Engineering Analysis with Boundary Elements 65 (2016) 101–111

Contents lists available at ScienceDirect

Engineering Analysis with Boundary Elements

journal homepage: www.elsevier.com/locate/enganabound

Solving a scattering problem in near field optics by a least-squares method

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ARTICLE INFO

Article history:
Received 20 September 2015
Received in revised form
22 December 2015
Accepted 12 January 2016
Available online 2 February 2016

Keywords:
Fundamental solution
Plane wave functions
Least-squares technique
Near field scattering

ABSTRACT

Motivated by the Trefftz method, a numerical algorithm is proposed based on the least-squares technique for a scattering problem in near field optics. Fundamental solutions and plane wave functions are used to approximate the scattering field toward infinity and the local properties, respectively. Whilst evanescent wave functions are introduced to enrich the plane wave functions to capture the sub-wavelength feature of the field. The continuity across the element boundaries is enforced by minimizing a simple quadratic functional. The method needs not truncate the domain and could obtain high accuracy with even coarse mesh by increasing the number of basis functions. Numerical experiments are also presented to show the effectiveness of the approach.

1. Introduction

As our recognition expanded into the nano-world, near field optics has developed dramatically and been applied in diverse aspects, including nano-technology, optics microscopy, non-destructive imaging in biology [1]. Since near field optics can provide an effective approach to improve the resolution [2,3], it is desirable to solve the underlying scattering problem in order to understand the physical mechanism. As marked in [11]: three important modalities that fall in the scenario of near-field optics are near-field scanning optical microscopy (NSOM) [5], total internal reflection microscopy (TIRM) [6,7], and photon scanning tunneling microscopy (PSTM) [11,8,9]. In NSOM, the light source is transmitted through both the fiber and the small aperture at the tip of a probe. The probe is scanned over the sample in the near-field zone. The field scattered by the sample is then collected and measured in the far-field zone as a function of the probe position. In TIRM, the sample is illuminated by high spatial frequency evanescent plane waves, which may be generated by total internal reflection from a prism [10]. The scattered field is measured in the far zone of the sample as the direction of the incident wave is varied. In PSTM, the sample is illuminated by an evanescent field generated at the face of a prism (similar to TIRM), but the scattered field is detected via a tapered fiber probe in the near zone of the sample (as in NSOM). See [4] for an account of other modalities as basic experiments of near-field optics and associated scattering theories.

In this work, we study an experimental mode in near field optics that models the TIRM. It is an important optical microscopy and is of great advantages such as high sinal to noise ratio, high resolution and less damage to the specimen. According to the imaging system, TIRM is classified into prism type and objective type. Here, we focus on the latter one, whose objective is used as an optical element to generate total internal reflection as well as a receiver to collect the signals of specimen. Specifically, a sample is deposited on a homogeneous substrate and illustrated below (transmission geometry) by time harmonic waves with incident angle greater than the critical value. Then the evanescent waves appearing at the other side of the interface are used as illumination to encode the sub-wavelength structure of the scattering object. This phenomenon is mathematically described by a time-harmonic wave equation, whose solution is oscillatory with the wave length. As a consequence, the problem becomes more difficult computationally as frequency of waves or computational domain grows [12], and prevents the traditional discretization methods from effective use, such as finite element and finite difference methods [13]. On the one hand, the domain must be truncated first. And it is essential to use an absorbing boundary condition to restrict spurious numerical reflections from the artificial exterior boundary. But, exact absorbing boundary conditions are usually non-local and thus involve large computational efforts. And the approximate absorbing conditions either do not necessary give an acceptable accuracy or have limitations to certain boundary geometries and incident directions. On the other hand, there

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http://dx.doi.org/10.1016/j.enganabound.2016.01.006
0955-7997/

must be sufficient number of discretization points to resolve the solution by these methods. A standard rule of thumb is to use at least ten grid points per wavelength. This dramatically increases the number of unknowns and entails an excessive computational efforts, eventually makes intractable using classical numerical methods. Furthermore, since the evanescent waves exponentially decay with distance from the interface, numerically capturing their information, which contains much more sub-scale features of the specimen, becomes a challenging task. When there is no sample, the problem is studied in [14–17].

In [18], the authors investigate the use of ultra weak variational formulation to solve such problem. In order to capture the sub-scale features of waves, we utilize evanescent wave functions together with plane wave functions to approximate the local properties of the field. Then analyze the global convergence and give an error estimation of the method. Motivated by the Trefftz method, in this paper we propose a least-squares method for this problem. The idea of the Trefftz method is to use the basis functions which are the solutions locally of the underlying partial differential equation (PDE) in each element. The main examples are the ultra weak variational formulation (UWVF) [19,20], the discontinuous enrichment method (DEM) [21], the discontinuous Galerkin method (DG) [22,23], the partition of unity method (PUM) [24,25], variational theory of complex rays (VTCR) [26], wave based method (WBM) [27] and many least-squares methods [28,29]. We also should note that the method of fundamental solutions is a Trefftz-like method, and the method of fundamental solutions for scattering and radiation problems are also investigated by Fairweather et al. [30] or Karageorghis and Lesnic [31,32].

In this paper, we attempt to solve a scattering problem in near field optics combining the fundamental solutions, plane wave functions, and the evanescent wave functions firstly. There are two main strategies in our scheme. One is to approximate the scattering field toward infinity by fundamental solutions instead of truncating the whole space. The other is to use plane wave functions combining evanescent wave functions for approximating the scattering field in near field. Since the information about the frequency is directly incorporated in the discrete space, only a small number of elements are needed and the size of the element even does not depend on the wavenumber. Whilst the information of the scattering filed in near field can be captured numerically. The proposed method can be implemented with less complexity, and various integrals can be evaluated in a closed form. When the wavenumber grows, it still can effectively resolve the problem with much fewer calculations.

The remainder of this paper is organized as follows. In Section 2, the model problem to be studied is formulated. In Section 3, we present our numerical method in detail. In Section 4, numerical experiments are performed to show the effectiveness of the approach. In Section 5, the concluding remarks are given for the proposed method.

2. Model problem

Throughout this paper, we assume nonmagnetic materials and transverse magnetic polarization, i.e., TM polarization. Meanwhile, the model Maxwell equations reduce to the two-dimensional Helmholtz equation. Thus in this paper, we mainly consider a near field scattering problem in $\mathbb{R}^2$ which models the total internal reflection microscopy (TIRM). The point in the plane is denoted by $\boldsymbol{x}=(x,y)\in\mathbb{R}^2$. $\Gamma=\{\boldsymbol{x}|y=0\}$ denotes the substrate interface and divides the whole space $\mathbb{R}^2$ into two parts $\mathbb{R}^2_+=\{\boldsymbol{x}|y>0\}$ and $\mathbb{R}^2_-=\{\boldsymbol{x}|y<0\}$, i.e., $\mathbb{R}^2=\mathbb{R}^2_+\cup\mathbb{R}^2_-\cup\Gamma$. The corresponding refractive indexes are constants n_+ and n_-, respectively, with $n_+<n_-$. A sample S with refractive n_s is deposited on the

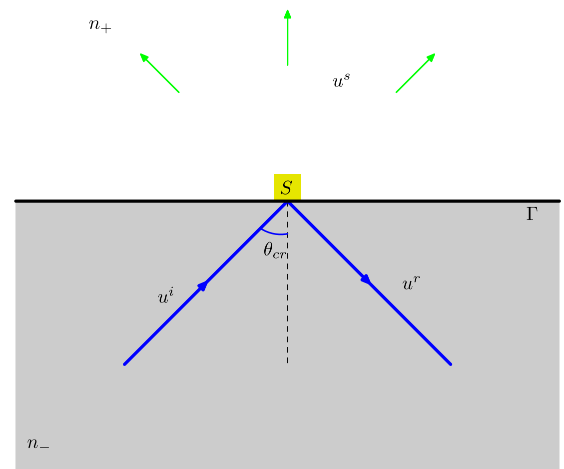

Fig. 1. A schematic of the problem geometry: the location of the sample S, the incident wave u^i, the scattering filed u^s, the refractive indexes n_+ and n_-, the substrate interface Γ.

substrate Γ and illustrated below by time harmonic plane wave $u^i=\exp(\mathrm{i}\alpha x+\mathrm{i}\eta y)$, where $\alpha=k_0 n_-\sin\theta$, $\eta=k_0 n_-\cos\theta$ with k_0 and θ denoting the free-space wavenumber and incident angle, respectively. We refer to Fig. 1 for the geometry illustration. Once θ becomes larger than the critical value θ_{cr}, the total inner reflection happens. Then the evanescent wave appears in $\mathbb{R}^2_+$, which exponentially decay with the distance from the substrate and oscillate with a wavelength in the directions along the interface. We try to compute the scattering field u^s caused by the sample.

When there is no sample, we denote the field by u^{ref} called the reference field. From [33], we know that u^{ref} has the following form:

$$u^{ref}=\begin{cases} u^t, & \boldsymbol{x}\in\mathbb{R}^2_+,\\ u^i+u^r, & \boldsymbol{x}\in\mathbb{R}^2_-, \end{cases} \tag{1}$$

where u^t and u^r are the transmitted wave and reflected wave, respectively. More precisely, we have

$$u^t=\frac{2\eta}{\eta+\gamma(\alpha)}\exp(\mathrm{i}\alpha x+\mathrm{i}\gamma(\alpha)y),\quad u^r=\frac{\eta-\gamma(\alpha)}{\eta+\gamma(\alpha)}\exp(\mathrm{i}\alpha x-\mathrm{i}\eta y), \tag{2}$$

where

$$\gamma(\alpha)=\begin{cases} \sqrt{k_0^2n_+^2-\alpha^2}, & \text{for } k_0n_+>|\alpha|,\\ \mathrm{i}\sqrt{\alpha^2-k_0^2n_+^2}, & \text{for } k_0n_+<|\alpha|. \end{cases} \tag{3}$$

From (2) and (3), it is easy to see that when the incident angle is larger than the critical value, i.e., $k_0n_+<|\alpha|$, $\gamma(\alpha)$ is purely imaginary. Whilst the transmitted wave becomes evanescent wave, which propagates in the directions along the substrate surface and exponentially decays in the y direction.

When the sample is deposited, the reference field u^{ref} is disturbed. Thus scattering field u^s emerges. Whilst the total field u is given by

$$u=u^{ref}+u^s. \tag{4}$$

Then from the electromagnetic theory of Maxwell, u satisfies the following equation:

$$\Delta u+k_0^2n^2(\boldsymbol{x})u=0,\quad \boldsymbol{x}\in\mathbb{R}^2, \tag{5}$$

with the wavenumber $\kappa=k_0n(\boldsymbol{x})$ and the refractive

$$n(\boldsymbol{x})=\begin{cases} n_+, & \boldsymbol{x}\in\mathbb{R}^2_+\backslash S,\\ n_s, & \boldsymbol{x}\in S,\\ n_-, & \boldsymbol{x}\in\mathbb{R}^2_-. \end{cases}$$