Computer Physics Communications 185 (2014) 3141–3150

Contents lists available at ScienceDirect

Computer Physics Communications

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

New scheme of the Discrete Sources Method for light scattering analysis of a particle breaking interface

Yuri Eremin [a], Thomas Wriedt [b,*]

[a] Lomonosov Moscow State University, Vorobyov's Hills, 119991 Moscow, Russia

[b] Institut für Werkstofftechnik, Badgasteiner Str. 3, 28359 Bremen, Germany

ARTICLE INFO

Article history:
Received 2 June 2014
Received in revised form
15 July 2014
Accepted 12 August 2014
Available online 20 August 2014

Keywords:
Discrete Sources Method
Numerical scheme
Light scattering
Partially embedded nanoparticle

ABSTRACT

The Discrete Sources Method (DSM) has been modified to analyze polarized light scattering by *an axial symmetric* penetrable nanoparticle partially embedded into a substrate. The new numerical scheme of the DSM enables to consider scattering from such substrate defects as flat particles, mounds, pits and voids. A detailed description of the numerical scheme is provided. The developed computer model has been employed to investigate scattering from a shallow particle and pit. Simulation results corresponding to the Differential Scattering Cross-Section and the integral response for P/S polarized light are presented.

1. Introduction

Multiple practical applications require considering a particle embedded into some media. Biosensors [1], optical antennas [2], solar cells [3], UV lithography [4] and plasmonics [5–7] are among the topics of interest. Partially embedded particles which are used as plasmonic structures [6,7] or surface features, which should be detected as a defect [8], require some optical simulation tools for their specification. In this context, interest has recently been aroused in the detection of nanoparticles partially embedded into a substrate [7,8]. In particular surface defects can arise in the chemical processing of a substrate surface [8]. The monitoring of such kind of surface features requires adequate tools for mathematical modeling that make it possible to detect and distinguish between different surface features. Additionally, modeling of the nanostructures' properties and analyzing their light scattering behavior can be used for a correct interpretation of experimental data in plasmonics.

For three-dimensional light scattering simulation, accurate modeling requires an appropriate choice of the specific numerical method. Various numerical techniques have been used to this end. Finite Difference Time Domain (FDTD) [9] solves Maxwell's equations in the differential form in the time domain. FDTD is a simple technique, which can be effectively implemented on a computer or a graphics processing unit (GPU). Unfortunately, these models might be not accurate enough in some interesting cases [10]. Additionally, a conventional FDTD scheme does not account for an infinite plane interface in its theoretical model and one has to apply special tricks to incorporate it [11]. The Finite Element Method (FEM) [12] solves Maxwell's equations in the differential form in the frequency domain. The FEM implementation leads to matrix equations with large sparse matrices. But direct application of the FEM to structures with surface features can cause problems related to a truncation of the simulation domain [13]. Besides, FDTD and FEM have the disadvantage that they require both the inhomogeneity and the background volume to be discretized, leading to higher computer demand.

Other suitable numerical approaches are commonly known as semi-analytical methods. This means that Green's theorem has to be applied to the system of Maxwell equations [14] to reduce the scattering problem formulated in the whole of 3D space to the impurity domain. There are volume-based methods, similar to Discrete Dipole Approximation (DDA) [15] and Volume Integral Equation (VIE) [16], which are suitable for modeling of light scattering by arbitrary impurities, and the surface based methods, such as the T-matrix method [17], Surface Integral Equation (SIE) [18], Multiple MultiPole Technique (MMP) [19] and Discrete Sources Method (DSM) [20]. While volume-based methods can handle any kind of inhomogeneity, they are pretty time consuming, especially if it is required to account for strong interaction between impurity and interface, which is the case considering flat attached particle.

* Corresponding author. Tel.: +49 0 42121851250; fax: +49 0 42121851211.
E-mail address: thw@iwt.uni-bremen.de (T. Wriedt).

http://dx.doi.org/10.1016/j.cpc.2014.08.010
0010-4655/

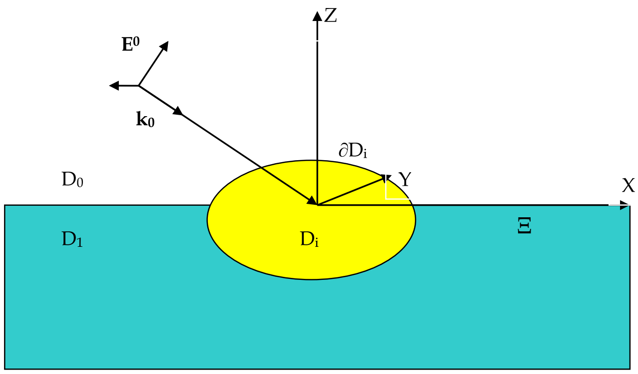

Fig. 1. Model geometry: a penetrable particle partially embedded into a plane substrate.

Surface-based methods seem to be more appropriate for the treatment of homogeneous features deposited near an interface. They allow incorporating of the Green Tensor (GT) of the plane interface to account for multiple interactions between impurity and the interface [21]. Most of them are direct methods. This means that they enables to solve a scattering problem for a whole set of incident angles and polarizations at the same time. This is an advantage with respect to FDTD, FEM, DDA and VIE which require to restart the entire computational process for any new incident angle or polarization. The T-matrix method also does not meet the problem to consider a flat particle attached the substrate, because it requires that a particle will be located inside subscribing sphere belongs completely to one of the half-spaces [22]. SIE might have a problem with very thin a particle attached to a plane interface as well because of strong interaction between an opposite surfaces of the particle.

Among the other mentioned methods, the MMP and the DSM have several advantages. First of all they are semi-analytical meshless methods that do not require any integration procedure over the impurity surface. Besides, MMP and DSM provide a unique opportunity for a reliable validation of the numerical results, as the errors of the solution can be evaluated explicitly by computing of the impurity surface residual [19,20]. The DSM outlines are similar to MMP. For non-axial symmetric structures they are almost identical. Essential difference between DSM and MMP appears for analysis of axial symmetric structures. The main difference consists in that DSM uses lowest order distributed multipoles deposited at the axis of symmetry or in adjoin complex plane [23]. This enables to account for the axial symmetry of the structure and polarization of an external excitation [24]. In the frame of MMP multipole deposited at an auxiliary surface inside a scatterer or ring currents are mostly employed [25].

In this paper we introduce a new scheme of the Discrete Sources Method (DSM) [20,23,24] that enables to consider polarized light scattering from a penetrable particle partially embedded into a plane substrate. The DSM is a semi-analytical surface based meshless method, which requires neither mesh generation, nor an integration procedure over the particle surface. In the frame of the DSM the scattered field everywhere outside a particle is represented as a finite linear combination of electromagnetic fields originated by dipoles and multipoles distributed inside the particle. Thus, the DSM solution satisfies Maxwell's equations, the radiation or attenuation conditions far away and the transmission conditions enforced at the plane interface analytically. To fit the transmission conditions at the interface we incorporate the Green Tensor of the half-space. Thus the unknown amplitudes of the discrete sources (DS) are to be determined from the boundary conditions enforced at the particle surface only. For to shallow bump or pit scattering analysis we employ the "fictitious" particle approach as suggested by Baryshev and Eremin [26] for the acoustic scattering problem. It consists in the following. Let us consider a shallow bump on a plane substrate and assume that the outer surface of the attached particle is a part of some larger particle embedded into the substrate which refractive index is equal to the substrate index. In this case we get a larger space for positioning of the DS and thus can avoid sharp edges of the attached particle. This idea is similar to Hafner's idea to handle with thin disc scattering analysis [27].

In the following chapter the new mathematical formalism of the DSM is presented, followed by the detailed description of the corresponding numerical scheme. In the final chapter of the paper some numerical results are demonstrated.

2. New scheme of the Discrete Sources Method

We start with the mathematical statement of the light scattering problem. Consider a configuration consisting of a plane substrate (half-space $D_1, z < 0$), and the other part of the space $(D_0, z > 0)$. Let an axial symmetric penetrable particle be partially embedded into the substrate. We denote the particle's internal domain as D_i and will refer to its surface as ∂D_i. Let us choose a Cartesian coordinate system with its origin O on the plane surface Ξ $(z = 0)$. Assume the Oz axis coincides with the axis of symmetry of the particle and directed into D_0. Let $\{\mathbf{E}^0, \mathbf{H}^0\}$ be an electromagnetic field of a linearly polarized plane wave propagating at an angle of $\pi - \theta_0$ with respect to the Oz axis (see Fig. 1). Then the mathematical statement of the scattering problem can be written in the following form

$$\begin{aligned}
&\nabla \times \mathbf{H}_\zeta = jk\varepsilon_\zeta \mathbf{E}_\zeta; \qquad \nabla \times \mathbf{E}_\zeta = -jk\mu_\zeta \mathbf{H}_\zeta \\
&\quad D_\zeta,\ \zeta = 0, 1, i, \\
&\left.\begin{aligned}\mathbf{n}_p \times \left(\mathbf{E}_i(p) - \mathbf{E}_{0,1}(p)\right) = 0,\\ \mathbf{n}_p \times \left(\mathbf{H}_i(p) - \mathbf{H}_{0,1}(p)\right) = 0,\end{aligned}\right. \quad p \in \partial D_i, \\
&\left.\begin{aligned}\mathbf{e}_z \times (\mathbf{E}_0(p) - \mathbf{E}_1(p)) = 0,\\ \mathbf{e}_z \times (\mathbf{H}_0(p) - \mathbf{H}_1(p)) = 0,\end{aligned}\right. \quad p \in \Sigma, \\
&\lim_{r\to\infty} r \cdot \left(\sqrt{\varepsilon_0}\mathbf{E}_0^s \times \frac{\mathbf{r}}{r} - \sqrt{\mu_0}\mathbf{H}_0^s\right) = 0, \quad r = |M| \to \infty,\ z > 0 \\
&\left(\left|\mathbf{E}_1^s\right|, \left|\mathbf{H}_1^s\right|\right) = o\left(\exp\{-|\mathrm{Im}\, k_1|\, r\}\right), \quad z < 0.
\end{aligned} \tag{1}$$

Here $\{\mathbf{E}_\zeta, \mathbf{H}_\zeta\}$ is the total field in the corresponding domain D_ζ, $\zeta = 0, 1$, $\{\mathbf{E}_\zeta^s, \mathbf{H}_\zeta^s\}$ is the scattered field, $k = \omega/c$, $\mathbf{n}_p$ is outer unit normal vector to the particle surface ∂D_i, $\mathbf{e}_z$ is the unit basis vector of the Cartesian coordinate system directed along the Oz axis, $k_\zeta = k\sqrt{\varepsilon_\zeta \mu_\zeta}$. We assume that the particle surface ∂D_i is smooth enough $\partial D_i \subset C^{(2,\upsilon)}$ and that the parameters of the media satisfy the following conditions: $\mathrm{Im}\, \varepsilon_0, \mu_0 = 0$, $\mathrm{Im}\, \varepsilon_1, \mu_1 < 0$, which correspond to the time dependence $\exp\{j\omega t\}$. Then, the boundary scattering problem (1) has a unique solution.

Let us solve the problem of reflection and transmission of the exciting plane wave $\{\mathbf{E}^0, \mathbf{H}^0\}$ at the plane interface $(z = 0)$. This can be done analytically to obtain the external excitation field $\{\mathbf{E}_\zeta^0, \mathbf{H}_\zeta^0\}$ in each domain D_ζ, $\zeta = 0, 1$ [28]. This field should satisfy the transmission conditions enforced at Ξ and the corresponding infinity conditions. We introduce the following notations

$$\left.\begin{aligned}\psi_\zeta^\pm &= \exp\left\{-jk_\zeta\left(x\sin\theta_\zeta \pm z\cos\theta_\zeta\right)\right\}\\ \mathbf{e}_\zeta^\pm &= \left(\mp\mathbf{e}_x\cos\theta_\zeta + \mathbf{e}_z\sin\theta_\zeta\right)\end{aligned}\right. \quad \zeta = 0, 1$$

where $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ are Cartesian basis, θ_1 is the angle at which the transmitted plane wave penetrates inside the substrate, according to Snell's law.

For P-polarization the incoming and outgoing waves are $\mathbf{E}_\zeta^{P(\pm)} = \mathbf{e}_\zeta^\pm \cdot \psi_\zeta^\pm$; $\mathbf{H}_\zeta^{P(\pm)} = -\mathbf{e}_y \cdot n_\zeta \cdot \psi_\zeta^\pm$ and, for S-polarization $\mathbf{E}_\zeta^{S(\pm)} = \mathbf{e}_y \cdot \psi_\zeta^\pm$; $\mathbf{H}_\zeta^{S(\pm)} = \mathbf{e}_\zeta^\pm \cdot n_\zeta \cdot \psi_\zeta^\pm$.