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ELECTROMAGNETIC WAVE SCATTERING: A MODERN BOUNDARY ELEMENT APPROACH FOR NDE APPLICATIONS

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INTRODUCTION

The modeling of electromagnetic scattering is becoming increasingly important to several industries largely due to their ability to simulate approximate procedures that are too complex and expensive to perform. One such application is the detection of contaminants such as dust particles on semiconductor devices and optical surfaces during manufacture. The presence of such contaminants can affect yield and cause reliability problems [1]. Optical techniques are beginning to find wide spread application as a tool for surface inspection and contamination detection in the integrated circuit and digital storage media industries. Current commercial detection instruments are available for scanning a smooth surface with a laser that counts individual contaminant scatterers of dimensions comparable to the laser wavelength, by detecting the scattered light. Although these instruments display high sensitivity to the presence of scatterers, the calibration process (i.e. the size vs. scatter relationship) must be experimentally determined for each substrate/contaminant combination [2]. Consequently, an accurate forward model predicting the calibration process is of significant interest to industry. The forward model presented in this paper is based on the boundary element method (BEM) for the solution of electromagnetic scattering in the presence of an dielectric object and is discussed below.

The problem geometry is shown in Figure 1. The goal is to solve for the scattered field in the external region. The problem is solved in three stages. First, the presence of the dust particle suspended in an infinite medium is studied. The numerical solutions obtained will be validated by comparing with those obtained using the analytical Mie theory. Next, another scatterer of indefinite size (half space) is introduced. The problem now consists of a particle adjacent to the surface of the half space with incident plane wave emanating from the external region. Results obtained will be compared with those presented in [3]. Lastly, the reduced half space plane S will be replaced by one with random surface roughness as shown in Figure 1. This configuration is currently under investigation and the results will be reported in later publications.

PROBLEM FORMULATION

The governing boundary integral equations (BIEs) for the first configuration are

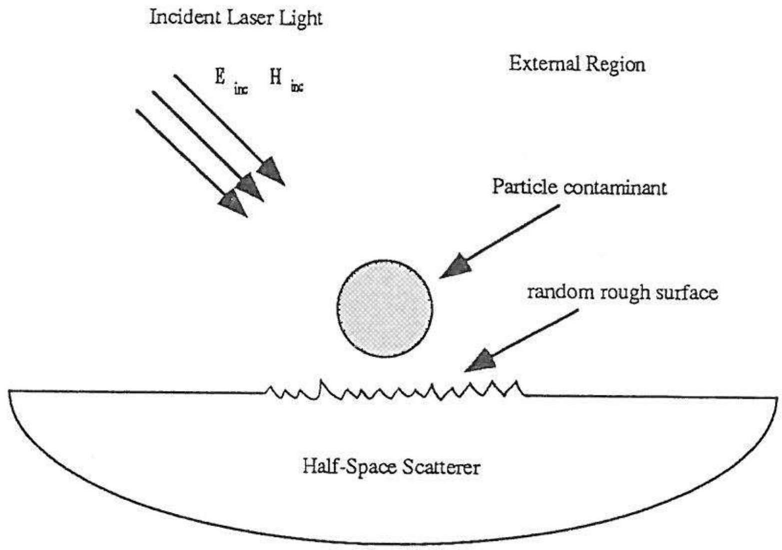

Figure 1. Overall Scattering Configuration

$$C_e\left\{\mathbf{n}\times\mathbf{E}\right\} + \frac{j}{\omega\varepsilon_e} F_e\left\{\mathbf{n}\times\mathbf{H}\right\} = \begin{pmatrix} -2\,\mathbf{E}_{inc}(p) & p \text{ inside } B_e \\ 2\,\mathbf{E}_e(p) & p \text{ outside } B_e \end{pmatrix} \tag{1}$$

$$C_e\left\{\mathbf{n}\times\mathbf{H}\right\} - \frac{j}{\omega\mu_e} F_e\left\{\mathbf{n}\times\mathbf{E}\right\} = \begin{pmatrix} -2\,\mathbf{H}_{inc}(p) & p \text{ inside } B_e \\ 2\,\mathbf{H}_e(p) & p \text{ outside } B_e \end{pmatrix} \tag{2}$$

$$C_i\left\{\mathbf{n}\times\mathbf{E}_i\right\} + \frac{j}{\omega\varepsilon_i} F_i\left\{\mathbf{n}\times\mathbf{H}_i\right\} = \begin{pmatrix} -2\,\mathbf{E}_i(p) & p \text{ inside } B_i \\ 0 & p \text{ outside } B_i \end{pmatrix} \tag{3}$$

$$C_i\left\{\mathbf{n}\times\mathbf{H}_i\right\} - \frac{j}{\omega\mu_i} F_i\left\{\mathbf{n}\times\mathbf{E}_i\right\} = \begin{pmatrix} -2\,\mathbf{H}_i(p) & p \text{ inside } B_i \\ 0 & p \text{ outside } B_i \end{pmatrix} \tag{4}$$

where four function operators are defined, for convenience, as

$$(C_\alpha\,\mathbf{a})\,(p) = \nabla_p \times \int_S \mathbf{a}(q)\; G_\alpha(p,q)\; dS_q \tag{5}$$

$$(M_\alpha\,\mathbf{a})\,(p) = \mathbf{n}(p) \times (C_\alpha\,\mathbf{a}) \tag{6}$$

$$(F_\alpha\, \mathbf{a})\,(p) = \nabla_p \times (C_\alpha\, \mathbf{a}) \tag{7}$$

$$(P_\alpha\, \mathbf{a})\,(p) = \mathbf{n}(p) \times (F_\alpha\, \mathbf{a}) \tag{8}$$

where $\mathbf{a}$ is a tangential vector, S is the boundary surface of the dust particle, $\mathbf{n}$ is an unit normal pointing out of the unit surface into the infinite medium, p is an observation point, q is a source point, B_e is the region outside the scatterer, B_i is the region inside the scatterer, and α = e or i denotes either exterior or interior quantity, respectively. For continuous $\mathbf{a}$, it can be shown that as an external (internal) point p approaches the surface point p

$$\mathbf{n} \times C_\alpha\, \mathbf{a} = \pm\, \mathbf{a} + M_\alpha\, \mathbf{a} \tag{9}$$

where the upper (lower) sign corresponds to p -> p on S from external (internal) region [4]. The boundary conditions on the surface of the scatterer are

$$\mathbf{n} \times \mathbf{E} = \mathbf{n} \times \mathbf{E}_i \tag{10}$$

$$\mathbf{n} \times \mathbf{H} = \mathbf{n} \times \mathbf{H}_i \tag{11}$$

where $\mathbf{E}$ is the total field in the external region (the incident field plus the scattered field) and $\mathbf{E}_i$ is the total internal field. Applying the boundary conditions described in equations (10) and (11) and taking the point p -> p on S, we get

$$(I - M_e)\{\mathbf{n} \times \mathbf{E}\} - \frac{j}{\omega\varepsilon_e} P_e\{\mathbf{n} \times \mathbf{H}\} = 2\, \mathbf{n} \times \mathbf{E}_{inc} \tag{12}$$

$$(I - M_e)\{\mathbf{n} \times \mathbf{H}\} + \frac{j}{\omega\mu_e} P_e\{\mathbf{n} \times \mathbf{E}\} = 2\, \mathbf{n} \times \mathbf{H}_{inc} \tag{13}$$

$$(I + M_i)\{\mathbf{n} \times \mathbf{E}\} + \frac{j}{\omega\varepsilon_i} P_i\{\mathbf{n} \times \mathbf{H}\} = 0 \tag{14}$$

$$(I + M_i)\{\mathbf{n} \times \mathbf{H}\} - \frac{j}{\omega\mu_i} P_i\{\mathbf{n} \times \mathbf{E}\} = 0 \tag{15}$$

Since we are solving for only the tangential components of $\mathbf{E}$ and $\mathbf{H}$ on the surface S, we can define these terms as a set of equivalent current densities capable of radiating the desired fields at points both inside and outside the scatterer. Thus, the magnetic surface current density $\mathbf{M}$ and the electric surface current density $\mathbf{J}$ are defined as

$$\mathbf{M} = -\,\mathbf{n} \times \mathbf{E} \tag{16}$$

$$\mathbf{J} = \mathbf{n} \times \mathbf{H} \tag{17}$$

Equations (12) through (15) now become

$$(I - M_e)\{\mathbf{M}\} + \frac{j}{\omega\varepsilon_e} P_e\{\mathbf{J}\} = 2\,\mathbf{M}_{inc} \tag{18}$$

$$(I - M_e)\{\mathbf{J}\} - \frac{j}{\omega\mu_e} P_e\{\mathbf{M}\} = 2\,\mathbf{J}_{inc} \tag{19}$$

$$(I + M_i)\{\mathbf{M}\} - \frac{j}{\omega\varepsilon_i} P_i\{\mathbf{J}\} = 0 \tag{20}$$

$$(I + M_i)\{\mathbf{J}\} + \frac{j}{\omega\mu_i} P_i\{\mathbf{M}\} = 0 \tag{21}$$

Equations (18) through (21) are four BIEs for the two unknowns **J** and **M**. A variety of ways exist for choosing two equations among the four. One way is to choose two linear combinations of the four equations. In this work, we have adopted the Muller linear combination [5] for the purpose of reducing the strongest (hyper)singularity in the BIEs. Scattered fields at any point p can subsequently be calculated using equations (1) through (4).

The second configuration of this work involves solving for the scattered fields in the presence of a particle near the half space scatterer, and is shown in Figure 2. Numerous approximate approaches for solving this problem have been taken by researchers in the past. The simplest considers the total scattered field as being made up of fields that are directly scattered from the particle plus fields reflected from the half space either before or after (one) interaction with the particle. The approach taken here makes no approximations regarding numbers of interactions. We consider the half-space as a secondary scattering obstacle bounded by the

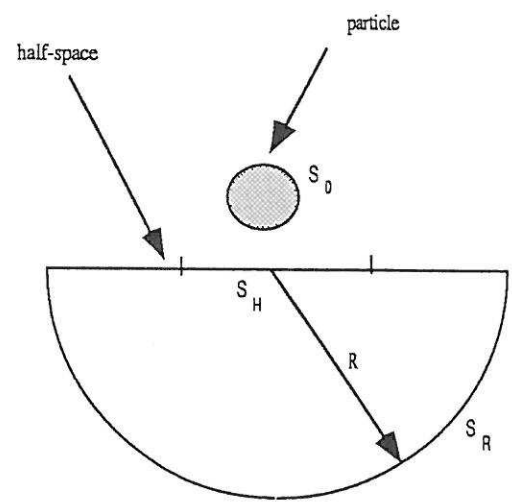

Figure 2. Second Problem Configuration

bowl-shape surface S_R and the top flat surface S_H. Using this technique, the free space Green's function can be used for the half-plane instead of the conventional half-space Green's function where the problems of instability and integration over infinitely many wave numbers are often encountered. Our model considers tthe radius of the bowl, in the limit, to go to infinity. Consequently, the total scattered **E** fields in the external region can be considered to be the sum of three fields.

$$\mathbf{E} = \mathbf{E}_{inc} + \mathbf{E}_{ref} + \mathbf{E}_e \tag{22}$$

where

$\mathbf{E}$ = the total scattered field in the external region
$\mathbf{E}_{inc}$ = the incident (plane) wave
$\mathbf{E}_{ref}$ = the reflected (plane) wave from the half-space in the absence of the particle
$\mathbf{E}_e$ = the scattered wave caused by the interaction between the particle and the half-plane (can be viewed as a perturbation term)

Due to the attenuating nature of the scattered field $\mathbf{E}_e$ with distance from the particle ($\mathbf{E}_e$ satisfies the radiation condition), the problem is formulated with $\mathbf{E}_e$ as the primary dependent variable, instead of the total field **E**. This requires only a finite surface area to be discretized on S_H. Similar remarks hold for $\mathbf{H}_e$ and **H** fields. Consequently, the governing integral equations for this problem are derived for $\mathbf{E}_e$ and $\mathbf{H}_e$ as follows:

$$(I - M_e)|_{S_H}\{\mathbf{M}_{eH}\} + P_e^*|_{S_H}\{\mathbf{J}_{eH}\} + \mathbf{n}(p_H) \times \left[- C_e|_{S_D}\{\mathbf{M}_{eD}\} + F_e^*|_{S_D}\{\mathbf{J}_{eD}\}\right] = 0 \tag{23}$$

$$(I - M_e)|_{S_H}\{\mathbf{J}_{eH}\} - P_e^{\Delta}|_{S_H}\{\mathbf{M}_{eH}\} + \mathbf{n}(p_H) \times \left[- C_e|_{S_D}\{\mathbf{J}_{eD}\} - F_e^{\Delta}|_{S_D}\{\mathbf{M}_{eD}\}\right] = 0 \tag{24}$$

$$(I - M_e)|_{S_D}\{\mathbf{M}_{eD}\} + P_e^*|_{S_D}\{\mathbf{J}_{eD}\} + \mathbf{n}(p_D) \times \left[- C_e|_{S_H}\{\mathbf{M}_{eH}\} + F_e^*|_{S_H}\{\mathbf{J}_{eH}\}\right]$$
$$= (I + M_e)|_{S_D}\{\mathbf{M}_{inc} + \mathbf{M}_{ref}\} - P_e^*|_{S_D}\{\mathbf{J}_{inc} + \mathbf{J}_{ref}\} \tag{25}$$

$$(I - M_e)|_{S_D}\{\mathbf{J}_{eD}\} - P_e^{\Delta}|_{S_D}\{\mathbf{M}_{eD}\} + \mathbf{n}(p_D) \times \left[- C_e|_{S_H}\{\mathbf{J}_{eH}\} - F_e^{\Delta}|_{S_H}\{\mathbf{M}_{eH}\}\right]$$
$$= (I + M_e)|_{S_D}\{\mathbf{J}_{inc} + \mathbf{J}_{ref}\} + P_e^{\Delta}|_{S_D}\{\mathbf{M}_{inc} + \mathbf{M}_{ref}\} \tag{26}$$

$$(I + M_D)|_{S_D}\{\mathbf{M}_{eD}\} - P_D^*|_{S_D}\{\mathbf{J}_{eD}\} = - (I + M_D)|_{S_D}\{\mathbf{M}_{inc} + \mathbf{M}_{ref}\} + P_D^*|_{S_D}\{\mathbf{J}_{inc} + \mathbf{J}_{ref}\} \tag{27}$$

$$(I + M_D)|_{S_D}\{\mathbf{J}_{eD}\} + P_D^{\Delta}|_{S_D}\{\mathbf{M}_{eD}\} = - (I + M_D)|_{S_D}\{\mathbf{J}_{inc} + \mathbf{J}_{ref}\} - P_D^{\Delta}|_{S_D}\{\mathbf{M}_{inc} + \mathbf{M}_{ref}\} \tag{28}$$

$$(I + M_H)|_{S_H}\{\mathbf{M}_{eH}\} - P_H^*|_{S_H}\{\mathbf{J}_{eH}\} = 0 \tag{29}$$

$$(I + M_H)|_{S_H}\{\mathbf{J}_{eH}\} + P_H^{\Delta}|_{S_H}\{\mathbf{M}_{eH}\} = 0 \tag{30}$$

where the superscripts * and Δ represent, respectively, multiplication with constants $\frac{j}{\omega\varepsilon}$ and $\frac{j}{\omega\mu}$.
The subscripts D, H, e, inc, and ref represent, respectively, the particle, the half-space, the external region, the incident, and the reflected quantities. Guideline for a sufficient size and fineness of the surface discretization for the half-space, needed for satisfactory approximation are yet to be determined by numerical experiments.

The problem of adding random surface roughness to the reduced plane surface of the half space is currently under investigation. The results obtained will be reported in subsequent publications.

SIMULATION RESULTS

The scattering cross section is calculated for the first two problem configurations. Numerical results obtained are compared with the analytical Mie theory to validate the program. The vertical axis of the plots represents the scattering cross section and the horizontal axis represent the scattering angle. Also, variables N represents the index of refraction of the scatterer (N=1 is assumed for the external region), ka represents the dimension less frequency and m represents the number of elements used in discretizing the surface. Results obtained for the first configuration indicate an agreement between our solution and the Mie solution are shown in Figure 3. The results for the second configuration are obtained by modeling the half-space as air and compared with Mie solutions. This was done for validation purposes and is shown in Figure 4.

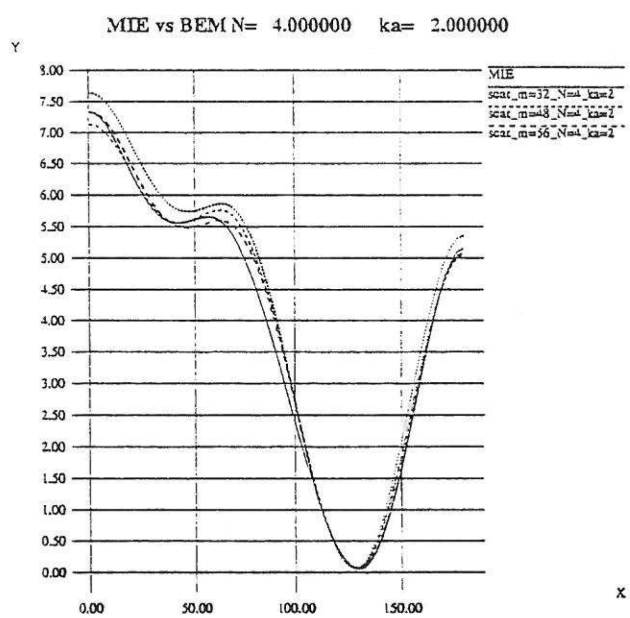

Figure 3. BEM vs. Mie Theory for the first configuration

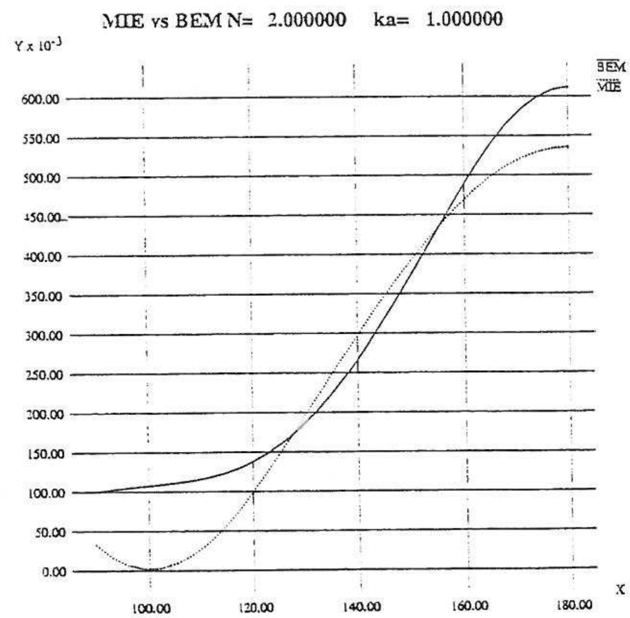

Figure 4. BEM vs. Mie Theory for the second configuration with radius of reduced space = 3ka, m=12

DISCUSSION

The problem of electromagnetic scattering in the presence of a dielectric scatterer resting on a half-space has been considered. The solution to this problem is important in the nondestructive evaluation (NDE) fields, particularly in the semiconductor industry where a forward model of contaminants resting on semiconductor surfaces is needed. Researchers have attacked this problem using several approximate methods. Others have obtained exact solutions but these solutions are limited to certain idealizations and physical restrictions. For the most part, finite element method (FEM) and finite difference method (FDM) have been used but these methods have proven to be computationally prohibitive. An alternative computational method, namely the BEM method, is well suited for this application since it requires discretization (elements) only over the surface of the scatterers and not throughout the indifinite volume. Also, BEM methods can handle objects of arbitrary shape which is generally the case for surface contaminants. This research is believed to be the first full three dimensional Muller combined field formulation for a three-phase electromagnetic scattering problem that can theoretically account for all interactions between the scatterer and the half-space with no physical limitations. This formulation is valid at all frequencies. Also, since a methodology is introduced to regularize both the strongly singular and hypersingular integrals, the approach need not depend on the cancellation of the hypersingularities provided by the Muller linear combination. Finally, quadratic isoparametric boundary elements in three dimensions are used which provide an improvement in computational accuracy over linear elements used by other current electromagnetic scattering work via integral equations. Nevertheless, the problems of interest in this work are still computationally intensive and the major difficulties are associated with the storage capacities and computer speed. These difficulties, however, should be overcome in the future as more computing power becomes available.

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