A Generalized Additional Boundary Condition for Mushroom-Type and Bed-of-Nails-Type Wire Media

Alexander B. Yakovlev, *Senior Member, IEEE*, Yashwanth R. Padooru, *Student Member, IEEE*, George W. Hanson, *Fellow, IEEE*, Arash Mafi, *Member, IEEE*, and Salman Karbasi, *Student Member, IEEE*

***Abstract*—An additional boundary condition (ABC) for mushroom or bed-of-nails metamaterials is generalized for thin 3-D or 2-D material patches or ground planes. It is shown that the usual ABC necessary for the homogenization of these wire-medium metamaterials fails for thin imperfect conductors, and a generalization is presented based on charge conservation. The new ABC leads to results that are in good agreement with full-wave simulations.**

***Index Terms*—Boundary conditions, composite material structures, electromagnetic (EM) analysis, EM modeling, nanostructures.**

I. INTRODUCTION

ARTIFICIAL wire media have been of interest for a long time [1], [2] due to their ability to form a negative permittivity solid-state plasma at microwave frequencies. It was shown in [3] that wire media exhibit strong spatial dispersion, necessitating additional boundary conditions for solving reflection and transmission problems for wire-medium homogenized metamaterials [4]–[6]. Mushroom structures comprised of perfectly conducting patches [7] tend to suppress spatial dispersion [8]–[11], but this is not the case for more general material patches, where charge buildup can occur at the wire-patch interface (as an extreme example, the patch can be transparent, and charge accumulates at the open wire end).

The geometry of a mushroom-type wire medium is shown in Fig. 1, where a TM-polarized plane wave is incident on the structure at angle θ. A bed-of-nails medium is obtained by omitting the patches.

In previous work, the ground plane, vertical wires, and patches have been assumed to be perfect electrical conductors (PECs). Here we assume that the vertical wires are PEC, but that the ground plane and/or the patches are arbitrary thin materials. With $k_0\sqrt{\varepsilon_r}a \ll \pi$ and $a/L > 1$, where k_0 is the free-space wavenumber, ε_r is the relative permittivity of the host medium of the wires, L is the thickness of the slab, and a is the period

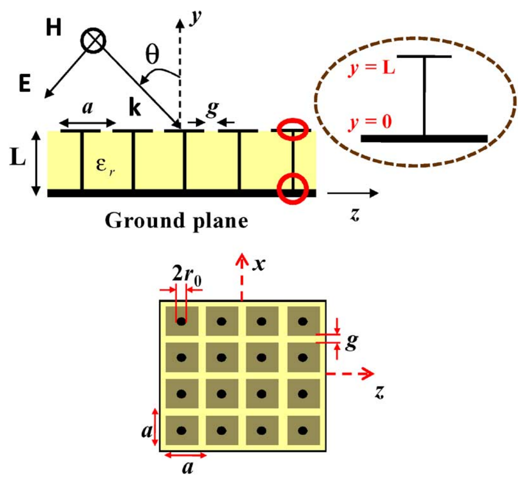

Fig. 1. Mushroom-type wire medium metamaterial. (*top*) Side-view showing incident TM plane wave. (*bottom*) Top view of structure.

of the 2-D lattice of square patches, the wire medium can be replaced with a homogenized, spatially dispersive material slab having thickness L and tensor permittivity $\underline{\boldsymbol{\epsilon}}(\mathbf{q},\omega)$, where $\mathbf{q} = \hat{\mathbf{y}}q$ is a vertical wavenumber [3], [6], [10]. In solving a plane-wave reflection/transmission problem, the presence of spatial dispersion necessitates an additional boundary condition at each material interface (i.e., at each wire termination). The purpose of this work is to present a generalized ABC (GABC) that is valid for wires terminated by an arbitrary, electrically thin material acting as ground plane and/or mushroom patches. We highlight the fact that for such thin metals, or for 2-D surfaces such as graphene, the presented generalization is necessary to obtain correct homogenization results. This was discussed and presented in [12], and here we extend that work by providing the derivation of the new ABC, as well as generalizing to the case of thin-metal patches, a two-sided mushroom configuration, and further comparisons with commercial full-wave codes with new results for the current distribution on the vias.

II. FORMULATION

Referring to Fig. 1, we assume that the wire is thin ($k_0 r_0 \ll 1$) so that we ignore azimuthal variations of wire current, as well as the azimuthal component of wire current. We then have a current density on the wire $J_c = J_c(y)$. Although the structure will support both $\mathrm{TM}^z(E_y, E_z, H_x)$ and $\mathrm{TE}^z(H_y, H_z, E_x)$ modes, we restrict attention to TM^z modes since TE^z modes will not interact with the wires and the resulting homogenized slab is local. Furthermore, in what follows, the term microscopic refers to currents and fields in the microstructure of the medium, i.e.,

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A. B. Yakovlev and Y. R. Padooru are with the Department of Electrical Engineering, The University of Mississippi, University, MS 38677 USA (e-mail: yakovlev@olemiss.edu; ypadooru@olemiss.edu).

G. W. Hanson, A. Mafi, and S. Karbasi are with the Department of Electrical Engineering, University of Wisconsin–Milwaukee, Milwaukee, WI 53211 USA (e-mail: george@uwm.edu; mafi@uwm.edu; karbasi2@uwm.edu).

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on the wires and patches of the actual physical structure. The term macroscopic refers to averaged (homogenized) fields, i.e., the fields in the equivalent homogenized medium.

For the case of an open-ended wire (not terminated by a ground plane or patch), the microscopic ABC for current on the wire is the vanishing of current at the wire end $y = y_0$ [5]

$$J_c(y_0) = 0 \tag{1}$$

or, in terms of macroscopic (homogenized) fields, $\varepsilon_r E_n$ must be continuous at y_0, where ε_r can be step-wise discontinuous at y_0 and E_n is the normal component of homogenized electric field. Equivalent to this is the macroscopic condition [5]

$$k_0 \varepsilon_r E_y(y_0) + k_z \eta_0 H_x(y_0) = 0 \tag{2}$$

where $k_z = k_0 \sin\theta$ is the propagation constant.

For the case where a perfect conductor is present at a wire end (either the ground plane or patch, assuming the patch is sufficiently large to ignore edge effects on the current at the center), the microscopic ABC for wire current is [10]–[13]

$$\left.\frac{\partial J_c(y)}{\partial y}\right|_{y_0} = 0 \tag{3}$$

(e.g., y_0 is 0 or L in Fig. 1) or, equivalently, written in terms of macroscopic fields

$$\left.\left(k_0 \varepsilon_r \frac{\partial E_y(y)}{\partial y} + k_z \eta_0 \frac{\partial H_x(y)}{\partial y}\right)\right|_{y_0} = 0. \tag{4}$$

However, this ABC only applies to a wire–PEC interface. When the skin depth is such that field penetrates throughout the material, the PEC model is a very poor approximation of the actual physics. In this case, we need an ABC for a wire connected to an imperfect conductor, or, more generally, to an arbitrary material characterized by its complex conductivity. The same problem occurs when trying to model the ground plane or patch as a 2-D material, such as graphene or a 2-D electron gas. Below we present the required generalization for electrically thin 3-D and 2-D materials.

The analysis is facilitated by considering a 2-D material having complex surface conductivity $\sigma_{2\mathrm{d}}$ (S). In the event of a sufficiently thin 3-D material having complex conductivity $\sigma_{3\mathrm{d}}$ (S/m), we can write $\sigma_{2\mathrm{d}} = \sigma_{3\mathrm{d}} t$ where $t \ll \delta$ is material thickness and $\delta = \sqrt{2/\omega\mu_0\sigma_{3\mathrm{d}}}$ is skin depth. On the 2-D material, assumed local and isotropic, the microscopic current and field are related as $\mathbf{J}_s(x,z) = \sigma_{2\mathrm{d}} \mathbf{E}_s(x,z)$, where $\mathbf{J}_s$ is the surface current density (A/m) and $\mathbf{E}_s$ is the tangential electric field. The surface charge density ρ_s on a PEC wire is given by $\rho_s(y) = \varepsilon_0 \varepsilon_r E_n(y)$, where E_n is the normal component of microscopic electric field at the wire surface. Then $\rho_s(y_0) = \varepsilon_0\varepsilon_r E_n(y_0) = \varepsilon_0\varepsilon_r E_s = \varepsilon_0\varepsilon_r J_s/\sigma_{2\mathrm{d}}$, where we used the fact that at the wire-material interface y_0 the electric field normal to the wire is tangential to the material (patch or ground plane). In addition, we have the continuity equation for the wire $\rho_s(y) = -(1/j\omega) dJ_c(y)/dy$. Equating the two expressions for surface charge and enforcing continuity of current between the wire and patch, $J_c(y_0) = J_s$, we have the desired generalized additional boundary condition for microscopic wire current

$$J_c(y_0) + \frac{\sigma_{2\mathrm{d}}}{j\omega\varepsilon_0\varepsilon_r} \left.\frac{dJ_c(y)}{dy}\right|_{y_0} = 0. \tag{5}$$

In terms of macroscopic fields,

$$\left.\left(1 + \frac{\sigma_{2\mathrm{d}}}{j\omega\varepsilon_0\varepsilon_r}\frac{\partial}{\partial y}\right)(k_0\varepsilon_r E_y(y) + k_z\eta_0 H_x y)\right|_{y_0} = 0. \tag{6}$$

Equations (5) and (6) are the main results of this paper. The boundary condition is seen to be a balance between the PEC (3) and transparent (1) material cases.

Upon homogenization, the material slab has a tensor effective permittivity [6] $\underline{\varepsilon}_{\mathrm{eff}}(q) = \varepsilon_0\varepsilon_r(\widehat{\mathbf{x}}\widehat{\mathbf{x}} + \varepsilon_{yy}(q)\widehat{\mathbf{y}}\widehat{\mathbf{y}} + \widehat{\mathbf{z}}\widehat{\mathbf{z}})$, where $\varepsilon_{yy}(q) = 1 - \beta_p^2/(k^2 - q^2)$, $k = k_0\sqrt{\varepsilon_r}$, and $\beta_p^2 = (2\pi/a^2)/(\ln(a/2\pi r_0) + 0.5275)$ with β_p being the plasma wavenumber. A TM^z plane wave incident on the homogenized slab with a PEC ground plane excites both transverse electromagnetic (TEM) and TM^z modes, and thus we can write

$$\begin{aligned} H_x(y,z) &= (e^{\gamma_0 y} + R\, e^{-\gamma_0 y}) e^{-jk_z z}, \qquad y > L \\ H_x(y,z) &= (B_{\mathrm{TEM}}\cos(ky) + B_{\mathrm{TM}}\cosh(\gamma_{\mathrm{TM}} y))\, e^{-jk_z z} \end{aligned} \tag{7}$$

$0 \le y \le L$, where $\gamma_0^2 = k_z^2 - k_0^2$, $\gamma_{\mathrm{TM}}^2 = \beta_p^2 + k_z^2 - k^2$. Field amplitudes B_{TEM} and B_{TM} and the reflection coefficient R are to be determined by enforcing the boundary conditions. Assuming that the material patches are replaced by a continuous surface impedance Z_g (discussed below), we enforce the macroscopic two-sided (or sheet) impedance boundary condition $E_z(y = L^-) = E_z(y = L^+) = -Z_g(H_x(y = L^+) - H_x(y = L^-))$. The GABC (6) is enforced at $y = L^-$, and, assuming a PEC ground plane, the ABC (4) is enforced at $y = 0^+$.

The grid impedance is [14], [15]

$$Z_g = \frac{a}{(a-g)\sigma_{2\mathrm{d}}} - j\frac{\pi}{\omega\epsilon_0(\epsilon_r + 1) a \ln\left(\csc\left(\frac{\pi g}{2a}\right)\right)}. \tag{8}$$

The resulting reflection coefficient is

$$R = \frac{K\coth(\gamma_{\mathrm{TM}} L)\cot(kL) - \left(\frac{1}{\gamma_0} + j\frac{\eta_0}{Z_g k_0}\right)}{K\coth(\gamma_{\mathrm{TM}} L)\cot(kL) + \left(\frac{1}{\gamma_0} - j\frac{\eta_0}{Z_g k_0}\right)} \tag{9}$$

where $K = N/D$,

$$\begin{aligned} N = &\left(\frac{1}{\varepsilon_{yy}^{\mathrm{TM}}} - 1\right)\left(\frac{\sigma_{2\mathrm{d}}\gamma_{\mathrm{TM}}}{j\omega\varepsilon_0\varepsilon_r}\tanh(\gamma_{\mathrm{TM}} L) + 1\right) \\ &+ \left(1 - \frac{\sigma_{2\mathrm{d}} k}{j\omega\varepsilon_0\varepsilon_r}\tan(kL)\right) \end{aligned} \tag{10}$$

$$\begin{aligned} D = &-\frac{k}{\varepsilon_r}\left(\frac{1}{\varepsilon_{yy}^{\mathrm{TM}}} - 1\right)\left(\frac{\sigma_{2\mathrm{d}}\gamma_{\mathrm{TM}}}{j\omega\varepsilon_0\varepsilon_r} + \coth(\gamma_{\mathrm{TM}} L)\right) \\ &+ \frac{\gamma_{\mathrm{TM}}}{\varepsilon_r}\left(\cot(kL) - \frac{\sigma_{2\mathrm{d}} k}{j\omega\varepsilon_0\varepsilon_r}\right) \end{aligned} \tag{11}$$

and where $\varepsilon_{yy}^{\mathrm{TM}}(q) = 1 - \beta_p^2/(k_z^2 + \beta_p^2)$. In the limiting case of $\sigma_{2\mathrm{d}} \to 0$, we have the wire medium (bed-of-nails) result [6], and for $\sigma_{2\mathrm{d}} \to \infty$, we have the PEC patch result [10], [11].

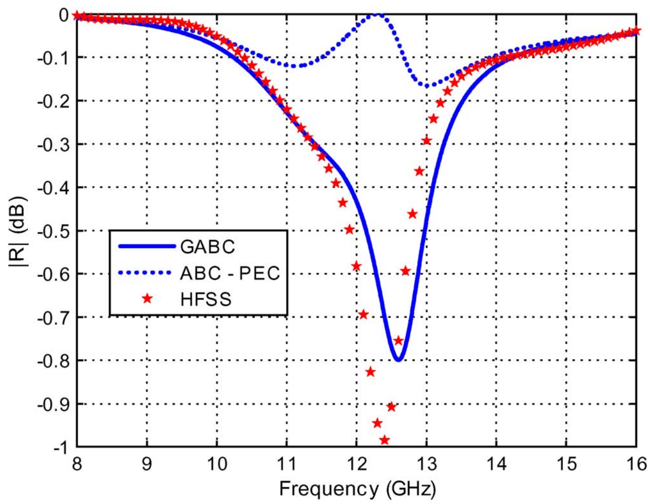

Fig. 2. Reflection coefficient for a TM-polarized incident wave ($\theta = 30^\circ$) when patches are 60-nm-thick copper. The ABC assuming PEC materials fails to reproduce the correct behavior, whereas the new GABC provides the correct result.

III. Results

To verify the new GABC, numerical results will be shown comparing homogenized result (9) with results obtained by a full-wave commercial finite-element simulator (HFSS).[1] In the full-wave simulator, one period of the structure is modeled, and periodic boundary conditions are applied to simulate an infinite structure. The thin metal patch is modeled as a 3-D object with finite bulk conductivity. Referring to Fig. 1, in all results, the period is $a = 2$ mm, the gap size is $g = 0.2$ mm, the wire radius is $r_0 = 0.05$ mm, the substrate thickness is $L = 1$ mm, and the relative permittivity is $\varepsilon_r = 10.2$.

Fig. 2 shows the reflection coefficient for a TM-polarized plane wave incident at 30° to the normal. The patches are copper and have a thickness of 60 nm. It can be seen that the result (9) arising from the GABC is in good agreement with the full-wave HFSS result, whereas the ABC for a PEC patch (4) gives erroneous results (results for a PEC patch showing good agreement with full-wave simulation are given in [10]).

Fig. 3 shows the reflection coefficient (9) for a metal with $\sigma_{3\mathrm{d}}t = 0.058$ S (e.g., $t = 20$ nm and $\sigma_{3\mathrm{d}} = 2.9 \times 10^6$ S/m). It can be seen that the PEC ABC (4) again results in significant errors, whereas the GABC provides the correct response. The slight disagreement between the analytical (GABC model) and full-wave HFSS results is likely due to discretization errors in the finite-element simulator, and could be improved by introducing a highly dense mesh. However, this would require large computational memory and time.

Fig. 4 shows the result for a two-sided mushroom structure (insert) with each patch having $\sigma_{3\mathrm{d}}t = 0.058$ S [the expression for R can be obtained in the same manner as (9)]. Again, excellent agreement for the reflection coefficient is provided by the GABC (top figure), as well as for the transmission coefficient (bottom figure), whereas, as with the previous figures, the ABC assuming PEC materials completely fails to reproduce the correct behavior.

[1]Ansoft Corporation, Pittsburgh, PA. [Online]. Available: http://www.ansoft.com/products/hf/hfss/

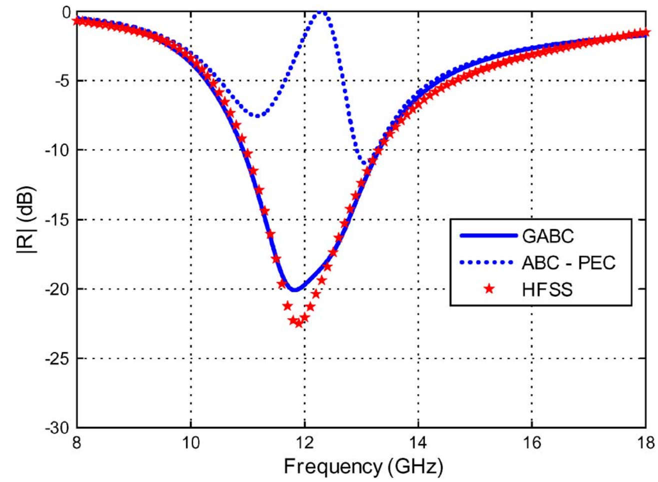

Fig. 3. Same as Fig. 2, but for a material patch having $\sigma_{3\mathrm{d}}t = 0.058$ S.

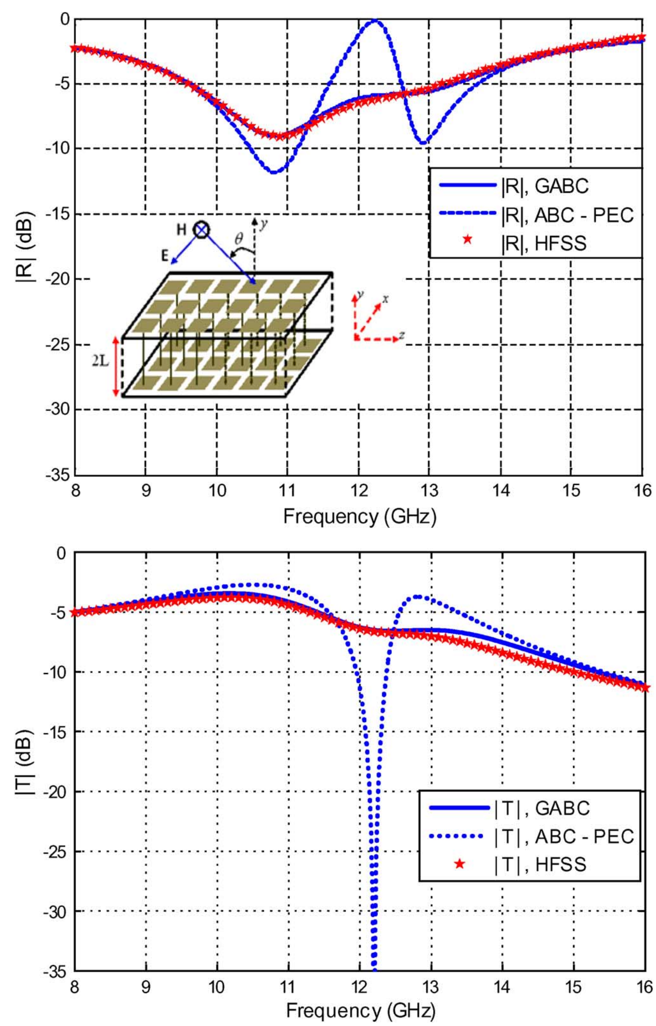

Fig. 4. Reflection (*top*) and transmission (*bottom*) coefficients for a two-sided mushroom geometry (insert). Each patch has $\sigma_{3\mathrm{d}}t = 0.058$ S. The ABC assuming PEC materials fails to reproduce the correct behavior, whereas the new GABC provides the correct result.

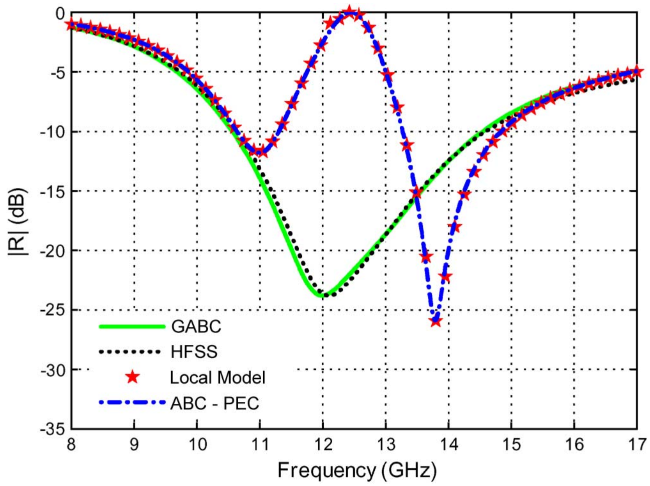

Fig. 5. Reflection coefficient for the one-sided mushroom structure when the patches are graphene. $\theta = 45^{\circ}$.

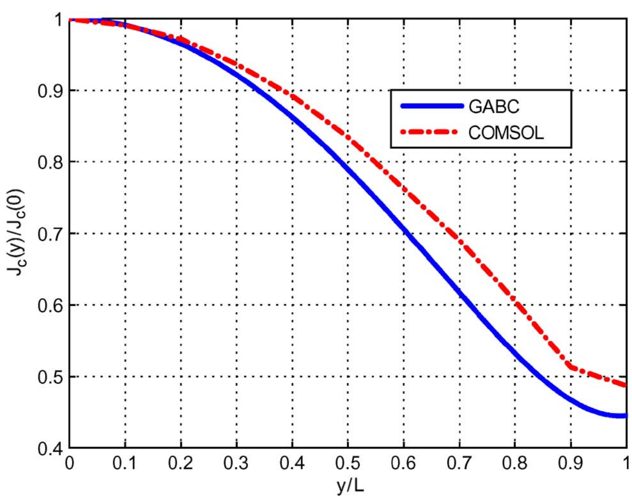

Fig. 6. Normalized wire current for a graphene patch mushroom structure at zero bias, $f = 14$ GHz.

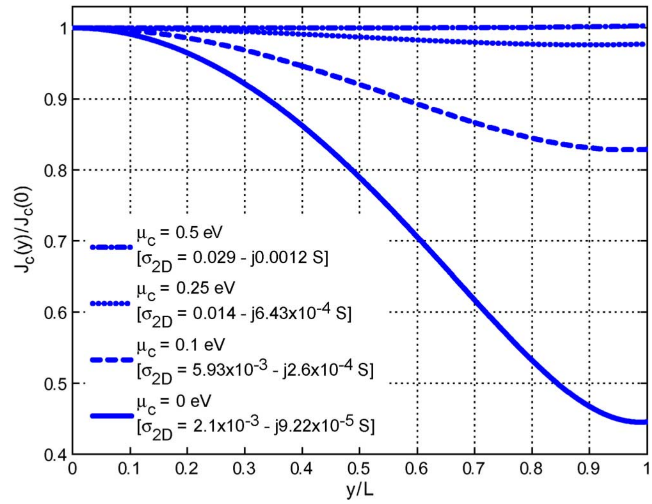

Fig. 7. Normalized wire current for a graphene patch mushroom structure for different values of bias at $f = 14$ GHz.

Fig. 5 shows the reflection coefficient for the one-sided mushroom structure (9) when the patches are graphene, assuming a Drude response and a chemical potential of $\mu_c = 0.5185$ eV (see [16] for the surface conductivity; e.g., at $f = 11.96$ GHz, $\sigma_{2\text{d}} = 0.0304 - j0.0011$ S) and an incident plane wave with $\theta = 45^{\circ}$. Excellent agreement is seen between the GABC and full-wave results. It can be seen that the nonlocal model with the PEC ABC and the local model [10] give erroneous results.

The failure of the ABC that assumes PEC materials is understandable since for the thin metals (or graphene surfaces) considered here, electric fields completely and uniformly penetrate the metal. Therefore, one would not expect the PEC model to be applicable. The new GABC has been derived by accounting for the uniform field behavior in the material. As can be seen from the results comparing the new GABC with full-wave simulation, the presence of a uniform field throughout the thin material has an important role in governing reflection and transmission properties of the homogenized slab. Furthermore, it should be mentioned that with the analytical GABC model results such as shown in these figures are generated essentially instantaneously, whereas the full-wave HFSS simulations take many hours of computation time.

Fig. 6 shows the normalized wire current for a graphene patch mushroom structure at $f = 14$ GHz for zero bias ($\mu_c = 0$ eV, $\sigma_{2\text{d}} = 0.0021 - j0.000092$ S), where a comparison was made with the result of the full-wave commercial simulator COMSOL.[2] It is seen that the GABC provides good agreement with the full-wave simulation.

Fig. 7 shows the normalized wire current on a graphene patch mushroom structure for different values of bias (the zero bias case is repeated from Fig. 6). It can be seen that for zero bias the current is quite nonuniform despite the electrical length of the via being electrically short. This is due to the fact that for this case, the electron density on the patch is relatively low ($\sigma_{2\text{D}}$ is low), and the patch resembles a dielectric more than a metal. As chemical potential is increased $\sigma_{2\text{D}}$ increases, and the current become more uniform, as expected for the patch being a good metal. It is interesting that, despite the uniformity of the current for $\mu_c = 0.5$ eV, as judged from Fig. 7, we still need the GABC rather than the ABC based on a PEC material to obtain the correct (and necessarily nonlocal) homogenization model. In this regard, it is understood that spatial dispersion is important for bed-of-nails type media because one wire end is open, and charge builds up at this point. Upon homogenization, this charge buildup is reflected in the nonlocal slab permittivity. The presence of PEC patches at the wire ends eliminates the charge buildup such that upon homogenization one can use a local slab permittivity [8], [10], [11]. For the case of bias $\mu_c = 0.5$ eV, conductivity is large enough so that the wire current appears nearly uniform, yet the field still completely penetrates the material, necessitating the use of the new GABC.

Referring to Fig. 5, it can be noted that the uniformity of the current for large bias also results in good agreement between the local model and the nonlocal model using the ABC for PEC materials (which would tend to suggest the suppression of spatial dispersion); however, it can be seen that the resulting reflection

[2]COMSOL-Multiphysics, Burlington, MA. [Online]. Available: http://www.comsol.com/

behavior is incorrect, and the GABC with the nonlocal homogenization model is essential in order to obtain the correct results.

IV. Conclusions

In summary, we have presented a generalized additional boundary condition applicable for modeling mushroom or bed-of-nails type metamaterials involving thin 3-D or 2-D conducting materials. We have shown that for this class of materials, the ABC based on the PEC condition yields incorrect results. The new condition was verified using full-wave finite-element commercial simulation codes.

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Alexander B. Yakovlev (S'94–M'97–SM'01) received the Ph.D. degree in radiophysics from the Institute of Radiophysics and Electronics, National Academy of Sciences, Kharkov, Ukraine, in 1992, and the Ph.D. degree in electrical engineering from the University of Wisconsin–Milwaukee, in 1997.

In 2000, he joined the Department of Electrical Engineering, The University of Mississippi, University, i as an Assistant Professor, and became an Associate Professor in 2004. He coauthored *Operator Theory for Electromagnetics: An Introduction* (Springer, 2002). From 2003 to 2006, he was an Associate Editor-in-Chief of the *ACES Journal*. His research interests include mathematical methods in applied electromagnetics, homogenization models for metamaterials, artificial impedance surfaces, and electromagnetic-bandgap structures, theory of leaky waves, and catastrophe and bifurcation theories.

Dr. Yakovlev is a member of URSI Commission B. From 2005 to 2008 he was an associate editor of the IEEE Transactions on Microwave Theory and Techniques. He was the recipient of the Young Scientist Award of the 1992 URSI International Symposium on Electromagnetic Theory, Sydney, Australia, and the Young Scientist Award of the 1996 International Symposium on Antennas and Propagation, Chiba, Japan.

Yashwanth R. Padooru (S'08) was born in Hyderabad, India, in 1985. He received the Bachelors degree in electronics and communication engineering from the Jawaharlal Nehru Technological University, Hyderabad, India, in 2006, the M.S.E.E. degree from the University of Mississippi, University, in 2009, and is currently working toward the Ph.D. degree in electrical engineering at The University of Mississippi.

He is currently a Research Assistant with the Department of Electrical Engineering, The University of Mississippi. His research interests include electromagnetic wave propagation in periodic structures.

George W. Hanson (S'85–M'91–SM'98–F'09) was born in Glen Ridge, NJ, in 1963. He received the B.S.E.E. degree from Lehigh University, Bethlehem, PA, in 1986, the M.S.E.E. degree from Southern Methodist University, Dallas, TX, in 1988, and the Ph.D. degree from Michigan State University, East Lansing, in 1991.

From 1986 to 1988, he was a Development Engineer with General Dynamics, Fort Worth, TX, where he was involved with radar simulators. From 1988 to 1991, he was a Research and Teaching Assistant with the Department of Electrical Engineering, Michigan State University. He is currently a Professor of electrical engineering and computer science with the University of Wisconsin–Milwaukee. He coauthored *Operator Theory for Electromagnetics: An Introduction* (Springer, 2002) and authored *Fundamentals of Nanoelectronics* (Prentice-Hall, 2007). His research interests include nanoelectromagnetics, mathematical methods in electromagnetics, electromagnetic wave phenomena in layered media, integrated transmission lines, waveguides, and antennas, and leaky wave phenomena.

Dr. Hanson is a member of URSI Commission B, Sigma Xi, and Eta Kappa Nu. He was an associate editor for the IEEE Transactions on Antennas and Propagation from 2002 to 2007. He was the recipient of the 2006 S. A. Schelkunoff Best Paper Award of the IEEE Antennas and Propagation Society.

Arash Mafi (M'07) received the Ph.D. degree from the Ohio State University, Columbus, in 2001.

From 2001 to 2005, he was a Research Associate with the Optical Sciences Center, Physics Department, and Arizona Center for Mathematical Sciences, University of Arizona, where he was involved with single-core and multicore double-clad and photonic crystal fiber (PCF) lasers. From 2005 to 2008, he was a Senior Research Scientist with Corning Inc. He is currently an Assistant Professor with the Department of Electrical Engineering and Computer Science, University of Wisconsin–Milwaukee.

Salman Karbasi (S'10) received the B.S. degree in electrical engineering from Yazd University, Yazd, Iran, in 2006, the M.S. degree in electrical engineering (fields and waves) from the Tarbiat Modares University, Tehran, Iran, in 2008, and is currently working toward the Ph.D. degree in electrical engineering at the University of Wisconsin–Milwaukee.

He is currently a Research Assistant with the University of Wisconsin–Milwaukee. His research interests include wave propagation in disordered media and plasmonic grating sensors.