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Adaptive Finite Element Method for Simulating Graphene Surface Plasmon Resonance

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Abstract. In this paper, we present the design of a posteriori error estimator for the plasmon phenomenon on the graphene surface and propose a method to achieve local high-precision numerical calculations when plasmon phenomena occur on the graphene surface. We provide a lower bound estimate for the posteriori error estimator, along with a proof of convergence. Specifically, the constructed posterior error estimator enables local refinement in regions where the error is significant at the graphene interface. Firstly, we outline the construction of the posterior error estimator and provide the proof of its lower bound. Secondly, we establish the convergence of the Adaptive Edge Finite Element Method (AEFEM). Finally, we present numerical results that validate the effectiveness of the error estimator.

AMS subject classifications: 35R30, 65N30

Key words: Surface plasmon phenomenon, time-harmonic Maxwell's equations, AEFEM, residual type posteriori error estimator.

1 Introduction

Assuming a bounded, Lipschitz polygonal domain denoted as $\Omega \subset \mathbb{R}^2$ with a boundary $\partial\Omega$ and an inner interface denoted as Σ, where $\boldsymbol{n}$ represents the unit outward normal vector of $\partial\Omega$, and ν represents the normal vector of Σ. In this study, we investigate the

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variable coefficient time-harmonic Maxwell's equations given by:

$$\begin{cases} \nabla\times\left(\mu_r^{-1}\nabla\times\boldsymbol{E}\right)-k^2\varepsilon_r\boldsymbol{E}=\boldsymbol{f} & \text{in } \Omega, \\ \boldsymbol{n}\times\boldsymbol{E}=0 & \text{on } \partial\Omega, \\ \left[\left[\nu\times\left(\mu_r^{-1}\nabla\times\boldsymbol{E}\right)\right]\right]_\Sigma=i\sigma_r^\Sigma\boldsymbol{E}_t & \text{on } \Sigma. \end{cases} \tag{1.1}$$

Here, $\boldsymbol{E}$ represents the electric field, $k>0$ is the wave number of the electromagnetic wave. The subscript t denotes the tangential part of the given vector, and $[[\cdot]]_\Sigma$ represents the jump over Σ, defined as:

$$\boldsymbol{f}_t=(\nu\times\boldsymbol{f})\times\nu \quad \text{and} \quad [[\boldsymbol{f}]]_\Sigma(\mathbf{x})=\lim_{s\to 0^+}(\boldsymbol{f}(\mathbf{x}+s\nu)-\boldsymbol{f}(\mathbf{x}-s\nu)).$$

In the above equations, $\boldsymbol{f}\in[L^2(\Omega)]^2$ represents a given known function, $i=\sqrt{-1}$, μ_r represents the permeability, which is a positive bounded function with values bounded between M_1 and M_2. That is, $0<M_1\le\mu_r(x)\le M_2$ for all $x\in\Omega$. ε_r is a 2×2 symmetric positive definite (SPD) matrix. For any given $x\in\Omega$ and $\xi\in\mathbb{R}^2$, the following inequalities hold:

$$0<\lambda_1(x)|\xi|^2\le\xi\varepsilon_r(x)\xi^{\mathrm{T}}\le\lambda_2(x)|\xi|^2<\infty,$$

where λ_1 and λ_2 are the two eigenvalues of ε_r, satisfying $0<\lambda_1\le\lambda_2<\infty$. Additionally, σ_r^Σ represents an appropriately chosen surface conductivity, specifically used to represent graphene's surface conductivity. It is a matrix-valued and symmetric function denoted as $\sigma_r^\Sigma\in L^\infty(\Sigma)^{2\times 2}$, possessing semidefinite real and complex parts and $\sigma_r^\Sigma=0$ on $\partial\Sigma$. Similar to ε_r, σ_r^Σ satisfies the bounded property: for any given $x\in\Omega$ and $\xi\in\mathbb{R}^2$, hold that:

$$0<M_3(x)|\xi|^2\le\xi\sigma_r^\Sigma(x)\xi^{\mathrm{T}}\le M_4(x)|\xi|^2<\infty.$$

Numerical solutions to Maxwell's equations play a crucial role in various applications. When it comes to solving Maxwell's equations numerically, there are several methods available, such as the finite difference time domain method [12,27,28] and the finite element method [1,6,13]. This paper primarily focuses on discussing the finite element method for solving Maxwell's equations, along with its adaptive mesh refinement technique [8,14].

In the traditional finite element method, nodal basis functions are commonly used as a basis set for the finite element space. However, when dealing with electromagnetic field problems, the use of nodal basis functions can lead to incorrect solutions. One particular issue is the failure to satisfy the divergence condition. This discrepancy arises because we assume that $\boldsymbol{E}$ and $\boldsymbol{H}$ are quadratically differentiable during the integration by parts, while our nodal basis functions only fulfill the continuity condition. To overcome this challenge, Nédélec edge finite elements can be introduced, as discussed in [4,5,15]. These elements address the problem by incorporating edge-based basis functions that ensure the satisfaction of the divergence condition and provide accurate solutions for electromagnetic field problems.