INTEGRAL EQUATIONS FOR SCATTERING BY A PARTICLE IN A LAYER

Egon Marx
National Institute of Standards and Technology
Gaithersburg, MD 20899

INTRODUCTION

In applications such as the alignment of layers in an integrated circuit or the application of a coating to a surface we may need to determine the light scattered by a dielectric or conducting particle of size comparable to the wavelength in a dielectric layer. We apply the method of the single integral equation to solve this problem and find that the minimum number of required unknown surface fields depends on the geometrical configuration of the system. This method, originally applied to gratings [1], involves the definition of auxiliary fields that coincide with physical fields in one region, obey the same equations everywhere, obey the radiation condition, and satisfy certain boundary conditions involving jumps that are the unknown surface functions in the integral equations. We have applied this method to a number of two-dimensional and three-dimensional configurations [2]-[7], and here we apply it to particles in layers. We find that for certain configurations the number of unknowns exceeds the number of boundaries. We also estimate the memory requirements for such a three-dimensional problem.

TARGET IN A SILICA LAYER

Fig. 1. Particle inside a layer on a substrate.

This is the simplest configuration of this group of problems, shown in Fig. 1. We choose the z-axis normal to the plane interfaces and we assume that the incident wave is plane and monochromatic. We subtract the homogeneous fields that would occur in each region in the absence of the target from the total fields to obtain the scattered fields that obey the radiation condition. We have to determine the reflected magnetic field, $\vec{H}_1^+$, in V_1 , the refracted field, $\vec{H}_3^-$, in V_3 , and the two homogeneous fields, $\vec{H}_2^+$, in V_2 in terms of the incident field $\vec{H}_1^-$. The index + or - indicates the direction of propagation. The electric field of a plane wave is determined from the magnetic field by $\vec{E}_0 = -\vec{k} \times \vec{H}_0 / \epsilon \omega$. To determine the wave vectors, we note that the frequency and the x- and y- components are the same for all waves, that is, we use $\omega^2 = k_j^2 / \epsilon_j \mu_j$ for $j = 1, 2, 3$, while the z-components are determined from $k_{jz}^2 = k_j^2 - k_x^2 - k_y^2$. The amplitudes are determined by the boundary conditions at the interfaces. The twelve components of the magnetic field can be obtained solving the equations

$$H_{0x}^{i+} + H_{0x}^{i-} = H_{0x}^{j-}, \quad i = 1, 2, \quad j = 2, 3, \quad (1)$$

U.S. Government Work Not Protected by U.S. Copyright

$$H_{0y}^{i+} + H_{0y}^{i-} = H_{0y}^{j-}, \quad i = 1, 2, \quad j = 2, 3, \quad (2)$$

$$\kappa_{ji} [k_y(H_{0z}^{i+} + H_{0z}^{i-}) - k_{iz}(H_{0y}^{i+} - H_{0y}^{i-})] = k_y H_{0z}^{j-} - k_{jz} H_{0y}^{j-}, \quad i = 1, 2, \quad j = 2, 3, \quad (3)$$

$$\kappa_{ji} [k_{iz}(H_{0x}^{i+} + H_{0x}^{i-}) - k_x(H_{0z}^{i+} - H_{0z}^{i-})] = k_{jz} H_{0x}^{j-} - k_x H_{0z}^{j-}, \quad i = 1, 2, \quad j = 2, 3, \quad (4)$$

where $\kappa_{ji} = \epsilon_j/\epsilon_i$ which together with $\vec{k}_j \cdot \vec{H}_0^j = 0$, $j = 1+, 2\pm, 3-$ form a set of the required twelve equations.

The auxiliary fields $\tilde{\mathcal{E}}_i$ and $\tilde{\mathcal{H}}_i$, $i = 1, 2, 3$, are equal to the scattered fields in V_1 , V_2 , and V_3 and obey the Maxwell equations with constants ϵ_i and μ_i everywhere. The fields $\tilde{\mathcal{E}}_2$ and $\tilde{\mathcal{H}}_2$ vanish in V_1 and $\tilde{\mathcal{E}}_3$ and $\tilde{\mathcal{H}}_3$ vanish outside of V_3 . Since the region V_4 is finite, the auxiliary fields $\tilde{\mathcal{E}}_4$ and $\tilde{\mathcal{H}}_4$ are equal to the total fields in V_4 and vanish elsewhere. The auxiliary fields are functionals of the unknown surface functions are the tangential components of the jumps $\tilde{\eta}_{ij}$ of the fields $\tilde{\mathcal{H}}_i$ on S_i as shown in Fig. 1, while the $\tilde{\mathcal{E}}_i$ are continuous on those surfaces. The other jumps are obtained [2] from the boundary conditions and the vanishing of the fields give the integral equations

$$\begin{aligned} & \left[\left(\frac{1}{2} + \bar{L}_{21}^{t1} \right) \bar{M}_{11}^{t1} \{ \tilde{\chi}_{11} \} + \bar{M}_{21}^{t1} \left(\frac{1}{2} + \bar{L}_{11}^{t1} \right) \right] \{ \tilde{\chi}_{11} \} - \bar{M}_{22}^{t1} \{ \tilde{\chi}_{22} \} - \bar{M}_{23}^{t1} \{ \tilde{\chi}_{23} \} \\ & = \left(\frac{1}{2} + \bar{L}_{21}^{t1} \right) \{ \hat{n}_1 \times \Delta \bar{E}^{h2} \} + \bar{M}_{21}^{t1} \{ \hat{n}_1 \times \Delta \bar{H}^{h2} \}, \end{aligned} \quad (5)$$

$$\begin{aligned} & \left[\left(\frac{1}{2} + \bar{L}_{32}^{t2} \right) \bar{L}_{21}^{t2} \bar{M}_{11}^{t1} + \left(\frac{1}{2} + \bar{L}_{32}^{t2} \right) \bar{M}_{21}^{t2} \left(\frac{1}{2} + \bar{L}_{11}^{t1} \right) + \bar{M}_{32}^{t2} \bar{L}_{21}^{t2} \left(\frac{1}{2} + \bar{L}_{11}^{t1} \right) + \bar{M}_{32}^{t2} \bar{M}'_{21} \bar{M}_{11}^{t1} \right] \{ \tilde{\chi}_{11} \} \\ & - \left[\left(\frac{1}{2} + \bar{L}_{32}^{t2} \right) \bar{M}_{22}^{t2} + \bar{M}_{32}^{t2} \left(\frac{1}{2} + \bar{L}_{22}^{t2} \right) \right] \{ \tilde{\chi}_{22} \} - \left[\left(\frac{1}{2} + \bar{L}_{32}^{t2} \right) \bar{M}_{23}^{t2} + \bar{M}_{32}^{t2} \bar{L}_{23}^{t2} \right] \{ \tilde{\chi}_{23} \} \\ & = - \left(\frac{1}{2} + \bar{L}_{32}^{t2} \right) \{ \hat{n}_2 \times \Delta \bar{E}^{h3} - \bar{L}_{21}^{t2} \{ \hat{n}_1 \times \Delta \bar{E}^{h2} \} - \bar{M}_{21}^{t2} \{ \hat{n}_1 \times \Delta \bar{H}^{h2} \} \} \\ & - \bar{M}_{32}^{t2} \{ \hat{n}_2 \times \Delta \bar{H}^{h3} - \bar{L}_{21}^{t2} \{ \hat{n}_1 \times \Delta \bar{H}^{h2} \} - \bar{M}'_{21} \{ \hat{n}_1 \times \Delta \bar{E}^{h2} \} \}, \end{aligned} \quad (6)$$

$$\begin{aligned} & \left[\left(\frac{1}{2} + \bar{L}_{43}^{t3} \right) \bar{L}_{21}^{t3} \bar{M}_{11}^{t1} + \left(\frac{1}{2} + \bar{L}_{43}^{t3} \right) \bar{M}_{21}^{t3} \left(\frac{1}{2} + \bar{L}_{11}^{t1} \right) + \bar{M}_{43}^{t3} \bar{L}_{21}^{t3} \left(\frac{1}{2} + \bar{L}_{11}^{t1} \right) + \bar{M}_{43}^{t3} \bar{M}'_{21} \bar{M}_{11}^{t1} \right] \{ \tilde{\chi}_{11} \} \\ & - \left[\left(\frac{1}{2} + \bar{L}_{43}^{t3} \right) \bar{M}_{22}^{t3} + \bar{M}_{43}^{t3} \bar{L}_{22}^{t3} \right] \{ \tilde{\chi}_{22} \} - \left[\left(\frac{1}{2} + \bar{L}_{43}^{t3} \right) \bar{M}_{23}^{t3} + \bar{M}_{43}^{t3} \left(\frac{1}{2} + \bar{L}_{23}^{t3} \right) \right] \{ \tilde{\chi}_{23} \} \\ & = \left(\frac{1}{2} + \bar{L}_{43}^{t3} \right) \{ \hat{n}_3 \times \bar{E}^{h2} + \bar{L}_{21}^{t3} \{ \hat{n}_1 \times \Delta \bar{E}^{h2} \} + \bar{M}_{21}^{t3} \{ \hat{n}_1 \times \Delta \bar{H}^{h2} \} \} \\ & + \bar{M}_{43}^{t3} \{ \hat{n}_3 \times \bar{H}^{h2} + \bar{L}_{21}^{t3} \{ \hat{n}_1 \times \Delta \bar{H}^{h2} \} + \bar{M}'_{21} \{ \hat{n}_1 \times \Delta \bar{E}^{h2} \} \}, \end{aligned} \quad (7)$$

where $\Delta \bar{E}$ and $\Delta \bar{H}$ are differences of homogeneous fields, $\bar{L}$, $\bar{M}$, and $\bar{M}'$ are functionals that give the fields in terms of the jump of the magnetic field [2] and, for instance, $\bar{L}_{ij}^{tm}(\tilde{\chi}_{ij}) = \hat{n}_m \times \bar{L}_{ij}^{tm}(\tilde{\chi}_{ij})$ is a tangential vector functional evaluated on S_m , where $\tilde{\chi}_{ij} = \hat{n}_j \times \tilde{\eta}_{ij}$. We thus have three integral

equations for the three unknown surface fields $\bar{\chi}_{11}$, $\bar{\chi}_{22}$, and $\bar{\chi}_{23}$. We thus have six unknown field components, two per surface, which equals the number of variables required for perfect conductors, one surface current density per surface.

This formulation also applies to a paint coating with particles in a base. The region V_4 can consist of several disconnected subregions for several particles. The use of the model is limited by the size of the memory required to cover all particles and the corresponding parts of the surfaces.

TARGET IN A SILICA LAYER WITH PHOTORESIST

Fig. 2. Particle on the substrate, with a partial top layer.

We now consider the more complicated case depicted in Fig. 2, where a layer of photoresist V_2 covers part of the silica V_3 and the target V_5 rests on the substrate V_4 . The homogeneous fields are determined as before with additional fields in the photoresist.

When a finite region is not isolated, as is the case with a strip on a substrate [3], the definition of the auxiliary fields needs to be modified. This is also the case when a layer does not cover completely the previous one. There is now an additional pair of homogeneous fields in the resist layer, but they are determined by the same method. We define auxiliary fields $\bar{\mathcal{E}}_1$ and $\bar{\mathcal{H}}_1$ that are equal to the scattered fields in V_1 and obey the Maxwell equations with constants ϵ_1 and μ_1 in all space; the electric field is continuous and the magnetic field has jumps $\bar{\eta}_{11}$ across S_1 and $\bar{\eta}_{13}$ across S_3 . The auxiliary fields $\bar{\mathcal{E}}_2$ and $\bar{\mathcal{H}}_2$ are equal to the scattered fields in V_2 and vanish elsewhere. The auxiliary fields $\bar{\mathcal{E}}_3$ and $\bar{\mathcal{H}}_3$ are equal to the scattered fields in V_3 and obey the Maxwell equations with constants ϵ_3 and μ_3 in all space; the electric field is continuous and the magnetic field has jumps $\bar{\eta}_{32}$ across S_2 , $\bar{\eta}_{33}$ across S_3 , $\bar{\eta}_{34}$ across S_4 , and $\bar{\eta}_{35}$ across S_5 . The auxiliary fields $\bar{\mathcal{E}}_4$ and $\bar{\mathcal{H}}_4$ are equal to the scattered fields in V_4 and satisfy the Maxwell equations with the constants ϵ_4 and μ_4 in all space; the electric field is continuous and the magnetic field has jumps $\bar{\eta}_{44}$ across S_3 and $\bar{\eta}_{46}$ across S_6 . The auxiliary fields $\bar{\mathcal{E}}_5$ and $\bar{\mathcal{H}}_5$ are equal to the total fields in V_5 and vanish elsewhere. We note that two boundary functions have been defined on S_3 and S_4 , which increases the memory requirements over the ideal minimum. We have not been able to find a definition of the auxiliary fields that reduces the number of unknown surface fields further to one per surface.

The boundary conditions are now used both to give other jumps in the fields and to obtain integral equations on S_3 and S_4 . The equations that result from the continuity of the tangential fields on S_3 are

$$\bar{M}_{11}^{13} \{\bar{\chi}_{11}\} + \bar{M}_{13}^{13} \{\bar{\chi}_{13}\} - \bar{M}_{32}^{13} \{\bar{\chi}_{32}\} - \bar{M}_{33}^{13} \{\bar{\chi}_{33}\} - \bar{M}_{34}^{13} \{\bar{\chi}_{34}\} - \bar{M}_{35}^{13} \{\bar{\chi}_{35}\} = 0, \quad (8)$$

$$\bar{L}_{11}^{(3)}\{\bar{\chi}_{11}\} + \left(\frac{1}{2} + \bar{L}_{13}^{(3)}\right)\{\bar{\chi}_{13}\} - \bar{L}_{32}^{(3)}\{\bar{\chi}_{32}\} + \left(\frac{1}{2} - \bar{L}_{33}^{(3)}\right)\{\bar{\chi}_{33}\} - \bar{L}_{34}^{(3)}\{\bar{\chi}_{34}\} - \bar{L}_{35}^{(3)}\{\bar{\chi}_{35}\} = 0, \quad (9)$$

where the homogeneous fields do not appear because they cancel when the boundary does not deviate from the plane. There is a similar pair of equations for S_4 . The derivation of the other integral equations remain essentially unchanged and the resulting four equations have the form of (5) to (7). We now have eight integral equations for $\bar{\chi}_{11}$, $\bar{\chi}_{13}$, $\bar{\chi}_{32}$, $\bar{\chi}_{33}$, $\bar{\chi}_{34}$, $\bar{\chi}_{35}$, $\bar{\chi}_{44}$, and $\bar{\chi}_{46}$.

MEMORY REQUIREMENTS

We can estimate the memory requirements for the problem shown in Fig. 1. To solve the integral equations, we use the point-matching method. We cover each surface with patches and compute the values of the surface fields at the center of each patch. We need about ten patches per wavelength λ to obtain accurate results. Thus, for a particle with a radius $n\lambda$, we need about $400\pi n^2$ patches. The scattered fields on the plane interfaces vanish far from the scatterer, which means that on the surface we need patches over two circles of radius $(n+6)\lambda$ for a total of $200\pi[2n^2 + (n+6)^2]$ patches. There are two independent components for each complex surface field, whence there are $400\pi(3n^2 + 12n + 36)$ unknowns. The memory required for the complex matrix of coefficients is then $2.88 \times 10^6 \pi^2 (n^2 + 4n + 12)^2$ words. For $n=1$, this expression gives approximately 8×10^9 words, which is rather large but not out of range for today's computers. A similar analysis for the more complicated problem results in a memory requirement of about 3×10^{10} words.

Numerical experiments can be used to estimate the size of the errors if, for instance, we go from ten patches per wavelength to six, reducing the size of the matrix by a factor of ten. We can also try using larger patches at the edges of the regions on the planes, where the surface fields are small. An out-of-core solver for a linear system of equations would be helpful too. The same functional is used more than once, and one can save computing time by saving them on disk. One then needs memory for a smaller matrix to calculate these functionals and a correspondingly large amount of disk space.

CONCLUDING REMARKS

Three-dimensional problems in the resonance region are marginally within the memory availability of computers when using the method of the single integral equation. It might be possible to reduce the memory requirements of the more complicated problem by a better definition of the auxiliary fields. Approximation of a three-dimensional problem by a two-dimensional one is possible if, for instance, the target resembles a long cylinder. Other approximations are useful when the scatterer is either small or large compared to the wavelength.

REFERENCES

- [1] D. Maystre, "Integral equations" in *Electromagnetic Theory of Gratings*, R. Petit, Ed. Berlin: Springer, 1980.
- [2] E. Marx, "Integral Equation for Scattering by a Dielectric," *IEEE Trans. Antennas Propagat.* **32**, 166-172 (1984).
- [3] E. Marx, "Fields Scattered by a Dielectric Strip on a Dielectric Half-Space," 1987 Int. Symposium Digest Antennas and Propagation, 1138-1141 (1987).
- [4] E. Marx, "Scattering by an Arbitrary Cylinder at a Plane Interface: Broadside Incidence," *IEEE Trans. Antennas Propagat.* **37**, 619-628 (1989).
- [5] E. Marx, "Computed Fields Near the Edge of a Dielectric Wedge," *IEEE Trans. Antennas Propagat.* **38**, 1438-1442 (1990).
- [6] E. Marx, "Radiation Scattered by Two Touching Spheres," 1994 Int. Symposium Digest Antennas and Propagation, 664-669 (1994).
- [7] E. Marx, "Integral Equation for Scattering by a Rough Surface" 1996 Digest of the IEEE Antennas and Propagation Society International Symposium, 462-465 (1996).