Method of Moment Analysis of Carbon Nanotubes Embedded in a Lossy Dielectric Slab Using a Multilayer Dyadic Green’s Function

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Abstract— Modeling the electromagnetic response of carbon nanotube (CNT) reinforced composites is inherently a 3-D multiscale problem that is challenging to solve in real time for nondestructive evaluation (NDE) applications. This article presents a fast and accurate full-wave electromagnetic solver based on a multilayer dyadic Green’s function approach. In this approach, we account for the effects of the dielectric slab, where the CNTs are embedded, without explicitly discretizing its interfaces. Due to their large aspect ratios, the CNTs are modeled as arbitrary thin wires (ATWs), and the method-of-moment (MoM) formulation with distributed line impedance is used to solve for their coupled currents. The accuracy of the in-house solver is validated against the commercial MoM and the finite element method (FEM) solvers over a broad range of frequencies (from 1 GHz to 10 THz) and for a wide range of dielectric slab properties. Examples of 100 nm-long vertical and horizontal CNTs embedded in a 1 μm-thick lossy dielectric substrate are presented. The in-house solver provides more than 50× speed up while solving the vertical CNT and more than 570× speed up while solving the horizontal CNT than a commercial MoM solver over the GHz-to-THz frequency range.

Index Terms— Arbitrary thin wire (ATW), carbon nanotubes (CNTs), electric field integral equation (EFIE), method of moment (MoM), multilayer dyadic Green’s function, Sommerfeld integrals (SI).

I. INTRODUCTION

OVER the past decade, carbon nanotube (CNT) reinforced composites have been used in a wide range of applications, including automotive and aerospace materials, electromechanical actuation and sensing, packaging,

adhesives, conductive ink, coatings, electromagnetic interference (EMI) shielding, and many more [1]–[5]. The unique carbon atom arrangements of metallic CNTs provide them with a unique high electrical conductivity [1], [2]. The inclusion of a small volume fraction of CNT fillers can produce lightweight, durable, ultrathin, and flexible composites with high dielectric constants [6], [7].

Several factors control the electromagnetic response of CNT composites, such as the spatial distribution of CNTs [8]–[10], CNT volume fraction [11], average length of embedded CNTs [12], [13], interaction among CNTs [13], [14], conductivity of CNTs (single wall/multiwall) [11], [15], waviness of CNTs (nearly straight to highly crumpled) [16], [17], CNT interaction with matrix, matrix properties, and dimensions [18], [19]. Thus, finding an efficient method capable of accurately quantifying the interactions among CNTs, interactions of CNTs with the embedding layers, and with the incident electromagnetic excitation is critical for understanding and optimizing the electromagnetic response of CNT reinforced composites. This will help guiding the process of composite fabrication and monitoring composite health during their service life and check for any structural degradation [5], [20].

To predict the effective permittivity and permeability of composite materials, many theories have been proposed and extended, such as the Waterman–Truell [21]–[24] and Maxwell–Garnett (MG) approximations [25], [26]. These theories are commonly known as the dilute limit effective medium approximation (EMA) theory, which assumes low filler density and operates at a low-frequency range. EMA theories do not incorporate the effects of the finer distribution of the fillers, interaction among fillers when in close proximity, and filler interaction with the embedding matrix. For example, Hassan et al. [27] recently used two independent commercial full-wave solvers, the method-of-moment (MoM)-based FEKO,\textsuperscript{1} and the finite element method (FEM)-based CST Microwave Studio (MWS) to verify that, even at small volume fractions, dilute limit EMA fails to account for the strong interactions between adjacent CNTs and differs significantly

\textsuperscript{1}Certain commercial equipment, instruments, or materials are identified in this article to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Manuscript received 23 June 2021; revised 1 February 2022; accepted 1 March 2022. Date of publication 28 March 2022; date of current version 8 September 2022. This work was supported in part by the National Institute of Standards and Technology (NIST) “Multi-Scale Computational Modeling of Carbon Nanostructure Composites” under Grant 70NANB15H285 and in part by the National Science Foundation for Computer and Information Science and Engineering Research Infrastructure (NSF CRI) “II-NEW: Experimental Characterization and CAD Development Testbed for Nanoscale Integrated Circuits” under Award 1629908. (Corresponding author: Sumitra Dey.)

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Color versions of one or more figures in this article are available at https://doi.org/10.1109/TAP.2022.3161316.

Digital Object Identifier 10.1109/TAP.2022.3161316

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from the full-wave simulations, especially at higher terahertz frequencies [27].

The full-wave electromagnetic analysis ensures the high accuracy of the solution, provided that the system under observation is discretized with adequate size and the number of mesh elements. The main bottleneck in discretizing CNT composites arises due to their multiscale nature. The CNTs are high aspect ratio pipe-like structures whose diameter varies from a few nm to hundreds of nm and length varies from hundreds of nm to several μm. Embedding matrix thicknesses vary from several μm to several mm, and lateral extents may go beyond the cm range. In 1 cm³ composite volume, the number of CNTs may vary from several thousands to billions. Thus, volume/surface discretization of the entire composite structure tremendously increases the computational cost. For example, Wang et al. [8] used finite element analysis (FEA)-based COMSOL Multiphysics software to study the effects of CNT orientation on the resulting relative permittivity of CNT composites. They modeled multiple 600 nm–long CNTs inside a 3-D unit cell (1.5 μm x 1.5 μm x 0.6 μm) and applied periodic boundary condition to simulate the composite. According to that study, the tetrahedral mesh per unit cell increased from 413702 to 1903693 elements when the number of embedded CNTs was increased from 5 to 40 with approximately a 134-fold increase in computational time. Hassan et al. [27] have also discussed the increase in the computational time necessary to accurately simulate a realistic distribution of a large number of 3-D CNTs.

In this article, we propose an alternate full-wave approach for analyzing multiscale CNT composites that reduce the computation time by several orders of magnitude compared to a commercial full-wave solver. The approach studied herein adopts the following strategies.

1) To eliminate the need for volume/surface discretization of the dielectric slab or substrate interfaces, we use a multilayer dyadic Green’s function (DGF) formulation where the substrate is simulated as a finite thickness lossy dielectric slab with infinite lateral extent [28], [29].
2) The embedded high-aspect-ratio CNTs are modeled as 1-D arbitrary thin wires (ATW) and discretized into 1-D segments [13], [16]. This eliminates a huge number of surface/volume mesh elements required for the explicit modeling of 3-D cylindrical CNTs.
3) The ATW CNTs are assigned distributed frequency-dependent complex impedances [30], and their corresponding induced currents are calculated using the MoM based on the electric field integral equation (EFIE) technique [31].

The DGFs are defined for lossy three-layer stratified media, which includes a special class of integrals known as the Sommerfeld integrals (SI) that have no direct analytical solutions [32], [33]. The accuracy and the computational speed of the solver depend directly on the efficiency and accuracy of the SI evaluation method. A large number of different numerical techniques and different contour deformations have been reported to evaluate the SIs associated with the DGFs [34]–[38]. However, this work proposes a modified semianalytical method that enjoys the following salient/novel features.

1) It avoids the requirement to locate the surface wave poles by deforming the contour in the first quadrant. The contour is frequency adaptive semielliptic contour, which allows the technique to be directly applicable to multilayer/multiscale problems.
2) The Bessel/Hankel functions are never approximated for their large arguments, as in [39], and therefore, the proposed computational approach for the multilayer Green’s function applies to arbitrary separation between source and receiver. Thus, our proposed method applies to the coupling between closely-spaced CNTs and mutual coupling between widely spaced CNTs.
3) The SI tail is evaluated in closed forms that circumvents time-consuming slow convergence issues [40]. The closed forms involve Bessel transforms [41], which can be expected to further allow computationally superior forms to be obtained compared to [39].

The in-house full-wave 1-D MoM solver was developed on the MATLAB [42] platform and was validated in two phases. First, the DGFs are validated using an infinitesimal embedded dipole for a vast range of embedding media properties from 1 GHz to 10 THz against the planar substrate solver of FEKO [43]. Next, the absorption power spectrum of horizontal and vertical embedded CNTs is computed using the in-house solver and is validated against the 3-D MoM solver FEKO [43] and the 3-D FEM solver CST MWS [44]. The comparison shows that the in-house solver is more efficient and several orders of magnitude faster than the commercial solvers, which requires explicit discretization of the 3-D CNT surface and/or the interfaces of the dielectric slab. This demonstrates the potential of the in-house solver for real-time interpretation of the scattering measurements typically performed during nondestructive evaluation (NDE) of CNT reinforced composites or any layered composites with wire-like fillers.

II. FORMULATION

The formulation of the proposed full-wave MoM solver is outlined in this section. The problem is defined by electric field integral equations (EFIE) with proper boundary conditions pertaining to the embedded CNTs. Detailed expressions of the dyadic Green’s functions (DGF) are provided, and their solution with a semianalytic approach is discussed. Different interpolation techniques and lookup tables are implemented to reduce the computation time for the MoM matrices.

A. EFIE for Embedded Arbitrarily Thin CNTs

A generic case of a lossy three-layer stratified planar structure is illustrated in Fig. 1, where the CNTs are embedded in layer 2, which has a finite thickness (d) and is backed by two other lossy semi-infinite layers (layer 1 and layer 3). The layered structure is illuminated by a plane wave excitation (Einc) incident on the top of layer 1. The interface between layer 1 and layer 2 is defined by the z = d plane, and the interface between layer 2 and layer 3 is defined by the z = 0 plane. The layers have real values of permittivity εi = ε0ρri, permeability μi = μ0μri, and conductivity σi, where the
layer number is given by \(i\) in layer 2.

![Fig. 1. General planar stratified three-layer structure with embedded CNTs in layer 2.](image)

**PARAMETER RANGE FOR THE MULTISCALE CNT COMPOSITE PROBLEM**

| Physical lengths | \(f = 1\) GHz | \(f = 10\) THz |
|------------------|----------------|----------------|
| free-space wavelength (\(\lambda_0\)) | 0.3 m | 3 \times 10^{-2} m |
| \(|\vec{R} - \vec{R}'|_{\min}\) | 0.033 \(\lambda_0\) | 0.033 \(\lambda_0\) |
| \(|\vec{R} - \vec{R}'|_{\max}\) | 3.33 \(\lambda_0\) | 3.33 \(\lambda_0\) |
| \(d_{\text{min}} = 10\) nm | 6.66 \times 10^{-3} \(\lambda_0\) | 66.66 \(\lambda_0\) |
| \(d_{\text{max}} = 2\) mm | | |

layer 2 experiences multiple reflections and transmissions at top and bottom interfaces and, eventually, sets up an equivalent electric field in layer 2 (\(E_{\text{inc}}^2(\vec{R})\)). When CNTs are present in layer 2, \(E_{\text{inc}}^2(\vec{R})\) will act as an excitation field and induce current (\(I_{\text{cnt}}\)) on the CNT surface, which, in turn, will produce scattering electric fields (\(E_{\text{sc}}^2(\vec{R})\)). The boundary condition that relates the total tangential electric field to the induced axial current on the CNT is given in the following:

\[
\left[ E_{\text{inc}}^2(\vec{R}) + E_{\text{sc}}^2(\vec{R}) \right]_{\text{inc}} = Z_{\text{cnt}} I_{\text{cnt}}.
\]

One needs to solve (1) for every operating frequency to find the value of \(I_{\text{cnt}}\), that is required to compute the absorbed power spectrum of the embedded CNTs in the composite structure. We first compute the scattered electric field (\(E_{\text{sc}}^1(\vec{R})\)) from the CNT surface, which is expressed as [28]

\[
E_{\text{sc}}^1(\vec{R}) = -j \omega \mu_2 \int G^{(23)}_{\text{eo}}(\vec{R}, \vec{R}') \cdot I_{\text{cnt}}(\vec{R}') \, dl
\]

where \(\vec{R}\) is the observation vector (see Fig. 1) that locates the electric field scattering point on the CNT surface. \(\vec{R}'\) is the source vector, which locates the point on the CNT where the unknown axial current \(I_{\text{cnt}}(\vec{R}')\) is excited on an infinitesimal CNT length \(dl\). The integration is computed over the contour length of the CNT (\(l\)). The term \(G^{(23)}_{\text{eo}}(\vec{R}, \vec{R}')\) is the spatial domain electric dyadic Green’s function (DGF) of the third kind defined in layer 2, which will be discussed next.

**B. Spatial Domain DGF**

For a stratified three-layer medium with embedded radiating source, there exists a total of nine electric DGF of the third kind, represented as \(G^{(pq)}_{\text{eo}}(\vec{R}, \vec{R}')\) with \(p, q = 1, 2, 3\), where \(p\) denotes the observation layer and \(q\) denotes the source layer [29]. In our present study, we are interested in analyzing interactions among the buried CNTs in layer 2. Thus, the source points (\(\vec{R}'(\vec{x}', \vec{y}', \vec{z}')\)) and observation points (\(\vec{R}(x, y, z)\)), whether on the same CNT or on two different CNTs, are both located in layer 2 \((p = q = 2)\), as shown in Fig. 1. Thus, out of nine electric DGF, only \(G^{(22)}_{\text{eo}}(\vec{R}, \vec{R}')\) is required to calculate scattering electric fields (\(E_{\text{sc}}^2\)) in layer 2, as declared in (2). Following the method of scattering superposition, \(G^{(22)}_{\text{eo}}(\vec{R}, \vec{R}')\) can be expressed in its generic form as given in [28] and [29]

\[
G^{(22)}_{\text{eo}}(\vec{R}, \vec{R}') = G^{(22)}_{\text{eo}}(\vec{R}, \vec{R}) + G^{(22)}_{\text{es}}(\vec{R}, \vec{R}')
\]

where the first term on the right-hand side denotes the free-space electrical DGF defined in a medium of the same constitutive constants as that of layer 2, and the second term defines the scattered DGF in layer 2. Considering the coordinate system and generic medium properties of Fig. 1, we derived the expression for \(G^{(22)}_{\text{eo}}(\vec{R}, \vec{R}')\), as given in the following. However, for brevity, the intermediate steps are skipped here and can be followed in [28].

For \(z > z'\) in layer 2

\[
G^{(22)}_{\text{eo}}(\vec{R}, \vec{R}') = -\frac{1}{k_2} \sum_{n=0}^{\infty} \frac{j(\delta n - 2)}{4\pi \lambda h_2} \times \left[ M (+h_2) + \rho_2 e^{-2j\lambda h_2} M (-h_2) \right] \times \left[ M' (+h_2) + \rho_2' e^{-2j\lambda h_2} M' (-h_2) \right] \times \left[ \hat{N} (+h_2) + \rho_2' e^{-2j\lambda h_2} \hat{N} (-h_2) \right] + \frac{1}{V} \left[ \hat{N} (+h_2) + \rho_2' e^{-2j\lambda h_2} \hat{N} (-h_2) \right]
\]
and for $z < z'$ in layer 2

\[
\tilde{G}^{(22)}_\varepsilon(\vec{R}, \vec{R}') = -\frac{1}{k_2^2} \sum_{\alpha} 2i \delta(\vec{R} - \vec{R}') + \int_0^\infty d\lambda \sum_{n=0}^{\infty} \frac{j(\delta_0 - 2)}{4\pi i \lambda} h_2 \left[ \frac{\rho_{23} M(\pm h_2) + M(-h_2)}{\sin \phi} \right] \times \left[ M'(\pm h_2) + \rho_{21} e^{-2i h_d} M'(-h_2) \right] + \frac{1}{\rho_{j} \sin \phi} \left[ \tilde{N}'(\pm h_2) + \tilde{N}(-h_2) \right] \times \left[ \tilde{N}'(\pm h_2) + \tilde{N}(-h_2) \right].
\]

(5)

The parameters and functions in (4) and (5) are defined as follows. $\lambda$ is the lateral wave vector in all three layers and also the Fourier–Bessel integral variable, and $h_i$ is the $z$-directed wave vector for the $i$th layer ($i = 1, 2, 3$), which defines the radiation condition

\[
h_i = \begin{cases} \sqrt{k_i^2 - \lambda^2}, & \text{for } \lambda \leq k_i \\ \mp j \sqrt{2^2 - k_i^2}, & \text{for } \lambda > k_i \end{cases}
\]

where the − sign and the + sign in front of the second condition in (6) must be chosen appropriately to identify poles in the top or bottom Riemann sheet, respectively. Condition (6) (if − sign) ensures that the Sommerfeld radiation conditions are obeyed [32]. $M$ and $\tilde{N}$ are the cylindrical wave vector functions, which are solutions to the wave equation in layer 2, describing the TE mode and the TM mode, respectively, and are expressed as [29]

\[
\begin{align*}
M(h_2) &= M_{\varepsilon,n}(h_2) = \nabla \times \left[ J_n(\lambda r) \cos \phi e^{-j h_2 z} \right] \\
&= \left[ \frac{n J_n(\lambda r)}{r} \cos \phi \hat{r} - \frac{\partial J_n(\lambda r)}{\partial r} \cos \phi \hat{\phi} \right] e^{-j h_2 z} \\
\tilde{N}(h_2) &= \tilde{N}_{\varepsilon,n}(h_2) = \frac{1}{k_2} \nabla \times M_{\varepsilon,n}(h_2) \\
&= \frac{1}{k_2} \left[ -j h_2 \frac{\partial J_n(\lambda r)}{\partial r} \cos \phi \hat{r} + \frac{j h_n}{r} J_n(\lambda r) \cos \phi \hat{\phi} \right. \\
&\left. + \lambda^2 J_n(\lambda r) \cos \phi \hat{z} \right] e^{-j h_2 z}
\end{align*}
\]

(7)

where the subscript $\varepsilon$ denotes the even mode and $\phi$ denotes the odd mode. $J_n$ is the Bessel function of order $n$. The primed functions in (4)-(5), $M'$ and $\tilde{N}'$, are the excitation coefficients defined with respect to the source coordinate ($r', \phi', z'$) pertaining to $\vec{R}'$. $M'(\pm h_2)$ and $\tilde{N}'(\pm h_2)$ represent wavelets traveling downward for the TE and TM modes, respectively. Similarly, $M'(-h_2)$ and $\tilde{N}'(-h_2)$ represent wavelets traveling upward for the TE and TM modes, respectively, $\delta_0 = 1$ for the null mode ($n = 0$), and $\delta_0 = 0$ for other modes ($n \neq 0$).

For waves traveling from layer-$i$ toward layer-$j$, their Fresnel’s coefficients of reflection for electric fields at the interface for TE modes and TM modes are given, respectively, as

\[
\rho_{ij} = \frac{\mu_j h_i - \mu_i h_j}{\mu_j h_i + \mu_i h_j}, \quad \rho_{ij}' = \frac{k_2^2 \mu_j h_i - k_1^2 \mu_i h_j}{k_2^2 \mu_i h_i + k_1^2 \mu_j h_j}.
\]

(9)

Finally, the expressions for the terms (1/$\Gamma$) and (1/$\Gamma'$) are given by [29]

\[
\begin{align*}
\frac{1}{\Gamma} &= \left( 1 - \rho_{23} \rho_{21} e^{-2i h_d} \right)^{-1} \\
\frac{1}{\Gamma'} &= \left( 1 - \rho_{23}' \rho_{21}' e^{2i h_d} \right)^{-1}.
\end{align*}
\]

(10a, 10b)

Substituting the expressions of (7)–(10) into (4) and (5) will lead to the final expression for $\tilde{G}^{(22)}_\varepsilon$ in layer 2 for $z \gtrless z'$.

For any arbitrary current distribution with $xyz$ variation, there are nine associated components of $\tilde{G}^{(22)}_\varepsilon$ present in the EFIE, as shown in the following:

\[
\begin{bmatrix}
E_{2x}^i \\
E_{2y}^i \\
E_{2z}^i
\end{bmatrix} = -j \omega \mu_2 \int_j \begin{bmatrix}
G_{x,x} \delta \hat{x} \\
G_{y,y} \delta \hat{y} \\
G_{z,z} \delta \hat{z}
\end{bmatrix} \cdot \begin{bmatrix}
J_{2x} \\
J_{2y} \\
J_{2z}
\end{bmatrix} dl.
\]

(11)

Fig. 2. (a) Horizontal CNT in layer 2 aligned parallel to the x-axis and (b) vertical CNT aligned parallel to the z-axis illuminated by a plane wave excitation polarized in the x-z-plane.

Presently, we are interested in studying horizontal (aligned in x-axis) and vertical (aligned in z-axis) embedded CNTs, as shown in Fig. 2. We choose the $xz$ plane as the plane of incidence for ($\vec{E}_1$ inc) that maximizes the field coupling to the CNTs in Fig. 2. Based on the thin wire approximation, the x-directed horizontal CNT in Fig. 2(a) couples only to the $E_{2x}^i$ component of the excitation field. Other components of $E_{2x}^i$ have no effect on the x-directed horizontal CNT and so do not contribute to the net electric field on the CNT surface, which then simply reduces to

\[
E_{2x}^i(\vec{R}) = -j \omega \mu_2 \int G_{xx}(\vec{R}, \vec{R}') J_{2x}(\vec{R}') dl.
\]

(12)

Similarly, the z-directed vertical CNT in Fig. 2(b) couples only to the $E_{2z}^i$ component of the incident excitation, and thus, the net electric field on the z-directed CNT surface reduces to

\[
E_{2z}^i(\vec{R}) = -j \omega \mu_2 \int G_{zz}(\vec{R}, \vec{R}') J_{2z}(\vec{R}') dl.
\]

(13)

To evaluate the scattered electric fields, we first need to evaluate the DGFs present in integrals (12) and (13). For planar stratified media, the DGFs are laterally invariant, and thus, while deriving $G_{xx}(\vec{R}, \vec{R}')$ and $G_{zz}(\vec{R}, \vec{R}')$ in layer 2, we consider the source point located at $\vec{R}(x' = 0, y' = 0, z')$ and choose an arbitrary observation point $\vec{R}(x, y, z)$. The
expressions are given in the following:

\[
G_{xx}(\mathbf{r}, \mathbf{r'}) = \left[ \begin{array}{c} G^{(2)}(\mathbf{r}, \mathbf{r'}) \\ \frac{1}{h_2} \end{array} \right]_{(0,0,x)} \cdot \hat{x}
\]

\[
= -\frac{j}{4\pi k_z^2} \int_0^{\infty} d\lambda \left\{ \lambda J_0(\lambda r) \sin^2(\phi) + \frac{J_1(\lambda r)}{r} \cos(2\phi) \right\} G_{xx} \quad \text{even} \quad \int_0^{\infty} d\lambda \left\{ \lambda J_0(\lambda r) \cos^2(\phi) - \frac{J_1(\lambda r)}{r} \cos(2\phi) \right\} G_{xx}
\]

where \( \hat{x} = \hat{r} \cos(\phi) - \hat{\phi} \sin(\phi) \) and

\[
G_{xx}^{TE} = \left( \frac{1}{h_2} \right) \left\{ \rho_{23} e^{-j h_2|x-z'|} + e^{-j h_2|x-z'|} \rho_{21} e^{-j h_2|x-z'|} \right\}
\]

\[
G_{xx}^{TM} = \left( \frac{h_2}{1} \right) \left\{ \rho_{23} e^{-j h_2|x-z'|} - e^{-j h_2|x-z'|} \rho_{21} e^{-j h_2|x-z'|} \right\}
\]

\[
\bar{G}_{xx}^{TM} = \left( \frac{h_2}{1} \right) \left\{ \rho_{23} e^{-j h_2|x-z'|} - e^{-j h_2|x-z'|} \rho_{21} e^{-j h_2|x-z'|} \right\}.
\]

The DGFs of (14) and (16) incorporate semi-infinite complex SI [32], which have no direct analytical solutions. Section II-C discusses a semianalytic approach in conjunction with special numerical treatments for efficient SI evaluation.

C. Evaluation of Sommerfeld Integrals With Semianalytic Approach

The generic form of a SI is given in the following [32]:

\[
G(r, z, z') = \int_0^\infty \{ J_n(\lambda r) \lambda^{n+1} \} \bar{G}(\lambda; z, z') d\lambda
\]

which connects the spatial domain Green’s function \( G(r, z, z') \) to its spectral domain counterpart \( \bar{G}(\lambda; z, z') \). The spectral domain Green’s function, \( \bar{G}(\lambda; z, z') \), also known as the layer/medium function, can take specific algebraic forms depending on the precise nature of the problem, such as in (15) and (17). The orders of the Bessel function that survives the derivation from (3) to (17) are \( n = 0, 1, 2 \). \( J_2(\lambda r) \) can be reduced to the lowest order Bessel functions \( J_0(\lambda r) \) and \( J_1(\lambda r) \) by using the recurrence relationship [46].

\[
J_2(\lambda r) = \frac{2}{\lambda r} J_1(\lambda r) - J_0(\lambda r).
\]

The fast and accurate evaluation of the Sommerfeld type integral is a classical problem that still draws a lot of attention from the computational EM community. Several computational techniques have emerged from decades of rigorous research to solve these semi-infinite integrals with competing performances in solution accuracy and computational speed [34]–[36], [38]–[40], [47]–[57]. There exists no such single optimum integration strategy that works well for all types of Green’s function problems. The solution strategy has to be adaptive following the nature of the particular problem in hand [58]. Especially when dealing with a multiscale multilayer problem with a wide frequency range, it becomes necessary to consider several factors that impact the behavior of the spectral domain Green’s function \( \bar{G}(\lambda; z, z') \).

While evaluating SI on the complex \( (\lambda) \) plane, severe numerical problems occur when the source and observation points lie on the same plane. As \( |z - z'| \to 0 \), the numerical integration begins to accumulate round off errors due to severe oscillatory behavior of the integrand induced by the Bessel functions [36], [51], [55].

If \( |z - z'| \neq 0 \), and the integration path stays on the proper Riemann sheet, then the overall integrand may have a fast or slow convergence depending on the distribution of the exponential terms and the lateral separation of source and observation points. In this case, the integration along the semi-infinite \( \mathcal{R}(\lambda) \)-axis still remains challenging, particularly when singularities of the integrand lie on or close to the \( \mathcal{R}(\lambda) \)-axis, such as the case of low-loss layered structures [36], [51], [55].

There are finite numbers of surface wave poles (SWPs) and infinite numbers of leaky-wave poles (LWPs) associated with \( \bar{G}(\lambda; z, z') \) [59]. The number of contributing poles increases with the electrical thickness of the embedding layer or with increasing operating frequency [37], [56], [59]. The pole locations depend on the constitutive parameter values, such as the material properties \( [\varepsilon_i, \mu_i, \sigma_i] \) and layer thickness \( (d) \) [37], [56], [59]. In order to integrate the SI on the \( \mathcal{R}(\lambda) \)-axis, maintaining a high numerical accuracy from near field to far-field calculations, one needs to identify all contributing pole locations accurately and evaluate their residue effects [55]–[57]. This is a very complex iterative time-consuming task that will hinder the goal of fast computation of the MoM matrix especially when the structure is lossy, multiscale, and multilayer.

Fortunately, these poles are dispersed in the shaded strip region, as shown in Fig. 3, confined by the branch points and branch cuts in the lower half-plane (considering all media are right-handed). To obviate the need for pole extraction and residue calculations, we chose to lift the contour of integration over the pole region in the first quadrant of the complex \( (\lambda) \) plane and split the SI into two parts following [38], [52]:

\[
\int_0^\infty \{ J_n(\lambda r) \lambda^{n+1} \} \bar{G}(\lambda; z, z') d\lambda
\]

\[
= \int_0^{k_M} \{ \cdots \} \bar{G}(\lambda; z, z') d\lambda + \int_{k_M}^\infty \{ \cdots \} \bar{G}(\lambda; z, z') d\lambda. \quad (20)
\]

The first finite integral on the right-hand side from 0 to \( k_M \) (with \( k_M \geq \max(\mathcal{R}(k_{1,2,3})) \)) is computed following a deformed contour (see Fig. 3) in the upper half-plane, which avoids all branch points and singularities lying in the fourth
of the reflection coefficients. The first condition of (21) leads in the closed form.

The integrand subtraction appearing in the first integral on the right-hand side of (20), as follows:

$$
\int_{k_M}^{\infty} \left\{ \cdots \right\} \tilde{G}(\lambda; z, z') \, d\lambda \\
\approx \int_{0}^{k_M} \left\{ \cdots \right\} \tilde{G}(\lambda \geq k_M; z, z') \, d\lambda \\
- \int_{0}^{k_M} \left\{ \cdots \right\} \tilde{G}(\lambda \geq k_M; z, z') \, d\lambda.
$$

Substituting (22) into (20) and rearranging terms under similar integration limits, one can obtain the approximate relationship for general numerical evaluation of SI appearing in various classes of multilayer media problems. This relationship reads

$$
\int_{0}^{k_M} \left\{ \cdots \right\} \tilde{G}(\lambda; z, z') \, d\lambda \\
\approx \int_{0}^{k_M} \left\{ \cdots \right\} \left[ \tilde{G}(\lambda; z, z') - \tilde{G}(\lambda \geq k_M; z, z') \right] \, d\lambda \\
+ \int_{0}^{\infty} \left\{ \cdots \right\} \tilde{G}(\lambda \geq k_M; z, z') \, d\lambda.
$$

The integrand subtraction appearing in the first integral on the right-hand side is a key step toward efficient SI evaluation, as it serves two purposes.

1) After subtraction, the resultant integrand in the contour integral \([0, k_M]\) decays faster with \(\lambda\), which accelerates the numerical integration process. Without subtraction, the original integrand for \([0, k_M]\) decays very slowly with \(\lambda\), especially when the source and field points are close to each other (\(d z \to 0\)) and close to an interface between two adjacent layers. In such cases, the exponential terms like \(e^{\mp j \mu d z}\) present in \(\tilde{G}(\lambda; z, z')\) approach 1 and do not decay with increasing \(\lambda\) [51].

2) The SI tail integration limit is now modified to \((0, \infty)\), which eases the search for an exact closed-form expression for the SI tail using the Fourier–Bessel transform relationships given in [41].

It is important to note that, unlike [39] and [47], the present method does not approximate the Bessel terms of (14) and (16) while searching for closed-form expressions for the SI tails. Asymptotic approximation of the Bessel/Hankel functions enhances inaccuracies for small separation between source and observation. The above techniques are unjustified for CNTs that have source points in nm scale proximity of observation points (\(k r \approx 10^{-8}\) at 1 GHz). Thus, in the present method, the asymptotic condition (21) is imposed only on the spectral domain Green’s functions of (15) and (17). For \(\lambda \geq k_M\), we first substitute (21) into (10) and expand it into power

\[\lim_{\lambda \to \infty} \begin{cases} h_1 \approx h_3 \approx h_2 = -j\sqrt{\lambda^2 - k^2} \\ p_{ij} \approx q_{ij} = \frac{\mu_j - \mu_i}{\mu_j + \mu_i}; \quad p'_{ij} \approx q'_{ij} = \frac{k^2_j \mu_i - k^2_j \mu_j}{k^2_j \mu_i + k^2_j \mu_j} \\ \tilde{G}(\lambda; z, z') \approx \tilde{G}(\lambda \geq k_M; z, z') \end{cases} \]

where \(q_{ij}\) and \(q'_{ij}\) become independent of the integration variable \(\lambda\) and are indeed the low-frequency approximation of the reflection coefficients. The first condition of (21) leads to more accurate asymptotic approximation for \(\tilde{G}(\lambda; z, z')\) compared to what was reported in [51]. Arnautovski-Toseva and Greve [50] used a similar approximation but neglected the entire contour integration contribution so that their approach was restricted only to the low frequency regime (\(\omega \to 0\)). In contrast, our approach is full-wave and works accurately from low frequency through tens of THz.

Fig. 3. Semianalytical approach for SI evaluation. The semielliptic contour deformation skips the region containing the integrand singularities lying in the range \(k_0 \leq \lambda \leq k_{\text{max}}\). The tail part of the SI \((k_M \leq \lambda \leq \infty)\) is evaluated in the closed form.
series as follows:
\[
\frac{1}{\Gamma} \approx \left( 1 - \varrho_{21} \varrho_{23} e^{-2d \sqrt{(z^2 - k_x^2)}} \right)^{-1}
\]
\[
\approx \sum_{n=0}^{\infty} \left( \varrho_{21} \varrho_{23} e^{-2d \sqrt{(z^2 - k_x^2)}} \right)^n
\]
\[
\frac{1}{\Gamma} \approx \left( 1 - \varrho_{21}' \varrho_{23}' e^{-2d \sqrt{(z^2 - k_x^2)}} \right)^{-1}
\]
\[
\approx \sum_{n=0}^{\infty} \left( \varrho_{21}' \varrho_{23}' e^{-2d \sqrt{(z^2 - k_x^2)}} \right)^n.
\]  
(24a)

(24b)

Similarly, by inserting (26) into (16), we get
\[
G_{zz}(\vec{R}, \vec{R}') \approx \frac{1}{k_z^4} \delta(\vec{R} - \vec{R}') + \left( G_{zz}^{TM \text{ contour}} + G_{zz}^{TM \text{ closed}} \right)
\]
\[
G_{zz}^{TM \text{ contour}} = -\frac{j}{4\pi k_z^2} \int_{0}^{k_M} \left\{ \lambda J_0(\lambda r) \right\} \left[ G_{zz}^{TM} - \tilde{G}_{zz}^{TM} \right] d\lambda
\]
\[
G_{zz}^{TM \text{ closed}} = -\frac{j}{4\pi k_z^2} \int_{0}^{\infty} \left\{ \lambda J_0(\lambda r) \right\} \tilde{G}_{zz}^{TM} d\lambda.
\]  
(28)

In (27), we find two finite and two infinite integrals, whereas, in (28), there is one finite and one infinite integral. All these integrals include infinite series in their integrands coming from the \( \tilde{G} \) terms. However, the infinite series can be truncated to a finite series without losing accuracy by judiciously choosing a sufficiently large value of \( n \). In our present study, we use \( n = 500 \) to eliminate any cumulative approximation error in the MoM calculation. However, this is not an ultimate value of \( n \) and can be optimized to reduce the SI tail computation time while maintaining required solution accuracy. As indicated by the subscripts, the finite integrals \( G_{xx}^{TE \text{ contour}}, G_{xx}^{TM \text{ contour}}, \) and \( G_{zz}^{TM \text{ contour}} \) and \( G_{zz}^{TM \text{ closed}} \) are computed numerically by integrating over the semielliptical contour. In this case, each \( \tilde{G} \) is computed first as a finite series up to \( n \)th terms and then subtracted from \( \tilde{G} \) giving the resultant spectral domain Green’s function, which is then multiplied with Bessel terms followed by contour integration. For the infinite integrals, \( G_{xx}^{TE \text{ closed}}, G_{xx}^{TM \text{ closed}}, \) and \( G_{zz}^{TM \text{ closed}} \), fortunately no integration is needed as we find exact closed-form solutions from [41] using the Fourier-Bessel transform relationships, as listed in Appendix B. To do so, we move the summation operator in front of the integration. This step is valid since the summation coefficients \( b_{mn}, c_{mn} \), and \( d_{mn} \) are independent of the spectral variable \( \lambda \). This step allows us to express \( G_{xx}^{TM \text{ closed}} \) as a sum of exponential terms by using the Sommerfeld identity (B.1) and its derivative (B.2). Similarly, we can express \( G_{xx}^{TM \text{ closed}} \) as a sum of exponential terms by using the identities (B.3) and (B.4). \( G_{zz}^{TM \text{ closed}} \) is expressed as a sum of exponential terms by using (B.5).

As we, now, have the closed-form solutions for the SI tails in (27) and (28), we, finally, turn our attention to evaluate the finite integrals over the semielliptical contour in the upper half of the complex \( \lambda \) plane. As depicted in Fig. 3, we first transform the finite integrals from \( \lambda : [0, k_M] \) space to \( \alpha : [0, \pi] \) space by applying the following semielliptic relations:
\[
\lambda = a - a \cos \alpha + j b \sin \alpha
\]
\[
d\lambda = a \sin \alpha + j b \cos \alpha
\]
\[
\frac{d\alpha}{d\lambda} = a \sin \alpha + j b \cos \alpha
\]  
(29)

where \( a = (k_M/2) \) is the semimajor axis and \( b \) is the semiminor axis of the semielliptic contour. The value of \( k_M \), or the major axis length, should be large enough to skip any singularities near the path of integration and also ensure the validity of the asymptotic condition (21). The minor axis height \( b \) dictates the convergence of the integrands, which are highly oscillatory along the \( \Re(\lambda) \)-axis and exponential along the \( \Im(\lambda) \)-axis [55]. A large value of \( b \) will cause both \( J_0(\lambda r) \) terms to diverge. Reducing \( b \) significantly can bring the contour down to the vicinity of singularities lying close to or on the \( \Re(\lambda) \)-axis [36], [55]. Thus, an optimal choice of
TABLE II
CONTROLLING MINOR AXIS HEIGHT (b)

| Reference          | Choice of b                                                                 |
|--------------------|------------------------------------------------------------------------------|
| [37], [38]         | \( b = \left\{ \begin{array}{ll} k_0 \times \min \left( 1, \frac{1}{k_0 r} \right) & \text{for } r > |z-z'| \\ k_0 & \text{for } r \leq |z-z'| \end{array} \right. \) |
| [36], [51]         | \( b = 10^{-3} \times 1.2 \times \max \{\text{Re}(k_z)\} \) \( = 10^{-3} \times 1.2 \times \text{Re}(k_z) \) |
| This work          | \( b = \left\{ \begin{array}{ll} 20 \text{ m}^{-1} & \text{for } 1 \text{ GHz} \leq f \leq 2 \text{ THz} \\ 10 \times \frac{f}{10 \text{ THz}} \text{ m}^{-1} & \text{for } 2 \text{ THz} < f \leq 10 \text{ THz} \end{array} \right. \) |

| Value of b         | \( f = 1 \text{ GHz} \) | \( f = 10 \text{ THz} \) |
|--------------------|------------------------|------------------------|
| \( r = 0.61 \text{ nm} \) | 20.95                  | 2.09 \times 10^5       |
| \( r = 1 \text{ cm} \) | 20.95                  | 2.09 \times 10^5       |

Considering \( \varepsilon_r = 10, \mu_r = 1, \sigma = 1 \text{ S/m} \). Air for layer1 and layer3.

\( b \) that minimizes the effect of the poles and the oscillations of the Bessel function should be somewhere in between these two extreme limits. A few studies can be found in this context, which discuss how to control the semiminor axis height and are given in Table II. However, none of these guidelines are fully compatible for a GHz-to-THz frequency range and nm to cm lateral range of operation. As shown in Table II, if we follow [37], [38], at 10 THz, the value of \( b \) will become too large, and the integrand will diverge. If we follow [36], [51], at 1 GHz, the value of \( b \) will become too small, and the contour will come very close to the \( \text{Re}(\lambda) \)-axis, at 10 THz, the value of \( b \) will be large enough to cause the integrand to diverge. Thus, in our present study, we propose a new adaptive contour height that is suitable for our multiscale scenario (see Table I). The contour height variation with frequency is shown in Fig. 4, and the relation is given in the last row in Table II. The contour maintains a constant low value of \( b \) as long as the operating frequency lies below 2 THz. Further increase in frequency enhances the effects of singularities near the \( \text{Re}(\lambda) \)-axis, and it becomes necessary to push the contour further into the upper half-plane. This is unavoidable because with increasing frequency layer 2 becomes electrically thick and more higher order poles pop up near \( \text{Re}(\lambda) \)-axis. Thus, eventually, \( a \) and \( b \) are increased to avoid the effects of singularities. This effect is more concerning when the source is close to an interface as it induces convergence problems. Our proposed choice of \( b \) has been tested for all possible scenarios of operating frequency, physical length, and material properties given in Table I. The validation results will be shown in Section III.

D. MoM-ATW for Embedded CNTs

The calculated scattered electric field value \( \bar{E}_s^2(\bar{R}) \) is inserted into the \( E \)-field boundary condition on the CNT surface (1) to solve the unknown current density flowing axially in the ATW CNT \( \hat{I}_{\text{cnt}} \). We first assume that the individual ATW CNT structure is subdivided into multiple number of connected small segments \( S \), and (1) is solved for each of these segments. The unknown \( I_{\text{cnt}} \), thus, can be approximately expressed as a linear weighted summation of

\[ \bar{I}_{\text{cnt}} \approx \sum_{n=1}^{N} I_n \bar{f}_n(\bar{R}) \] (30)

where \( I_n \) is the unknown weighting current coefficient for the \( n \)th triangular basis \( \bar{f}_n \) that expands over \( n \)th and \( (n+1) \)th segments [31]. To satisfy the ATW condition with reasonable accuracy, the discretization should be optimized. At least 20 segments per wavelength are desired, but individual segment length should not fall below twice the diameter of the CNT [13], [16]. This sets an upper and lower limit on the choice of segment number \( (S) \)

\[ \frac{20 l}{\lambda} < S < \frac{l}{4 r_{\text{cnt}}} \] (31)

Substituting (30) into (1) results in a matrix equation as given in the following, which needs to be solved for each operating frequency [31]

\[ [Z]_{N \times N} [I]_{N \times 1} = [V]_{N \times 1}. \] (32)

On the right-hand side, \( V = [\bar{E}_2^{\text{inc}}(\bar{R})]_{\text{tan}} \) is the tangential \( E \)-field component of the incident excitation that couples to the CNT. On the left-hand side, \( Z \) is the resultant complex impedance matrix, also known as the MoM impedance matrix. To find \( Z \), we have followed the procedure described in [31]. We first set the right-hand side of (1) to zero, which gives
us the solution of the impedance matrix of a perfect electric conductor (PEC) wire. Next, we add the distributed line impedance value of CNT ($Z_{cnt}$) along with the diagonal elements of the PEC impedance matrix calculated in the previous step. Imposing the right impedance condition along the thin wire structure is the key step that differentiates the CNT electromagnetic response from that of a similar PEC wire. The total axial current ($I_{cnt}$) flowing in the CNT is determined by solving the matrix equation (32). Once the current is solved, we can finally calculate the total extinction power ($P_{ext}$), absorbed power ($P_{abs}$), and scattered power ($P_{scat}$) for the embedded CNTs following the given relations [13]

$$P_{ext} = 0.5 \Re(e^{\int_0^l I_{cnt} \cdot E_{inc} (\vec{R}) \, dl})$$
$$P_{abs} = 0.5 \int_0^l |I_{cnt}|^2 \Re(Z_{cnt}) \, dl$$
$$P_{scat} = P_{ext} - P_{abs}$$

where the $^\dagger$ notation refers to conjugate transpose. For PEC and conventional metals, such as gold, silver, or aluminum, $P_{scat}$ dominates over $P_{abs}$, whereas conductors with complex conductivity, such as the CNTs, show higher values of $P_{abs}$ compared to $P_{scat}$. The resonant peaks found in the absorption power spectrum have various applications in CNT-based nanosensing platforms.

Filling the impedance matrix $[Z]_{N \times N}$ in (32) is a time-consuming task. To give an idea, the matrix size or the number of bases ($N$) may range from tens (for a single CNT) to several thousand (for a cluster of CNTs). For more accurate numerical integration, we have subdivided each basis into 64 Legendre–Gauss quadrature points. Thus, to calculate $[Z]_{N \times N}$ for a single operating frequency, one needs to compute the source observation interactions for $64 \times N \times 64 \times N$ times. However, considering the source observation reciprocity and lateral invariance properties of Green’s function of multilayered structures, we can reduce the burden of repetitive calculations. To accelerate the filling of $[Z]_{N \times N}$, we have adapted different interpolation and lookup table (LUT) strategies. In general, if all other constitutive parameter values remain constant, then a spatial domain Green’s function $G(r, z, z')$ needs a 3-D LUT for varying lateral separation between source and observation points ($r$), the observation height ($z$), and the source height ($z'$). For a horizontal CNT, $z$ and $z'$ are fixed, and thus, for $G_{zz}$, a 1-D LUT with varying $r$ is sufficient. However, for a vertical CNT, only $r$ is fixed; thus, for $G_{xx}$, a 2-D LUT with varying $z$ and $z'$ is required. In our present study, an LUT is built only for the contour integration part of the SI, which is otherwise a laborious task, especially at THz frequencies. Spline interpolation is used to populate the contour integration LUT for intermediate locations between the node points. The closed-form expressions for the SI tail are easy to compute and require minimal time; thus, no separate LUT was used for them. For the self-terms (diagonal entries in $[Z]$ matrix) and terms adjacent to them, which, inherently, have a large order of magnitude, their closed parts are filled by exhaustive calculations. Source and observation bases that are at least a segment apart are filled by a $5 \times 5$ spline interpolation for each segment consisting of $32 \times 32$ Legendre–Gauss quadrature points. This strategy ensures the high accuracy of the full-wave solver and, at the same time, maintains a fast computing speed. Details of the computational speed and accuracy of the solution compared to commercial solvers are discussed in the following sections.

**III. ELECTRIC FIELD EVALUATION AND VALIDATION**

We first demonstrate the validity of the Green’s function formulated in (27) and (28). We consider an $x$-directed HED (horizontal electric dipole) and $z$-directed VED (vertical electric dipole) of the unit magnitude current embedded in a lossy dielectric slab, as shown schematically in Figs. 5(a) and 5(a), respectively. The dielectric slab is $d = 2\text{ mm}$ thick and is backed by air ($\varepsilon_{r1, 3} = 1$, $\mu_{r1, 3} = 1$, and $\sigma_{1, 3} = 0 \text{ S/m}$) on either side. The electric dipoles are placed $\delta z = 0.25\text{ mm}$ below the top interface. The dominant electric field $E_{z}$ for $x$-directed HED is computed directly following (12), which
is nothing but $G_{zz}$ multiplied with a factor of $(-j\omega \mu_2)$. Similarly, the dominant electric field $E_{zz}$ for $z$-directed VED is computed directly following (13), which is actually $G_{zz}$ multiplied with a factor of $(-j\omega \mu_2)$. The dominant field components are shown specifically as they will be required to solve the embedded $x$-directed and $z$-directed CNTs of Fig. 2. The in-house field calculations are validated against the results generated by the FEKO planar multilayer substrate solver, which also uses a multilayer Green’s function formulation.

We validate the field computation rigorously for the wide frequency range from 1 GHz to 10 THz and parameters, as given in Table I. However, for brevity, we select $f = 1$ THz as an intermediate frequency value and select two different sets of slab dielectric properties to present the validation study, as shown in Figs. 5(b) and (c) and 6(b) and (c). The electric fields produced by HED in Fig. 5(b) and VED in Fig. 6(b) consider a dielectric slab having electrical properties close to that of lossless air ($\varepsilon_r = 1.1, \mu_r = 1$, and $\sigma = 10^{-9}$ S/m).

In Figs. 5(c) and 6(c), the slab is assigned high values of permittivity and conductivity ($\varepsilon_r = 20, \mu_r = 1$, and $\sigma = 20$ S/m). The $E$-fields were computed at the source height ($z = \ell$) for the source-observation lateral separation starting from $r_{cnt} = 0.61$ nm to 1 cm. For a clean comparison, the computed real and imaginary parts of the electric fields are plotted separately along with the corresponding FEKO results. The relative percentage error/difference between the in-house field calculation and FEKO result is calculated as follows:

$$\text{Relative error} = \frac{E - E_{\text{FEKO}}}{E_{\text{FEKO}}} \times 100\%.$$  \hspace{1cm} (34)

The relative error remains less than 1% (≤−2 dB) (gray dashed line) throughout the lateral range. The validation study clearly shows that the in-house DGF implementation is robust, accurate, and suitable for the multiscale composite environment, which includes extremely thick layers, variable media properties, and THz-range operating frequency.

IV. ABSORPTION POWER SPECTRUM OF EMBEDDED CNTs

In this section, we perform a full-wave analysis of both horizontal and vertical embedded CNTs in a lossy dielectric slab.

A. Horizontal Embedded CNT

The schematic of a horizontal embedded CNT in lossy three-layer media was shown previously in Fig. 2(a). For validation, we consider a simple CNT composite, where the top and bottom layers are considered as air, and the middle layer is $d = 1$ μm-thick dielectric with relative permittivity $\varepsilon_r = 10$ and conductivity $\sigma = 1$ S/m. The horizontal CNT is $l = 100$ nm long, with a radius $r_{cnt} = 0.61$ nm, and placed at a height $z_0 = 0.75$ μm from the bottom interface. The composite structure in Fig. 2(a) is illuminated by a transverse magnetic (TM) plane wave excitation normally incident on the top interface, i.e., with zero incidence angle ($\theta_i = 0^\circ$), so that the incident electric field has only $E_x$-component and couples maximally to the $x$-directed CNT. Following the ATW condition (31), the in-house solver discretizes the embedded 100 nm-long CNT into $S = 25$ small equal segments and assigns frequency-dependent complex distributed line impedance ($Z_{cnt}$) to each segment. No discretization is required for the layer as the in-house solver uses multilayer DGFs to account for the layer effect. The absorbed power spectrum ($P_{abs}$) of the horizontal embedded CNT is computed by the in-house solver from 1 to 10 THz and is shown as the black curve in Fig. 7. The 100 nm-long horizontal embedded CNT shows resonance at 6.9 THz. The unique complex conductivity of CNT and the presence of the layered media allow the CNT to resonate at a much lower frequency than a similar-sized PEC wire in free space. For example, the first resonance of an isolated 100 nm-long PEC wire in free space appears near 1500 THz, and that of a 100 nm-long CNT in free space appears near 22 THz, irrespective of their orientation [13]. While embedded in a dielectric layer, the same CNT resonates at a much lower frequency value depending on the layer characteristics.

We validate the in-house solver results against the MoM-based FEKO planar multilayer substrate solver, which
uses a similar multilayer Green’s function approach that avoids layer discretization complexity [43]. However, FEKO does not allow assigning complex impedance to 1-D wire structures, and thus, the CNTs are modeled as 3-D penetrable objects (cylinders), discretized by triangular surface mesh elements, and assigned a frequency-dependent equivalent complex permittivity profile, as given in Appendix A and (A.3). In the FEKO simulation setup, we used double-precision accuracy and a model extent of 500 μm. Different meshing densities were achieved for CNTs by defining custom mesh triangle edge length: (0.16 to 2.2) \( \times r_{\text{cnt}} \). Since the CNTs are inherently high aspect ratio wire-like structures, a large number of surface mesh elements is required to accurately define the wire curvature of the 3-D cylindrical model. In the present example, the 100 nm-long CNT with a radius \( r_{\text{cnt}} = 0.61 \text{ nm} \) has an aspect ratio (length/diameter) \( \approx 80 \). To study the meshing effect on solution accuracy and compare the computation time, we simulated different mesh densities for the 3-D CNT structure in FEKO. Two such discretizations in FEKO are shown by the zoomed-in view in Fig. 8(a) (using 3000 mesh elements) and Fig. 8(b) (using 6000 mesh elements). The FEKO results show overall good agreement with the in-house results except for the small red-shifts in resonance frequency (red and green curves in Fig. 7). We find that the red-shift decreases from 4.35% to 2.61% when the CNT surface mesh elements assigned by FEKO are doubled from 3000 to 6000 triangles. This means that, with increasing meshing density, the 3-D CNT resonance should converge to the 1-D CNT resonance. This is because increasing mesh elements in FEKO better approximates the wire curvature, and thus, we get increasingly accurate 3-D MoM solutions. It is obvious that the 3-D meshed cylindrical shape will always remain crude compared to the actual cylindrical shape (which ideally would need an infinite number of mesh elements), and thus, a small but finite red-shift will always persist in the FEKO generated resonance compared to the in-house solution. This observation is in accordance with our previously reported work [13], where the CNTs were investigated in a free space condition. To better visualize the convergence phenomena of embedded CNT resonance, we plot both the FEKO resonance and the in-house resonance with increasing mesh density in Fig. 9. The top \( x \)-axis shows the inverse of the number of linear segments used by the in-house solver to discretize the 1-D CNT, and corresponding resonances are plotted in black. The bottom \( x \)-axis shows the inverse of the square root of triangular mesh elements used by FEKO for 3-D cylindrical CNT. Composite parameters remain the same as in Fig. 7. We performed an extra validation step. We chose the finite element method (FEM)–based CST Microwave studio [44], a full-wave electromagnetic solver that uses a totally different approach than the

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**Fig. 7.** Validation of the absorbed power spectrum of an embedded horizontal CNT [see Fig. 2(a)] using three different solvers: 1) MoM-based 1-D in-house solver (this work); 2) MoM-based 3-D FEKO solver; and 3) FEM-based CST MWS. Composite parameters are given as follows: \( \varepsilon_r = \varepsilon_\infty = 1 \), \( \varepsilon_2 = 10 \), \( \mu_1 = \mu_2 = \mu_\infty = 1 \), \( \sigma_1 = \sigma_\infty = 0 \), \( \sigma_2 = 1 \text{ S/m} \), \( d = 1 \mu \text{m} \), \( z_0 = 0.75 \mu \text{m} \), \( l = 100 \text{ nm} \), and \( r_{\text{cnt}} = 0.61 \text{ nm} \). TM wave excitation with \( \theta = 0^\circ \).

**Fig. 8.** 3-D full-wave model in commercial solvers for a 100 nm-long single CNT embedded in a 1 μm-thick dielectric slab. (a) Zoomed-in view of the 3-D cylindrical model for CNT in FEKO MoM solver discretized by 3000 triangular surface mesh elements and (b) discretized by 6000 triangular surface mesh elements. The dielectric slab does not need discretization. (c) 3-D unit cell in the CST solver with periodic boundary condition assigned in \( x \)-and \( y \)-directions for the single CNT embedded in the dielectric slab where the whole setup is discretized by 1 145 026 tetrahedral mesh elements.

**Fig. 9.** Convergence of FEKO resonance toward the in-house solver resonance with increasing mesh density for an embedded 100 nm-long horizontal CNT. The top \( x \)-axis shows the inverse of the segment number used by in-house code for 1-D CNT. The bottom \( x \)-axis shows the inverse of the square root of triangular mesh elements used by FEKO for 3-D cylindrical CNT. Composite parameters remain the same as in Fig. 7.
MoM-based FEKO and the in-house solver. The FEM-based CST solver requires the discretization of the embedding layer surfaces and the embedded 3-D CNT with a large number of tetrahedral mesh elements. As shown in Fig. 8(c), we design the 1 μm-thick dielectric slab with embedded CNT confined in a 3-D unit cell of 4 μm × 4 μm × 5 μm. The \( z_{\text{min}}/\text{max} \) are set to open boundary conditions to simulate air above and below the dielectric interfaces. The periodic boundary condition is applied on \( x_{\text{min}}/\text{max} \) and \( y_{\text{min}}/\text{max} \) to simulate infinite lateral extent of all three layers. We chose the adaptive mesh refinement setting in CST and solved from 1 to 10 THz. In the CST simulation setup, we used double-precision, a maximum of eight passes in the adaptive mesh refinement, and a second-order frequency-domain solver of the accuracy of 0.0001.

The CST solution slowly converges to the in-house solution of \( P_{\text{abs}} \) with an increasing number of iterative passes. The CST computed \( P_{\text{abs}} \) is also plotted in Fig. 7 (magenta dashed curve), which shows excellent agreement with the in-house result. The CST resonance frequency value is less than 1% red-shifted compared to the in-house resonance frequency value. To achieve this result, CST assigned a total of 1145026 tetrahedral mesh elements to discretize the confined composite structure in a unit cell. Thus, it is evident that, with increasing mesh density, both the FEKO 3-D MoM solution and the CST 3-D FEM solution converge toward our in-house 1-D MoM solution of embedded CNT.

The disadvantage of increasing mesh density is the price of increased computation time. For a fair comparison, we only compared the time required by FEKO and our in-house solver. Both the solvers use multilayer Green’s function-based MoM technique that obviates the computational cost of layer discretization. We only consider the time to calculate and fill the impedance matrix at each operating frequency. An Intel Xeon CPU E5-2697A v4 at 2.60 GHz machine, with 512 GB installed RAM, was used to study the computation time. Since the in-house algorithm does not involve any parallel computation, FEKO was also operated in serial mode. Fig. 10 plots the CPU time (in second) elapsed until the \([Z]\) matrix is filled along the \( y \)-axis and increasing frequency (1 GHz–10 THz) along the \( x \)-axis. The red solid line refers to the computation time required by the FEKO 3000 mesh (\( t_{\text{FEKO}(3K)} \)), and the green solid line refers to the computation time required by the FEKO 6000 mesh (\( t_{\text{FEKO}(6K)} \)). The time required by the in-house algorithm (for \( S = 25 \) segment CNT) is plotted as the black solid curve (\( t_{A+B} \)), which is the sum of two independent times \( t_A \) and \( t_B \). \( t_A \) is the time required to build the LUT for contour integration on the axial mesh grid along the CNT length. \( t_A \) rises with increasing frequency as the upper limit of contour integration \( k_M \) in (27) and (28) increases, and more sampling points and iterations are needed to maintain a desired numerical accuracy. However, \( t_B \) is independent of frequency. \( t_B \) is the combined time required to compute the closed-form SI tail on the CNT axial mesh grid, followed by the interpolation of the full-wave solution and filling of the \([Z]\) matrix.

Observing the entire frequency range in Fig. 10, we see that \( t_{\text{FEKO}(3K)} \approx 2000 \text{ s} \) and \( t_{\text{FEKO}(6K)} \approx 8000 \text{ s} \). Thus, to reduce the resonant frequency red-shift approximately by a factor of two (from 2.61% to 4.35%), FEKO needs a twofold increase in surface mesh density (from 3000 to 6000), which, in turn, increases the computation time by fourfold (from 2000 to 8000 s). However, to solve a \([Z]\times2\times2\) matrix for the horizontal CNT, the in-house solver takes only \( t_A+B = 11.5 \text{ s} \) at 1 GHz and \( t_A+B = 16.7 \text{ s} \) at 10 THz. Thus, we achieve on average a computation speed up of \((t_{\text{FEKO}(6K)}/(t_{A+B}))/\approx 570\) for a 100 nm-long horizontal embedded CNT while using the in-house solver as compared to FEKO that still suffers from a 2.61% red-shift in resonant frequency.

**B. Vertical Embedded CNT**

To perform a similar full-wave analysis with a vertical embedded CNT, we keep every other composite parameter the same as mentioned in Fig. 7, except for the CNT orientation and incident excitation. The schematic of the vertical embedded CNT in lossy three-layer media was shown previously in Fig. 2(b), where the CNT was oriented along the \( z \)-axis and centered at a height \( z_0 = 0.75 \mu \text{m} \) from the bottom interface. The vertical embedded CNT [see Fig. 2(b)] is illuminated by a transverse electric (TE) plane wave excitation with oblique incidence (\( \theta_i = 80^\circ \)), which has a large \( E_z \) component that couples to the \( z \)-directed CNT.

The absorbed power spectrum (\( P_{\text{abs}} \)) for the embedded vertical CNT is computed using the in-house solver and FEKO from 1 to 10 THz, and the results are compared in Fig. 11. For ease of comparison, we keep the mesh settings similar to the previously discussed horizontal CNT case. From the in-house calculation, we find that the 100 nm-long vertical embedded CNT also resonates at 6.9 THz similar to the embedded horizontal CNT. However, due to the difference in incident electric field polarization and CNT orientation, the absorbed power spectrum of the vertical embedded CNT (see Fig. 11) is found to be approximately 19 dB lower than that of the horizontal embedded CNT (see Fig. 7). The FEKO simulation results for the vertical embedded CNT with 3000 and 6000 mesh show good agreement with the in-house results (see Fig. 11). In this case, also, we find small red-shifts in resonance frequency exhibited by FEKO compared to the in-house solver. The red-shift decreases from 4.35% to 2.61% when the number of FEKO surface mesh elements is doubled from 3000 to 6000 triangles.
A novel full-wave MoM solver was developed for accurate and efficient noninvasive evaluation of the electromagnetic response from multiscale CNT reinforced composites. The 3-D multiscale composite problem has been effectively reduced to a 1-D arbitrary thin wire problem by using the multilayer dyadic Green’s function (DGF), which accurately accounts for the lossy substrate effect. A modified semianalytical technique was conceived for fast evaluation of the associated Sommerfeld-type integrals. The integrand singularities were avoided by adaptive contour deformation. The slow converging tails were computed in the exact closed form. The reliability of the in-house solver was tested for a wide range of composite parameters, including GHz to tens of THz operating an average computation speed up of \( \frac{t_{\text{FEKO(6K)}}}{t_{A+B}} \approx 50 \) by using the in-house solver compared to FEKO. The computational experiments in Figs. 10 and 12 were conducted for a CNT with a fixed length and fixed number of segments \( S \). However, we tested our in-house solver for an increasing number of segments and showed that the computational complexity of our implementation is \( O(S \log(S)) \).

We also simulated a multi-CNT configuration, as shown in the inset in Fig. 13, to highlight the capability of our in-house solver to simulate complex CNT distributions. The CNTs are embedded in a 50 nm-thick dielectric slab \( (\varepsilon_{r1} = 10, \mu_{r1} = 1, \sigma_1 = 0, \sigma_2 = 1 \text{ S/m}, \ d = 1 \mu m, \ z_0 = 0.75 \mu m, \ l = 100 \text{ nm}, \text{ and } r_{\text{cnt}} = 0.61 \text{ nm}) \). TE wave excitation with \( \theta = 80^\circ \).

Using the same Intel Xeon CPU E5-2697A v4 at 2.60 GHz machine, with 512 GB installed RAM, we record the computation time required to solve the vertical embedded CNT. Fig. 12 shows the time comparison between FEKO and the in-house solver. The \( y \)-axis indicates the CPU time (in seconds) elapsed until the \([Z]\) matrix is filled, and the \( x \)-axis shows increasing frequency from 1 GHz to 10 THz. The definition of \( t_{\text{FEKO(3K)}}, t_{\text{FEKO(6K)}}, t_A, t_B, \text{ and } t_{A+B} \) remains the same as in Fig. 10. To solve a \([Z]\) \( 24 \times 24 \) matrix for the vertical embedded CNT, the in-house solver takes \( t_{A+B} = 140.2 \text{ s} \) at 1 GHz and \( t_{A+B} = 177.3 \text{ s} \) at 10 THz, as shown in Fig. 12. This is almost ten times more than what was observed in Fig. 10 for the horizontal CNT. To explain this tenfold increase in computation time, we can refer back to the last paragraph of Section II-D, where it was discussed that, for the horizontal CNT, a 1-D LUT is employed considering its lateral invariance property, but, for the vertical CNT, a 2-D LUT is required. The FEKO solution time for the embedded 3-D CNT remains similar irrespective of any CNT orientation. This is because FEKO fetches Green’s function data from a preformatted built-in LUT that works in a similar fashion for any orientation of the 3-D object. However, for the 100 nm-long vertical embedded CNT, we still achieve
frequency, nm to mm-thick substrate, nm to cm range of lateral separation between source and observation point, and also a wide variety of media properties to cover most CNT composite applications. The accuracy of the in-house algorithm was verified rigorously against multiple commercial 3-D full-wave solvers. The absorbed power spectrum of horizontal and vertical embedded CNTs is studied. It is observed that, with increasing mesh density, the results obtained from the 3-D commercial solvers gradually converge toward the results achieved by the solver proposed in this work. The in-house algorithm (in serial mode) solves a 100 nm-long embedded CNT ≈ 570 times faster for horizontal orientation and ≈ 50 times faster for vertical orientation compared to the FEKO 3-D MoM solver. Thus, for composite problems, the present approach will be more scalable than available commercial full-wave solvers. In its present form, the solver can be rigorously applied to investigate horizontal and vertical arrangements of embedded CNTs and study the effects of composite parameters on the total electromagnetic response. The algorithm is currently being expanded to include additional DGF components. Parallelization of the algorithm can further improve the solver speed.

In summary, the proposed full-wave solver overcomes the limitations of: 1) the dilute limit effective media approximations (EMAs) that are fast but inaccurate beyond low frequencies and 2) 3-D full-wave commercial solvers (FEM and MoM) that give comparable accuracy but at the expense of enormous computation resources and time. The proposed solver could enable the simulations of more complex composite structures that are engineered to produce tailored electromagnetic behavior. Future work will involve characterizing the distribution and location of the CNTs in the dielectric slab using tomographic transmission electron microscopy similar to [27]. This will allow us to compare our solver simulation results with the experimental measurements for the real-time interpretation of the spectroscopy data to facilitate the nondestructive evaluation (NDE) of CNT composites.

APPENDIX A

ELECTRICAL PROPERTIES OF SINGLE-WALLED CNTS

The ATW CNTs are assigned Drude-like axial surface conductivity as follows [30]:

\[ \sigma_{cnt} = \frac{\sigma_0}{1 + j \omega \tau_0}, \quad \sigma_0 = \frac{2 e^2 v_F \tau}{\pi \hbar r_{cnt}} \quad (A.1) \]

where \( \sigma_0 \) is the CNT static dc conductivity, \( \tau = 0.3 \) ps to 3 ps is the relaxation time, \( \epsilon_0 \) is the electronic charge, \( v_F = 9.71 \times 10^5 \) m/s is the Fermi velocity, \( \hbar \) is Plank’s constant divided by 2\( \pi \), and \( r_{cnt} \) is the CNT radius. The axial surface conductivity in (A.1) is valid in the microwave through 100 THz range for metallic CNTs with small chirality \( (n, m) < 50 \) [45]. In this study, we have considered only single-walled CNTs (SWCNTs) with a \((9, 9)\) armchair chirality resulting in a cross-sectional CNT radius of \( r_{cnt} = 0.61 \) nm. The relaxation time was set to \( \tau = 3 \) ps to generate sharp resonances in power spectrum. The CNT axial surface conductivity can be translated into a 1-D distributed complex impedance \( Z_{cnt} \) as follows [13]:

\[ Z_{cnt} = R_{cnt} + j \omega L_{cnt} = \frac{1}{2 \pi \frac{r_{cnt}}{\sigma_{cnt}}} \quad (A.2) \]

where

\[ R_{cnt} = \frac{1}{2 \pi \frac{r_{cnt}}{\sigma_0}}, \quad L_{cnt} = \frac{\tau}{2 \pi \frac{r_{cnt}}{\sigma_0}} \]

where \( R_{cnt} \) is the Ohmic distributed resistance and \( L_{cnt} \) is the kinetic inductance of the CNT.

While modeling the CNT as a penetrable 3-D cylindrical structure in FEKO, the region inside the cylinder was assigned an appropriate complex permittivity profile following the below steps

\[ \sigma_{cyl} = \frac{1}{Z_{cnt}} \pi r_{cnt}^2 \]

\[ \epsilon_{r,cyl} = \frac{\text{Im}(\sigma_{cyl}) - j \text{Re}(\sigma_{cyl})}{\omega \epsilon_0} \]

\[ \tan \delta_{cyl} = \frac{\text{Im}(\epsilon_{r,cyl})}{\text{Re}(\epsilon_{r,cyl})} \quad (A.3) \]

APPENDIX B

SOMMERFELD IDENTITIES

The following exact closed-form solutions of Sommerfeld type integrals are derived using the Fourier-Bessel transform relationships given in [41]:

\[ S_0 = \int_0^\infty d\lambda \left[ j_0(\lambda \rho) \right] \frac{e^{-\rho \text{rcyl} \sqrt{\frac{\lambda^2 - k_i^2}{\lambda^2 - k_i^2}}} - e^{-jk_i A}}{A} = \frac{1}{A^2} \quad (B.1) \]

where \( A = \sqrt{r^2 + \alpha_n^2} \)

\[ S_1 = \int_0^\infty d\lambda \left[ J_1(\lambda \rho) \right] \frac{e^{-\rho \text{rcyl} \sqrt{\frac{\lambda^2 - k_i^2}{\lambda^2 - k_i^2}}} - e^{-jk_i A}}{A} = \frac{1}{A^2} \quad (B.2) \]

\[ S_2 = \int_0^\infty d\lambda \left[ j_1(\lambda \rho) \right] \sqrt{\frac{\lambda^2 - k_i^2}{\lambda^2 - k_i^2}} = \frac{e^{-jk_i A}}{A^2} \left[ -jk_i - 1 - \frac{k_i^2 A^2}{3 \frac{a_n^2}{A^2} + \frac{3a_n^2}{A^2}} \right] \quad (B.3) \]

\[ S_3 = \int_0^\infty d\lambda \left[ J_1(\lambda \rho) \right] \sqrt{\frac{\lambda^2 - k_i^2}{\lambda^2 - k_i^2}} = \frac{1}{r^2} \left[ \frac{jk_i e^{-jk_i A} + e^{-jk_i A}}{A} \left( 1 - \frac{jk_i a_n^2}{A} - \frac{a_n^2}{A^2} \right) \right] \quad (B.4) \]

\[ S_4 = \int_0^\infty d\lambda \left[ j_2(\lambda \rho) \right] \sqrt{\frac{\lambda^2 - k_i^2}{\lambda^2 - k_i^2}} = \frac{e^{-jk_i A}}{A^2} \left[ 2jk_i + \frac{2 (jk_i)^2}{A} \right] - \frac{3jk_i r^2}{A^2} - \frac{3r^2}{A^2} \right]. \quad (B.5) \]

ACKNOWLEDGMENT

The author D. Chatterjee would like to thank the early discussions on this topic while as an ONR Summer Faculty Fellow, with Dale Zolnicker, formerly with the U.S. Naval Research Laboratory, Washington, DC, USA.
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DEY et al.: METHOD OF MOMENT ANALYSIS OF CNTs EMBEDDED IN LOSSY DIELECTRIC SLAB 6933