Fundamental Limitations on the Use of Open-Region Boundary Conditions and Matched Layers to Solve the Problem of Gratings in Metallic Screens

Babak Alavikia and Omar M. Ramahi

Department of Electrical and Computer Engineering
University of Waterloo, ON, N2L3G1, Canada
balaviki@maxwell.uwaterloo.ca, oramahi@uwaterloo.ca

Abstract **—** Interest in accurate modeling of the electromagnetic wave scattering from grating surfaces has been renewed due to recent advances in the manipulation and localization of the light in novel application of plasmonic resonance. This work briefly reviews the frequency-domain finite methods that have been used extensively to solve the grating problem. Emphasis will be placed on the finite methods that use local boundary operators or matched layers to truncate the computational boundary. It is shown that significant errors can be generated when using either of these two mesh truncation techniques even if the truncation boundaries are receded to avoid any evanescent waves emanating from the gratings. To quantify the error, the solutions obtained using the boundary condition or matched layers are compared to the solutions obtained using either mode matching or the surface integral equation method, both of which are devoid of truncation boundary related approximations and errors. Additionally, limitations on the use of the periodic boundary condition to truncate the mesh for periodic problems are also addressed.

Index Terms **—** Finite element method, global boundary condition, infinite structures, local boundary condition, surface integral equation.

I. INTRODUCTION

Recent advances in manipulation and localization of the light in novel applications of plasmonic resonance such as near-field microscopy, sub-wavelength lithography, surface defect detection, and development of tunable optical filters has renewed interest in accurate modeling of wave scattering from grating surfaces. Several methods such as field decoupling by equivalent magnetic current [1, 2], integral equation [3], and mode matching [4-10] are reported in the literature to solve the problem of scattering from cavities engraved in a metallic screen. Although these methods are powerful, they are not general enough to address cavities with general shapes or cavities having inhomogeneous and anisotropic fillings. In contrast, the methods based on finite mathematics, such as, the finite element method (FEM) and the finite-difference time-domain method (FDTD) are suitable for the problem of scattering from general-shape cavities with anisotropic and inhomogeneous fillings [11-14].

When solving the scattering problem from a bounded target using finite mathematics, it is essential to introduce an artificial boundary to truncate the solution region surrounding the target. Appropriate boundary condition must be imposed on the artificial boundary to guarantee a well-posed and unique solution to the wave equation. In addition, the boundary condition must model the behavior of the wave at infinity. In other words, the artificial boundary must be as transparent as possible for impinging waves from the interior region.

There are two types of boundary conditions to truncate the solution region, viz., (i) non-local or integral type; (ii) local or differential type. Non-local types of boundary conditions are *analytical* integral equations which accurately model the behavior of the wave at the boundaries [15]. Therefore, they are exact for all range of incident angles. In addition, they can be imposed on the boundary which is very close to the scatterer body.

The major drawback of those types of boundary conditions is that they result in dense system matrix, which spoils the sparsity of the FEM system matrix. In contrast, local types of boundary conditions are partial differential equations which *approximate* the exact behavior of the wave at the artificial boundary [16-18].

When solving the problem of scattering from infinite grating surfaces containing multiple cavities using non-local boundary conditions, the solution region can be truncated at the opening of the cavities [11-14]. In [11-14], the domain of the surface integral equation as a boundary constraint is limited to the aperture of the cavities, and, thus, the infinitely extended perfect electric conducting (PEC) walls have no contribution in calculating the boundary condition. On the other hand, a difficulty in truncating the solution region arises when using local boundary conditions or matched layers (typically referred to in the literature as absorbing boundary conditions, ABC, or perfectly matched layer, PML) in solving the problem of scattering from gratings in infinite PEC screens. Since it is impossible to fully enclose the scatterer's geometry by the ABC or PML, the behavior of the scattered field due to the infinite PEC wall outside of the computational domain boundary cannot be modeled properly. Therefore, errors can be generated in the solution when using ABC or PML even if the truncation boundary is receded.

In this paper, we analyzed the performance of commonly used ABC or PML in solving the problem of scattering from grating surfaces containing a single or multiple cavities engraved in an infinite PEC screen. In particular, we focused on the errors introduced in the solution due to grazing incident waves. Next, we analyzed the dependence of this error on the location of the ABC. Finally, we addressed the error when using periodic boundary conditions when solving the problem of scattering from an infinite periodic array of cavities engraved in a PEC screen. The errors were calculated by comparison to the solutions obtained using an FEM-based method where the surface integral equation is used as a boundary constraint [14] and the mode matching technique reported in [7].

II. GENERAL DESCRIPTION OF THE PROBLEM

As a representative example of the problem of scattering from gratings in metallic screens, we consider the problem depicted in Fig. 1 which shows an electromagnetic wave impinging on a cavity engraved in an infinite metallic wall. The solution region can be truncated using the ABC as a local boundary condition as it is shown in Fig. 1.

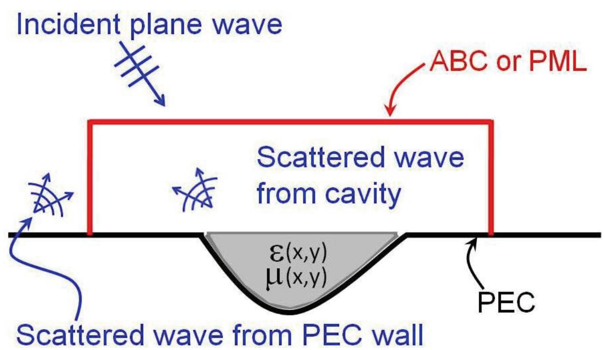

Fig. 1. Schematic of the scattering problem from a cavity with arbitrary shape in an infinite PEC surface. An ABC or PML is used to truncate the computational domain.

Because generic types of ABCs and PMLs are ineffective in absorption of evanescent waves, the introduced error due to these mesh truncation techniques is in general inversely proportional to the distance between the truncation walls and the cavity. Therefore, an ABC or PML cannot be located very close to the cavity. In addition, it is impossible to fully enclose the scatterer's geometry by an ABC or PML. Therefore, the behavior of the scattered field due to the PEC surface that lies outside of the computational domain boundary cannot be modeled properly and thus any consequential physical interaction cannot be included in the solution. In fact, more explicitly, as can be shown in Fig. 1, a portion of the scattered field from the PEC wall propagates into the solution region which causes error that would most likely depend on the incident angle. By increasing the incident angle, more energy is reflected into the solution region by the PEC walls located outside of the ABC, whereas, at zero angle of incidence, the reflected energy from the surface surrounding the cavity does not enter the computational domain depicted in Fig.1.

Therefore, this error is expected to increase as the incident angle increases.

To minimize this error, the domain truncating boundaries should be located far enough from the cavity to enclose a larger segment of the PEC wall in addition to the cavity. However, placing the boundary of the computational domain far from the cavity leads to prohibitive increase in the computational cost, in addition to inaccuracy in the solution due to the exclusion of a large part of the scatterer. The computational cost is most critical when considering cavities whose sizes are several wavelengths, and when loading the cavities to minimize the radar cross-section (RCS), requiring extensive optimizations. Notice, also, that enlarging the computational domain by including a larger segment of the PEC wall while keeping the upper boundary (the horizontal terminating boundary in Fig.1) very close to the PEC wall does not reduce the errors as in such scenario the upper boundary experiences a large concentration of waves incident at oblique angles, which cannot be absorbed effectively by typical PML or ABC methods. There are specialized ABC or PML methods that are designed to absorb waves incident at oblique angles, or even effectively absorb evanescent waves such as in [19, 20]. However, these truncation techniques are specialized and typically add additional computational overhead.

III. NUMERICAL EXPERIMENTS

To study the limitations on the use of ABC or PML to truncate the computational domain for the gratings problems considered in this work, we use the highly robust and widely used full-wave simulator, HFSS [21] which employs a highly effective implementation of PML. We emphasize that the purpose of the comparison is to accentuate the limitations of PML or ABC rather than the effectiveness of the simulator in general. Since the PML implementation in HFSS provides much higher accuracy than the ABC implementation in the same solver, we make comparison to the solution obtained using PML. This solution, henceforth, will be referred to as HFSS-PML. However, in the first example we showed the results obtained using ABC as a benchmark. This solution is referred to as HFSS-ABC. It is important to note that HFSS uses multilayer biaxial anisotropic materials in the PML implementation [22].

Absence of analytical solutions to the problem of scattering from cavities, the solutions generated by two methods will be used for gauging the errors caused by the HFSS-PML or HFSS-ABC solutions. The first method employs the surface integral equation to truncate the computational domain at the aperture of the cavity [14], and the second method employs the mode matching techniques [7]. These two solutions are considered highly accurate in the sense that the approximations used in their respective solution procedures involve discretization of the field rather than any boundary condition approximations.

The solutions presented here are made over a wide range of incident angles. For the transverse magnetic incident plane wave where the electric field vector lies along the axis of the cavities, the error in the magnitude of the total electric field at the aperture of the cavity is calculated as:

$$err = \sqrt{\frac{\int (E - E_0)^2 dl}{\int E_0^2 dl}} \times 100\%. \quad (1)$$

where E is total electric field obtained using the HFSS-PML or HFSS-ABC solutions and E_0 is total electric field calculated using the surface integral equation method reported in [14] (throughout this work we refer to this methods as FEM-TFSIE), or the mode matching technique [7], respectively. The integration domain is the aperture of the cavities.

In the first example, we considered an 0.8λ X 0.4λ (width X depth) rectangular cavity in a PEC sheet where λ is the wavelength in free space. The solution region using HFSS-PML or HFSS-ABC is truncated by a rectangular mesh. The vertical distance of the truncation boundary from the PEC screen is h=1λ and the distance of the lateral truncation walls D from the edge of the cavity is set to be 4λ (see inset of Fig.2). Figure 2 shows the error using the results calculated using FEM-TFSIE and mode matching technique for incident angle range of 0^0-85^0. It is observed that by increasing the incident angle, the error increases in an almost exponential trend. This is because by increasing the incident angle, more reflected waves from the PEC screen outside of the PML or ABC propagate into the solution region. As shown in Fig. 2, the increment trend is uniform in HFSS-PML case while it highly depends on incident angles in HFSS-ABC case for $\theta>30^0$. To validate this reason, we changed the distance of the lateral truncation walls (i.e. D) from the cavity. Figure 3 shows the effect of increasing D on the error for grazing incident angle of $\theta=85^0$. By increasing the D from 4λ to 16λ, the error decreases from 37% to 8% in HFSS-PML case. Notice that to achieve 8% solution accuracy, a computational space of approximately $32\lambda^2$ would be needed when using a PML-based truncation technique; whereas, the solution space using FEM-TFSIE which is confined to the cavity's area, would require a computational domain of $0.32\lambda^2$. (It is important to emphasize here that while approximate computational areas are used to highlight the efficiency and accuracy of the methods discussed here, other aspects of different code implementations are intentionally not discussed here such as the algorithm used to solve the systems matrix, the type of bases functions used in the FEM implementation, ...etc.)

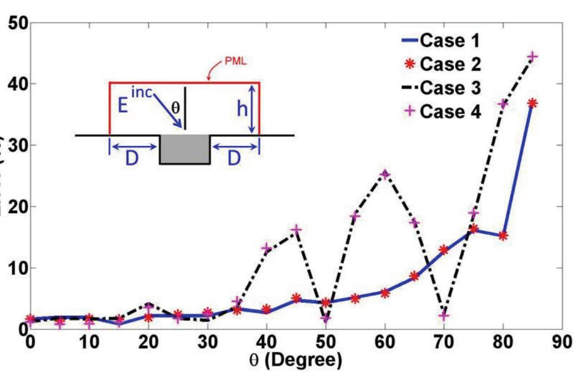

Fig. 2. Error versus incident angle θ for a 0.8λ X 0.4λ air-filled rectangular cavity, TM case, D=4λ, h=1λ. Error between results obtained using: Case1) HFSS-PML and FEM-TFSIE, Case2) HFSS-PML and Mode Matching Technique, Case3) HFSS-ABC and FEM-TFSIE, Case4) HFSS-ABC and Mode Matching Technique.

As a second example, we considered five identical cavities in a PEC screen. The cavities are rectangular with dimension of 0.8λ X 0.4λ and are separated by distance of 0.2λ. The vertical distance of the mesh truncation wall from the PEC screen is h=1λ and the distance of the lateral truncation walls from the cavities is set to be D=4λ (see the inset of Fig. 4). Figure 4 shows the error for incident angle varying from $\theta=0^0$ to $\theta=85^0$. Figure 5 shows the decrease in the cavity field error from 30% to 14% when D is increased from 4λ to 16λ. Notice that despite the excessive computational domain needed when D is increased to 1λ resulting in a computational domain of $37\lambda^2$, the error in the apertures field remains above 10%.

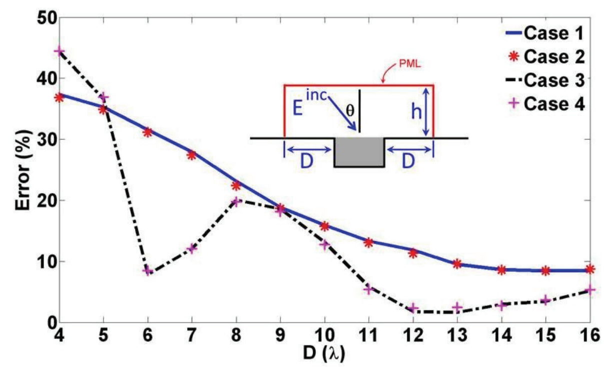

Fig. 3. Error versus distance D of the lateral PML walls from a 0.8λ X 0.4λ air-filled rectangular cavity, TM case, θ=85, h=1λ. Error between results obtained using: Case1) HFSS-PML and FEM-TFSIE, Case2) HFSS-PML and Mode Matching Technique, Case3) HFSS-ABC and FEM-TFSIE, Case4) HFSS-ABC and Mode Matching Technique.

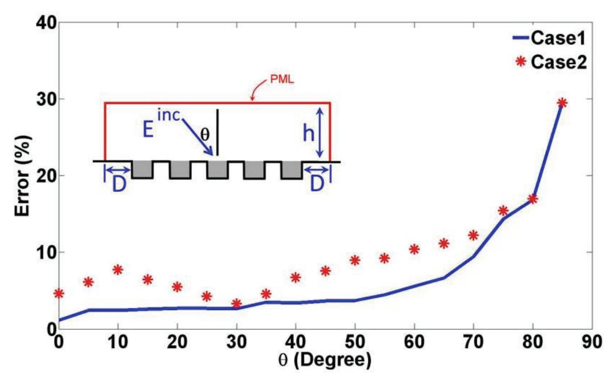

Fig. 4. Error versus incident angle θ for five identical 0.8λ X 0.4λ air-filled rectangular cavities, TM case, D=4λ, h=1λ. The cavities are separated by 0.2 λ. Error between results obtained using: Case1) HFSS-PML and FEM-TFSIE, Case2) HFSS-PML and Mode Matching Technique.

As the final example, we considered an infinite array of identical cavities in a metallic screen. The cavities are rectangular with dimension of 0.8λ X 0.4λ and are separated by a distance of 0.2λ. Therefore, the periodicity of the cavity is P=1λ. Using Floquet theorem, the solution region can be limited to one unit-cell containing one period of the infinite array (see inset of Fig. 6). In the HFSS solution, the periodic boundary condition and the PML are applied on the lateral walls and the top wall of the truncation boundaries, respectively.

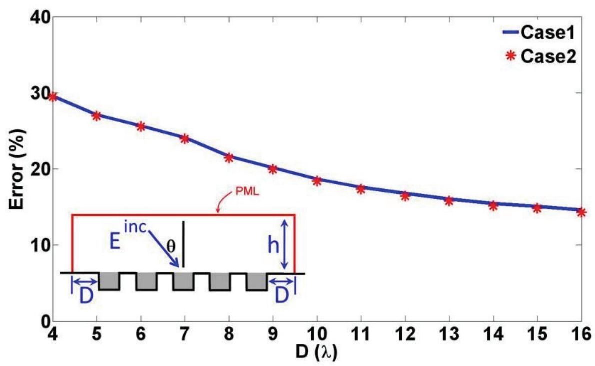

Fig. 5. Error versus distance D of the lateral PML walls from the marginal cavities in an array of five identical 0.8λ X 0.4λ air-filled rectangular cavities, TM case, θ=85, h=1λ. The cavities are separated by 0.2λ. Error between results obtained using: Case1) HFSS-PML and FEM-TFSIE, Case2) HFSS-PML and Mode Matching Technique.

As the final example, we considered an infinite array of identical cavities in a metallic screen. The cavities are rectangular with dimension of 0.8λ X 0.4λ and are separated by a distance of 0.2λ. Therefore, the periodicity of the cavity is P=1λ. Using Floquet theorem, the solution region can be limited to one unit-cell containing one period of the infinite array (see inset of Fig. 6). In the HFSS solution, the periodic boundary condition and the PML are applied on the lateral walls and the top wall of the truncation boundaries, respectively.

We calculated the truncation error in the electric field at the aperture of the cavities in the unit-cell using the results calculated for a finite array of 21 identical cavities with the same dimension using FEM-TFSIE. Figure 6 shows the error for a unit cell containing 1, 3 and 9 cavities for incident angle varying from $\theta=0^0$ to $\theta=85^0$. Notice that changing the size of the number of cavities in the unit cell does not change the physical problem at hand. We observe that by increasing the size of the unit cell to three and nine periods of array (see inset of Fig. 6), the error decreases significantly. We are not in a position to discuss the particular implementation of the periodic boundary condition in HFSS, however, what is quite interesting is that the error in the HFSS solution which directly depends on the periodic boundary condition implemented in HFSS, changes appreciably depending on the number of periods considered.

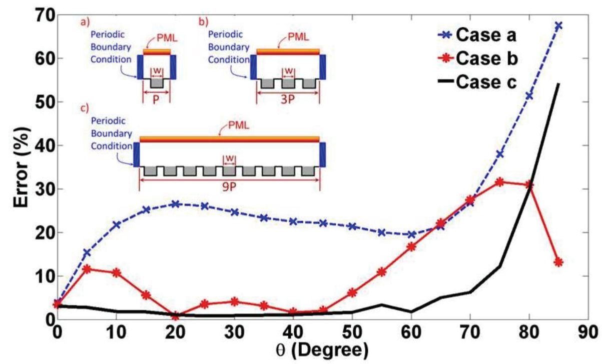

Fig. 6. Error in field calculation versus incident angle θ at the aperture of the center cavity of the unit-cell in an infinite array of identical 0.8λ X 0.4λ rectangular air-filled cavities, TM case. The cavities are separated by 0.2λ. Case a) 1 cavity in a unit-cell, Case b) 3 cavities in a unit-cell, Case c) 9 cavities in a unit-cell. Error between results is obtained using HFSS and FEM-TFSIE.

IV. CONCLUSION

In this study, we highlighted the inherent limitation in truncation the infinite structure using local boundary operators, such as ABC or PML, in context of the problem of scattering from gratings containing a single or multiple cavities engraved in an infinite PEC screen. In fact, we showed that there is an inherent error in the solution due to the truncation of the solution region and ignoring the portion of PEC walls located outside the solution region. Numerical examples of single and multiple cavities engraved in an infinite PEC wall were presented to calculate the error in field computation using PML. The root mean square error in the field computation using PML is calculated with respect to the FEM-based method using a non-local boundary condition and mode matching technique as the accurate solutions. First, we analyzed the error which introduced to the solution due to the grazing incident waves. We showed that the error in the solution due to truncation increases almost exponentially as the incident angle increases. Next, we analyzed the dependence of this error to location of the mesh truncation boundary. We showed that the error decreases by receding the boundary but cannot be eliminated completely while incurring prohibitive increase of computational resources. Finally, we addressed the error in solution while using periodic boundary condition in truncating the solution region into a unit-cell when solving the problem of scattering from an infinite periodic array of cavities engraved in a metallic screen.

REFERENCES

[1] R. F. Harrington and J. R. Mautz, "A generalized network formulation for aperture problems," *IEEE Trans. Antennas Propagt.*, vol. 24, no. 6, pp. 870-873, Nov. 1976.

[2] D. T. Auckland and R. F. Harrington, "Electromagnetic transmission through a filled slit in a conducting plane of finite thickness, TE Case," *IEEE Trans. Microwave Theory Tech.*, vol. 26, no. 7, pp. 499-505, Jul. 1978.

[3] Y. Shifman and Y. Leviatan, "Scattering by a groove in a conducting plane A PO-MoM hybrid formulation and wavelet analysis," *IEEE Trans. Antennas Propagt.*, vol. 49, no. 12, pp. 1807-1811, Dec. 2001.

[4] Y. -L Kok, "Boundary-value solution to electromagnetic scattering by a rectangular groove in a ground plane," *J. Opt. Soc. Am. A,* vol. 9, no. 2, pp. 302-311, Feb. 1992.

[5] T. J. Park, H. J. Eom, and K. Yoshitomi, "An analytic solution for transverse-magnetic scattering from a rectangular channel in a conducting plane," *J. Appl. Phys.*, vol. 73, no. 1, pp. 3571-3573, Apr. 1993.

[6] T. J. Park, H. J. Eom, and K. Yoshitomi, "An analysis of transverse electric scattering from a rectangular channel in a conducting plane," *Radio Science*, vol. 28, no. 5, pp. 663-673, Sep.-Oct. 1993.

[7] T. J. Park, H. J. Eom, and K. Yoshitomi, "Analysis of TM scattering from finite rectangular grooves in a conducting plane," *J. Opt. Soc. Am. A*, vol. 10, no. 5, pp. 905-911, May 1993.

[8] R. A. Depine and D. C. Skigin, "Scattering from metallic surfaces having a finite number of rectangular grooves," *J. Opt. Soc. Am. A*, vol. 11, no. 11, pp. 2844-2850, Nov. 1994.

[9] M. A. Basha, S. K. Chaudhuri, S. Safavi-Naeini, and H. J. Eom, "Rigorous formulation for electromagnetic plane-wave scattering from a general-shaped groove in a perfectly conducting plane," *J. Opt. Soc. Am. A*, vol. 24, no. 6, pp. 1647-1655, Jun. 2007.

[10] M. A. Basha, S. K. Chaudhuri, and S. Safavi-Naeini, "Electromagnetic scattering from multiple arbitrary shape grooves: a generalized formulation," *IEEE/MTT-S International Microwave Symposium*, pp. 1935-1938, June 2007.

[11] J. M. Jin and J. L. Volakis, "TM scattering by an inhomogeneously filled aperture in a thick conducting plane," *IEE Proceedings-H Microwaves, Antennas and Propagation*, vol. 137, no. 3, pp. 153-159, Jun. 1990.

[12] J. M. Jin and J. L. Volakis, "TE scattering by an inhomogeneously filled thick Conducting Plane," *IEEE Trans. Antennas Propagt.*, vol. 38, no. 8, pp. 1280-1286, Aug. 1990.

[13] O. M. Ramahi and R. Mittra, "Finite element solution for a class of unbounded geometries," *IEEE Trans. Antennas Propagt.*, vol. 39, no. 2, pp. 244-250, Feb. 1991.

[14] B. Alavikia and O. M. Ramahi, "Finite-element solution of the problem of scattering from cavities in metallic screens using the surface integral equation as a boundary constraint," *J. Opt. Soc. Am. A*, vol. 26, no. 9, pp. 1915-1925, Sep. 2009.

[15] B. H. Mcdonald and A. Wexler, "Finite-element solution of unbounded field problems," *IEEE Trans. Microwave Theory Tech.*, vol. 20, no. 12, pp. 841-847, Dec. 1972.

[16] B. Engquist and A. Majda, "Absorbing boundary condition for numerical simulation of waves," *Proceeding of the National Academy of Sciences of the United States of America*, vol. 74, no. 5, pp. 1765-1766, May 1977.

[17] A. Bayliss, M. Gunzburger, and E. Turkel, "Boundary condition for the numerical solution of elliptic equations in exterior regions," *Siam Journal On Applied Mathematics*, vol. 42, no. 2, pp. 430-450, Apr. 1982.

[18] O. M. Ramahi, A. Khebir, and R. Mittra, "Numerically derived absorbing boundary condition for the solution of open region scattering problems," *IEEE Trans. Antennas Propagt.*, vol. 39, no. 3, pp. 350-353, Mar. 1991.
[19] O. M. Ramahi, "The concurrent complementary operators method for FDTD mesh truncation," *IEEE Trans. Antennas Propagt.*, vol. 46, no. 10, pp. 1475-1482, Oct. 1998.
[20] J-P. Berenger, "Numerical reflection from FDTD-PMLs: A comparison of the split PML with the unsplit and CFSPMLs," *IEEE Trans. Antennas Propagt.*, vol. 50, no. 3, pp. 258-265, Mar. 2002.
[21] Ansoft HFSS Version 11.2, "Ansoft Corporation," http://www.ansoft.com.
[22] I. Bardi and Z. Cendes, "New directions in HFSS for designing microwave devices," *Microwave Journal*, vol. 41, no. 8, pp. 22, Aug. 1998.

Babak Alavikia received the B.Sc. degree in atomic and molecular physics from Tabriz University, Tabriz, Iran, in 1995, and the M.Sc. degree in the solid state physics, in 1998, from the University of Urmia, Urmia, Iran. He is currently working toward the Ph.D. degree in electrical and computer engineering at university of Waterloo, Canada. Since 2007, he has worked on developing an accurate method to model the electromagnetic scattering from the grating surfaces to study plasmonic resonance and extra ordinary transmission of light through sub-wavelength apertures. His research interests include numerical techniques in electromagnetic and full-wave analysis of electromagnetic scattering in electromagnetic compatibility and interference applications.

Omar M. Ramahi received the BS degrees in Mathematics and Electrical and Computer Engineering (summa cum laude) from Oregon State University, Corvallis, OR. He received his M.S. and Ph.D. in Electrical and Computer Engineering from the University of Illinois at Urbana-Champaign. Presently, he is a Professor in the Electrical and Computer Engineering Department. He holds cross appointments with the Department of Mechanical and Mechatronics Engineering and the Department of Physics and Astronomy. He has authored and co-authored over 240 journal and conference papers. He is a co-author of the book EMI/EMC Computational Modeling Handbook, 2nd Ed. (Springer-Verlag, 2001). Presently, he serves as an Associate Editor for the IEEE Transactions on Advanced Packaging and as the IEEE EMC Society Distinguished Lecturer. Dr. Ramah is an IEEE Fellow.