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Evanescent wave scattering by particles on a surface: Validation of the discrete dipole approximation with surface interaction against microwave analog experiments

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ABSTRACT

The discrete dipole approximation with surface interaction (DDA-SI) is analyzed and expanded for the modeling of far-field scattering by objects on a surface illuminated by an evanescent wave generated by total internal reflection. More specifically, the electric field scattered in the far zone predicted via the DDA-SI is compared against scaled microwave experiments; additional comparisons are also performed using results from a Finite Element Method (FEM). Three cases are considered: a lossless cube with a side length of $\lambda/1.79$ (size parameter $x=1.76$), a lossless sphere with a diameter of $\lambda/1.92$ ($x=1.63$) and an absorbing sphere with a diameter of $\lambda/0.87$ ($x=3.63$), where λ is the wavelength. For lossless scatterers, a good agreement between the DDA-SI, the FEM and scaled microwave analog experiments is observed, especially when modified Fresnel reflection coefficients are used for computing the surface interaction in the DDA-SI. For an absorbing sphere, the experimental and FEM results are in reasonable agreement, while the DDA-SI exhibits a different trend. This behavior might be due to the fact that the accuracy of the DDA decreases as the permittivity and the size parameter increase. This work suggests that the DDA-SI could be used as a forward model in an evanescent wave-based characterization framework given that a thorough convergence and accuracy analysis is carried on in order to improve the performance when dealing with objects having large permittivity and/or size parameter.

1. Introduction

The need for a real-time, non-obtrusive, nanostructure characterization system continues to rise as the use of nanoscale materials increases rapidly. Current imaging methods such as atomic force microscopy, scanning tunneling microscopy and scanning electron microscopy all provide excellent visual imaging of nanoscale materials, yet are unable to do so without having some effect on the sample. They are also unable to give precise particle characteristics in real time such as size, arrangement and composition. One promising characterization system currently being researched which is expected to provide such characteristics, and in real time, is the Polarized-Surface-Wave-Scattering System (PSWSS) [1–8]. This framework functions in a non-invasive manner through measuring the far-field scattering profiles (Mueller matrix elements) of nanostructures on a surface illuminated by an evanescent wave generated by total internal reflection (TIR) of a laser beam [8]. The measured scattering profiles, sensitive

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to the size, shape, arrangement and composition of the particles, can then be used to characterize nanostructures on a surface via inversion techniques [5–7]. These measurements can also be made in real time with the only limitation being the speed of the detector. This methodology is promising, yet in order for this system to provide accurate characterization results a strong forward model for calculating evanescent wave scattering by particles on a surface must also be present.

Prediction of evanescent wave scattering by particles on a surface is a challenging problem. The transfer matrix method combined with the normal incidence approximation (NIA) was used to predict scattering by a sphere on a surface illuminated by a propagating [9,10] and an evanescent [1–4] wave. An exact solution for the problem of multiple spheres on a surface was also proposed by Mackowski [11]. For characterization purposes, the forward model should be able to accommodate arbitrarily shaped objects on a surface. Numerical approaches such as the null-field method with discrete sources [12] and the finite-difference time-domain method [13] could be used for that purpose. In this work, evanescent wave scattering by particles on a surface is predicted via a discrete dipole approximation (DDA). The DDA is a widely accepted method for solving light scattering by particles from direct propagating illumination. The most well-known application is by Draine and Flatau in the open-source code DDSCAT written in *Fortran* [14,15]. Similarly, ADDA is an open-source *C* software package developed by Yurkin and Hoekstra [16,17]. These codes, however, do not accommodate for evanescent illumination of particles on a surface.

The method being evaluated for the forward model to be used in the PSWSS is the DDA with surface interaction (DDA-SI) implemented by Loke et al. [18,19]. The DDA-SI was created as an open-source *MATLAB* computational toolbox [20] and is based on the work of Schmehl [21] and Nebeker [22]. The DDA-SI has been chosen both for its accuracy as well as its flexibility. The method is based on discretizing the objects into cubical sub-volumes conceptualized as point electric dipoles. Since calculations are made for each individual sub-volume, the DDA-SI can easily accommodate any complex-shape inhomogeneous scatterer. This can vary from simple geometries such as cylinders, cubes and spheres, to more complex agglomerates or arrays of particles. Additionally, the DDA-SI can be used both for cases of propagating and evanescent illuminations.

The objective of this work is to use and expand the DDA-SI program package for calculations of far-field scattering by objects on a surface illuminated by an evanescent wave, and to validate the method against scaled microwave analog experiments. Results from a Finite Element Method (FEM) are also used for additional comparisons. In the next section, the physical and mathematical description of the problem is provided, and modifications performed in the DDA-SI package are highlighted. Scattered electric fields in the far zone calculated with the DDA-SI are then compared against measurements performed at microwave frequencies and predictions obtained with the FEM for two lossless particles (cube and sphere) and an absorbing sphere.

2. Physical and mathematical description of the problem

2.1. Description of the characterization framework

The characterization framework is schematically depicted in Fig. 1. Non-magnetic objects of various shapes, sizes, arrangements and compositions are placed in air (refractive index n_2 of 1) on a substrate with refractive index n_1 larger than the refractive index of air. A monochromatic radiation beam of wavelength λ is incident from within the substrate at an angle θ_{inc} measured from the normal to the surface. The incidence angle θ_{inc} is larger than the critical angle θ_{crit} for TIR ($\theta_{crit}=\sin^{-1}(n_2/n_1)$), such that the propagating beam is totally reflected back in the substrate at an angle $\theta_{ref}=\theta_{inc}$ while an evanescent wave, with a field decaying in air, is generated at the substrate–air interface [23]. Particles illuminated by the evanescent field scatter the energy in the far field as shown in Fig. 1. The far-field scattering profiles, quantified by the Mueller matrix elements in the characterization framework, can be used to retrieve the particle characteristics via an inversion algorithm. Calculation of far-field scattering is performed via the DDA-SI, as explained next.

2.2. Far-field scattering calculations via the DDA-SI

The formulation of the DDA-SI starts by expressing the total electric field as the sum of incident and scattered electric fields. A system of linear equations is then derived from the total electric field equation by discretizing the objects on the surface into N cubical sub-volumes conceptualized as electric point dipoles. After discretization into sub-volumes, the following system of linear equations is obtained [21]:

$$(\overline{\overline{\mathbf{A}}}+\overline{\overline{\mathbf{R}}})\cdot\overline{\mathbf{P}}=\overline{\mathbf{E}}_{inc} \tag{1}$$

where $\overline{\mathbf{E}}_{inc}$ is the $3N$ incident electric field vector due to an external illumination (propagating or evanescent), $\overline{\overline{\mathbf{A}}}$ is the $3N$ by $3N$ interaction matrix that accounts for dipole–dipole interactions, $\overline{\overline{\mathbf{R}}}$ is the $3N$ by $3N$ matrix due to surface interaction, and $\overline{\mathbf{P}}$ is the $3N$ vector containing the N unknown dipole moments $\mathbf{p}_j$ each with x-, y- and z-components. The dipole moment at a sub-volume j is

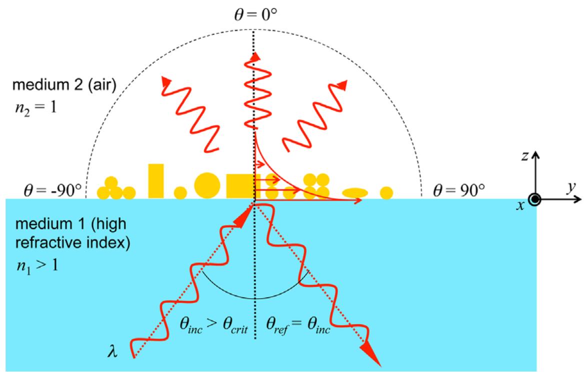

Fig. 1. Schematic representation of the characterization framework: particles on the substrate are illuminated by an evanescent wave generated by TIR of an external radiation beam.