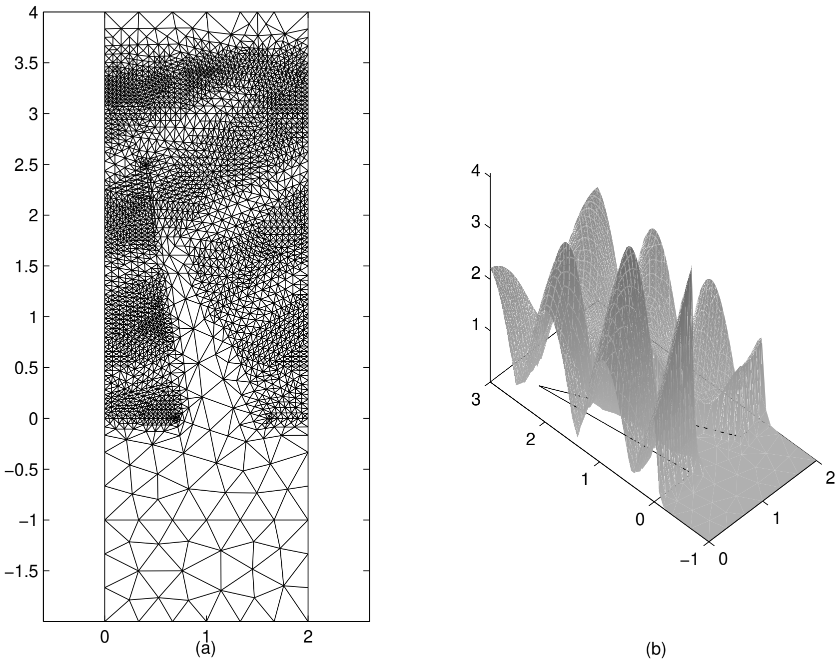

FIG. 6.6. *The mesh and the surface plot of the amplitude of the associated solution after 10 adaptive iterations. The mesh has 3585 nodes.*

and the a posteriori error estimate over which is 0.8189. The initial a posteriori error estimate is 3.0701. Again the meshes near the upper PML boundary is rather coarse, as a result of the exponential decay factor in our a posteriori error estimator.

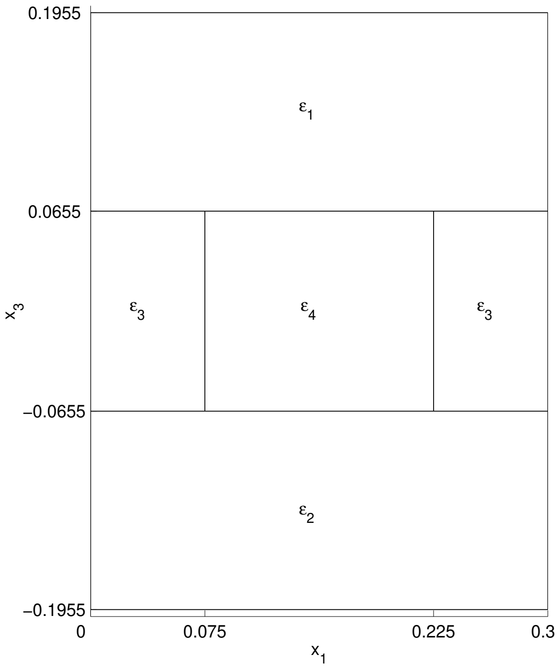

FIG. 6.7. *Geometry of the domain in Example 3.*

Acknowledgments. The authors wish to thank Gang Bao for many inspiring discussions on the physical background and the mathematical modeling of the grating problems.

REFERENCES

[1] T. Abboud. *Electromagnetic waves in periodic media,* in Second International Conference on Mathematical and Numerical Aspects of Wave Propagation, ed. by Kleinman et al, SIAM, Philadelphia, 1993, 1-9.

[2] I. Babuška and A. Aziz. *Survey Lectures on Mathematical Foundations of the Finite Element Method.* in The Mathematical Foundations of the Finite Element Method with Application to Partial Differential Equations, ed. by A. Aziz, Academic Press, New York, 1973, 5-359.

[3] I. Babuška and C. Rheinboldt. Error estimates for adaptive finite element computations. *SIAM J. Numer. Anal.* 15 (1978), 736-754.

[4] G. Bao, D.C. Dobson and J.A. Cox. Mathematical studies in rigorous grating theory. *J. Opt. Soc. Am. A* 12 (1995), 1029-1042.

[5] G. Bao. Variational approximation of Maxwell's equations in biperiodic structures, *SIAM J. Appl. Math.* 57 (1997), 364-381.

[6] G. Bao, L. Cowsar and W. Masters. *Mathematical Modeling in Optical Science.* SIAM, Philadelphia, 2001.

[7] G. Bao, Y. Cao and H. Yang. Numerical solution of diffraction problems by a least-square finite element method. *Math. Meth. Appl. Sci.* 23 (2000), 1073-1092.

[8] J.-P. Berenger. A perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Physics* 114 (1994), 185-200.

[9] Z. Chen and S. Dai. Adaptive Galerkin methods with error control for a dynamical Ginzburg-Landau model in superconductivity. *SIAM J. Numer. Anal.* 38 (2001), 1961-1985.

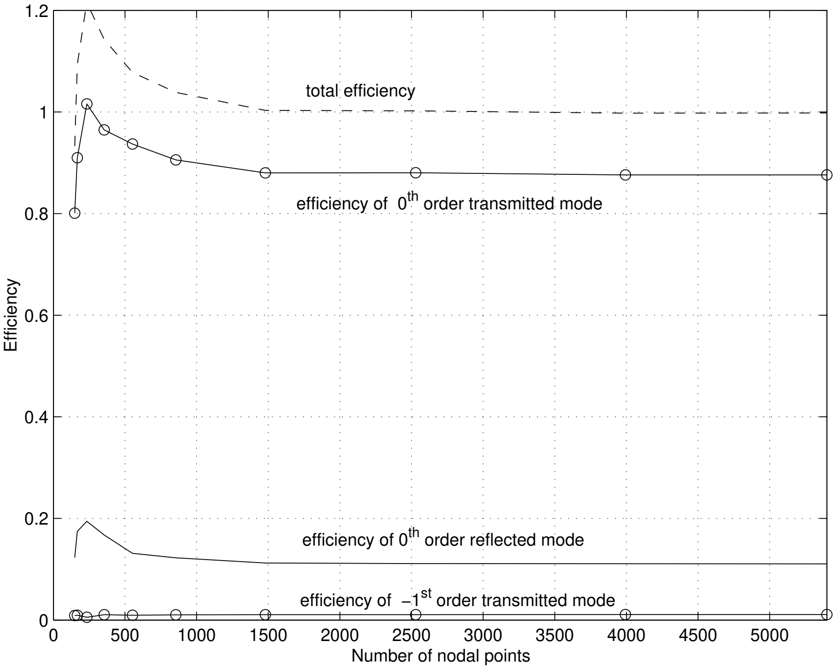

FIG. 6.8. *Grating efficiency of Example 3.*

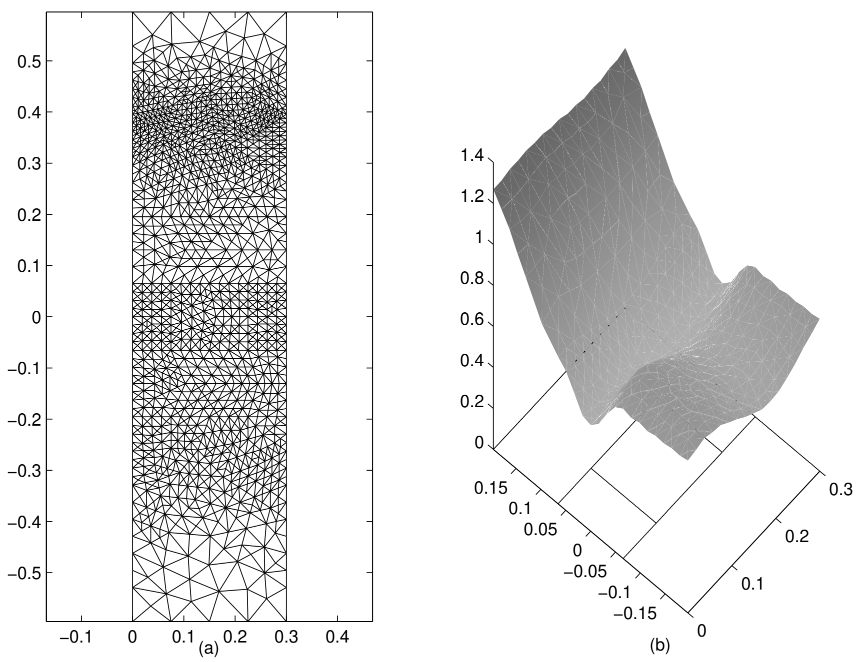

FIG. 6.9. *The mesh and the surface plot of the amplitude of the associated solution after 7 adaptive iterations. The mesh has 1480 nodes.*

[10] Z. Chen and S. Dai. On the efficiency of adaptive finite element methods for elliptic problems with discontinuous coefficients. *SIAM J. Sci. Comput.* 24 (2003), 443-462.

[11] Z. Chen, R.H. Nochetto and A. Schmidt. A characteristic Galerkin method with adaptive error control for continuous casting problem. *Comput. Methods Appl. Mech. Engrg.* 189 (2000), 249-276.

[12] F. Collino and P.B. Monk. Optimizing the perfectly matched layer. *Comput. Methods Appl. Mech. Engrg.* 164 (1998), 157-171.

[13] D. Dobson. A variational method for electromagnetic diffraction in biperiodic structures. *Math. Model. Numer. Anal.* 28 (1994), 419-439.

[14] D. Dobson and A. Friedman. The time-harmonic Maxwell equations in a doubly periodic structure. *J. Math. Anal. Appl.* 166 (1992), 507-528.

[15] M. Lassas and E. Somersalo. On the existence and convergence of the solution of PML equations. *Computing* 60 (1998), 229-241.

[16] P. Monk. A posteriori error indicators for Maxwell's equations. *J. Comput. Appl. Math.* 100 (1998), 173-190.

[17] P. Monk and E. Süli. The adaptive computation of far-field patterns by a posteriori error estimation of linear functionals. *SIAM J. Numer. Anal.* 36 (1998), 251-274.

[18] P. Morin, R.H. Nochetto and K.G. Siebert. Data oscillation and convergence of adaptive FEM, *SIAM J. Numer. Anal.* 38 (2000), 466-488.

[19] R. Petit, ed. *Electromagnetic Theory of Gratings,* Topics in Current Physics, Vol. 22, Springer-Verlag, Heidelberg, 1980.

[20] A.H. Schatz. An observation concerning Ritz-Galerkin methods with indefinite bilinear forms. *Math. Comp.* (1874), 959-862.

[21] L.R. Scott and S. Zhang. Finite element interpolation of nonsmooth functions satisfying boundary conditions. *Math. Comp.* (1990), 483-493.

[22] E. Turkel and A. Yefet. Absorbing PML boundary layers for wave-like equations. *Appl. Numer. Math.* 27 (1998), 533-557.

[23] R. Verfürth. *A Review of A Posteriori Error Estimation and adaptive Mesh Refinement Techniques*, Teubner, 1996.