Research on Terahertz Wave Reflection and Transmission of Carbon Nanotubes Slab Using FDTD

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Abstract **─** Terahertz wave reflection and transmission of carbon nanotubes slab are investigated in this paper. The wave and current equations that describe characters of terahertz wave in dispersive carbon nanotubes (CNTs) are presented and discretized by using the auxiliary differential equation (ADE) in the finite-difference time-domain method (FDTD), because the permittivity of CNTs are frequency-dependent. The ADE-FDTD method and program's efficiency is proved by the reference's analytical method. Numerical results show that the transmission coefficient of single wall carbon nanotubes (SWCNTs) does not show distinct peaks and dips at Terahertz frequency. The multiple transmitted pulses of silicon dioxide bi-covered with SWCNTs are observed. The electromagnetic interference (EMI) shielding effect of SWCNTs, double wall carbon nanotubes (DWCNTs) and Hydrogen doped CNTs are compared.

Index Terms **─** Auxiliary differential equation (ADE), carbon nanotubes, dispersive, finite-difference time-domain (FDTD), permittivity.

I. INTRODUCTION

Nowadays, carbon nanotubes (CNTs) [1-8] and grapheme, which are advanced engineering materials with unique structures and electrical properties, have attracted much attention. CNTs can be classified as single wall (SW), double wall (DW) and multiwall (MW) carbon nanotubes and modified as hydrogen (H) doped CNTs [5] and so on. CNTs [9-12] have some potential microwave, Terahertz (THz) wave, and optical applications, such as hydrogen storage devices, antennas, interconnects, electrochemical capacitors, and lightweight electromagnetic shields etc.

The electromagnetic interference shielding effectiveness [13-14] of carbon nanotubes structure at THz frequency regime has not yet been considerable studied. CNTs have the compound properties of metallic and semiconductor. The complex and frequency dispersive permittivity of CNTs at THz frequency regime are affected by the number of tube walls, thickness, aspect ratio, filling factor, and geometrical factor during the growth. Analytical and numerical methods [14-20] have been developed to investigate the electromagnetic characteristic of carbon nanotubes such as semi-classical approach [14], method of moments (MoM) [15], and finite-difference time-domain (FDTD) method [17-23] etc. FDTD method is a popular algorithm to predict the properties of materials in arbitrary shapes. Compared to other modeling approaches, FDTD method can study not only carbon nanotubes are made of hollow and long carbon cylindrical molecules, but also CNTs are equivalent to dispersive media. For simulating equivalent CNTs, the computational memory and cost requirement of auxiliary differential equation (ADE) FDTD method is relatively lower than shift operator [19], recursive convolution method and Z-transform methods and is generally used to simulate dispersive media.

In this paper, the electromagnetic interference shielding effectiveness of SWCNTs, DWCNTs and H-doped CNTs at THz frequency are computed with the ADE-FDTD method. Firstly, the ADE-FDTD method for dispersive Drude-Lorentzian model of carbon nanotubes is deduced. Then the accuracy of ADE-FDTD method and program is verified by analytical method in the reference [24]. The interaction of terahertz wave with stratified media containing single wall carbon nanotubes is simulated. The reflection and transmission coefficients for medium covered by SWCNTs, DWCNTs and H-doped CNTs are compared to discuss their application in EMI shielding.

II. ADE-FDTD FORMULA

As in Ref. [4], an extended Drude-Lorentzian model can be used to simulate the relative dispersive permittivity

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of carbon nanotubes at THz frequency [25], i.e.,

$$\varepsilon_r = \varepsilon_c - \frac{\omega_p^2}{\omega(\omega - \mathrm{j}\Gamma)} + \frac{\omega_{p1}^2}{-\omega^2 + \mathrm{j}\omega\Gamma_1 + \omega_1^2}, \tag{1}$$

where ε_c is the dielectric constant at infinite frequency. ω_p, ω_1, and ω_{p1} represent the electron plasma, phonon and oscillator frequency, respectively. Γ and Γ_1 are relaxation rate and spectral width, respectively.

The frequency-dependent constitutive relation for CNTs can be characterized as:

$$\boldsymbol{D} = \varepsilon_r\varepsilon_0\boldsymbol{E} = \varepsilon_c\varepsilon_0\boldsymbol{E} + \boldsymbol{P} + \boldsymbol{P}_1, \tag{2}$$

where the polarization intensities $\boldsymbol{P}$ and $\boldsymbol{P}_1$ are:

$$\boldsymbol{P} = \varepsilon_0\omega_p^2\boldsymbol{E} / [(\mathrm{j}\omega)^2 + \Gamma\mathrm{j}\omega], \tag{3}$$

$$\boldsymbol{P}_1 = \varepsilon_0\omega_{p1}^2\boldsymbol{E} / [(\mathrm{j}\omega)^2 + \Gamma_1\mathrm{j}\omega + \omega_1^2]. \tag{4}$$

By applying the transform relation ($\mathrm{j}\omega \rightarrow \partial/\partial t$) between frequency domain and time domain, we obtain:

$$\partial^2\boldsymbol{P} / \partial t^2 + \Gamma\partial\boldsymbol{P} / \partial t = \varepsilon_0\omega_p^2\boldsymbol{E}, \tag{5}$$

$$\partial^2\boldsymbol{P}_1 / \partial t^2 + \Gamma_1\partial\boldsymbol{P}_1 / \partial t + \omega_1^2\boldsymbol{P}_1 = \varepsilon_0\omega_{p1}^2\boldsymbol{E}. \tag{6}$$

By defining the induced electric currents $\boldsymbol{J}$ and $\boldsymbol{J}_1$,

$$\boldsymbol{J} = \partial\boldsymbol{P} / \partial t, \tag{7}$$

$$\boldsymbol{J}_1 = \partial\boldsymbol{P}_1 / \partial t. \tag{8}$$

The electromagnetic field and current equations discretized with the ADE-FDTD method for the CNTs are:

$$\nabla\times\boldsymbol{E} = -\mu\partial\boldsymbol{H} / \partial t, \tag{9}$$

$$\nabla\times\boldsymbol{H} = \varepsilon_c\varepsilon_0\partial\boldsymbol{E} / \partial t + \boldsymbol{J} + \boldsymbol{J}_1 + \boldsymbol{J}_s, \tag{10}$$

$$\partial^2\boldsymbol{J} / \partial t^2 + \Gamma\partial\boldsymbol{J} / \partial t = \varepsilon_0\omega_p^2\partial\boldsymbol{E} / \partial t, \tag{11}$$

$$\partial^2\boldsymbol{J}_1 / \partial t^2 + \Gamma_1\partial\boldsymbol{J}_1 / \partial t + \omega_1^2\boldsymbol{J}_1 = \varepsilon_0\omega_{p1}^2\partial\boldsymbol{E} / \partial t, \tag{12}$$

where $\boldsymbol{J}_s$ is the free current source.

The standard grid, leapfrog in time approach is used to discrtize the Eqs. (9)-(12). The electric field and electric current are sampled at the cell edge for integer and half integer time steps, respectively. The magnetic field is sampled at the cell center for half integer time steps. If $\partial/\partial x$=0 and $\partial/\partial y$=0, the iterative fields and currents for a one-dimensional (1D) CNTs slab are:

$$\begin{aligned} &H_y^{n+\frac{1}{2}}(i+\frac{1}{2}) = \\ &\quad H_y^{n-\frac{1}{2}}(i+\frac{1}{2}) - \frac{\Delta t}{\mu\Delta z}\left[E_x^n(i+1) - E_x^n(i)\right], \end{aligned} \tag{13}$$

$$\begin{aligned} &E_x^{n+1}(i) = E_x^n(i) \\ &+ \frac{\Delta t}{\varepsilon_c\varepsilon_0\Delta z}\left\{\begin{matrix} \left[H_y^{n+\frac{1}{2}}(i+\frac{1}{2}) - H_y^{n+\frac{1}{2}}(i-\frac{1}{2})\right] \\ -[J_x^{n+\frac{1}{2}}(i) + J_{x1}^{n+\frac{1}{2}}(i) + J_s^{n+\frac{1}{2}}(i)]\Delta z \end{matrix}\right\}, \end{aligned} \tag{14}$$

$$\begin{aligned} J_{x1}^{n+\frac{3}{2}}(i) &= \alpha_{x1}J_{x1}^{n+\frac{1}{2}}(i) + \beta_{x1}J_{x1}^{n-\frac{1}{2}}(i) \\ &+ \gamma_{x1}\left[E_x^{n+1}(i) - E_x^{n-1}(i)\right], \end{aligned} \tag{15}$$

$$\begin{aligned} J_x^{n+\frac{3}{2}}(i) &= \alpha_x J_x^{n+\frac{1}{2}}(i) + \beta_x J_x^{n-\frac{1}{2}}(i) \\ &+ \gamma_x\left[E_x^{n+1}(i) - E_x^{n-1}(i)\right], \end{aligned} \tag{16}$$

where

$$\alpha_{x1} = \frac{4 - 2\Delta t^2\omega_1^2}{2 + \Gamma_1\Delta t},\ \beta_{x1} = \frac{\Gamma_1\Delta t - 2}{2 + \Gamma_1\Delta t},\ \gamma_{x1} = \frac{\varepsilon_0\omega_{p1}^2\Delta t}{2 + \Gamma_1\Delta t},$$

$$\alpha_x = \frac{4}{2 + \Gamma\Delta t},\ \beta_x = \frac{\Gamma\Delta t - 2}{2 + \Gamma\Delta t},\ \gamma_x = \frac{\varepsilon_0\omega_p^2\Delta t}{2 + \Gamma\Delta t}. \tag{17}$$

The power reflection, transmission, and absorption coefficients in decibel scale are:

$$R_{\mathrm{dB}} = 20\lg R, \tag{18}$$

$$T_{\mathrm{dB}} = 20\lg T, \tag{19}$$

$$A_{\mathrm{dB}} = 10\lg(1 - |R|^2 - |T|^2). \tag{20}$$

III. NUMERICAL RESULTS

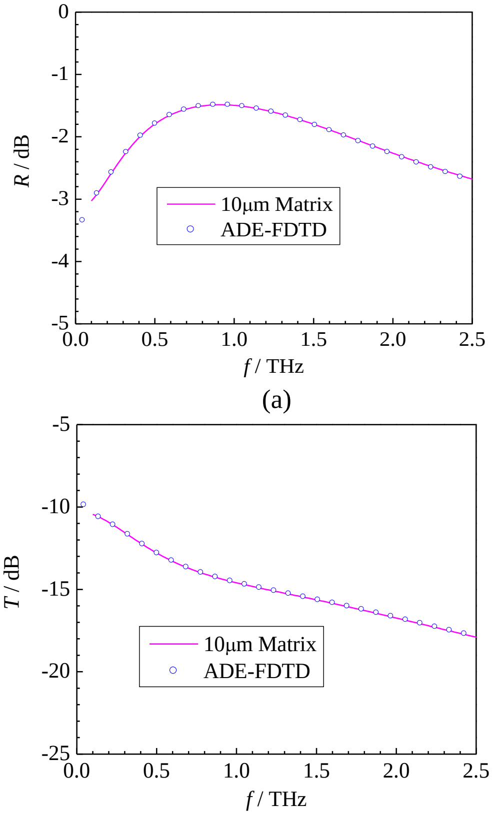
In the following section, FDTD numerical results about Terahertz wave reflection and transmission of stratified media containing various carbon nanotubes are illustrated. The EMI shielding effectiveness, which is generally dependent upon various material parameters characterized by CNTs' aspect ratio, filling factor, geometrical factor and working frequency etc. are discussed below.

To validate the auxiliary differential equation finite-difference time-domain method introduced above, Fig. 1 illustrates the reflection and transmission coefficients for one-layer single wall carbon nanotubes slab. The spatial discretization size is δ=0.1 μm and the time step size is $\Delta t=\delta/2c$. The incident differential Gaussian pulse in the time domain is $E_i(t)= \{(t-t_0)\cdot\exp[-4\pi(t-t_0)^2/\tau^2]\}/\tau^2$. The pulse peak occurs at $t_0=120\Delta t$. The pulse width of the pulse is influenced by the constant $\tau=150\Delta t$.

If no special instructions in this paper, the material parameters in Eq. (1) for SWCNTs [4] are ε_c=8.41, ω_p=2π×23 THz, ω_{p1}=2π×38.9 THz, ω_1=2π×5.9 THz, Γ=2π×24.5 THz, Γ_1=2π×29.6 THz. The CNTs' thickness is 10 μm. The reflection and transmission coefficients computed with analytical propagation matrix method in Ref. [4] and the ADE-FDTD method reach a good agreement in Fig. 1. Though the peak value of the reflection coefficient occur at 0.916 THz, the transmission coefficient for a 10-μm-thick SWCNTs slab does not show obvious peaks and troughs at 0.3-2.5 THz in Fig. 1. The variation trend is consistent with the experimental results in Ref. [9].

Figure 2 gives the ADE-FDTD method simulated the terahertz wave transmission coefficient and the time domain waveform of 1mm depth silicon dioxide (SiO_2) and silicon dioxide bi-covered by 15 μm depth SWCNTs respectively. The permittivity for SiO_2 is presumed constant ε_r=4 [26].

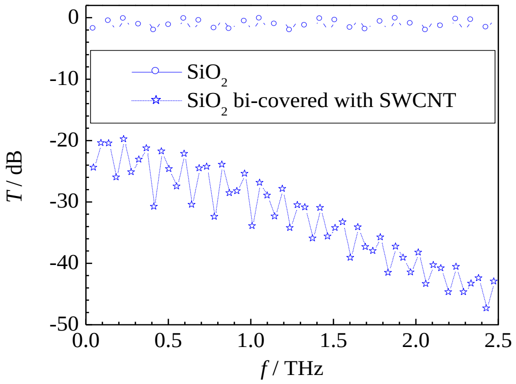
As shown in Fig. 2 (a), the SWCNTs can make the transmission coefficient greatly decrease. The single wall carbon nanotubes demonstrate high efficiency shielding at terahertz frequency range. The sampling points of the transmission time-domain waveform E_y in Fig. 2 (b) are 5δ away from the media boundary between SWCNTs and vacuum. Several transmitted pulses produced by the multi-reflection phenomena in the stratified media can be seen in Fig. 2 (b).



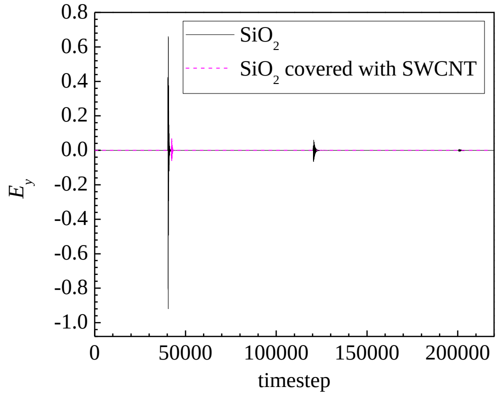
(a)

(b)

Fig. 1. Reflection and transmission coefficients for one-layer SWCNTs. (a) Reflection coefficient and (b) transmission coefficient.



(a)

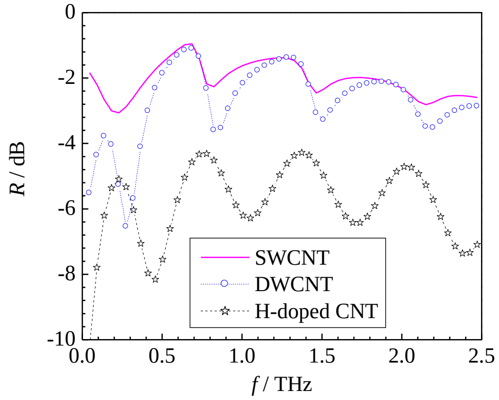


(b)

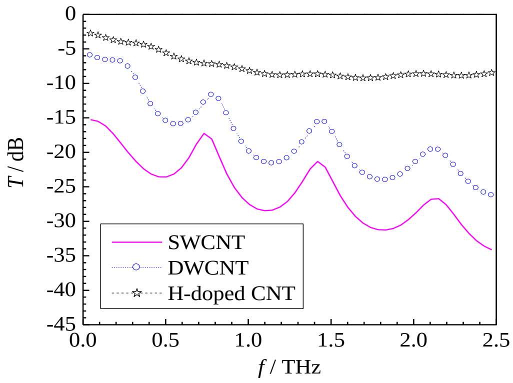
Fig. 2. FDTD predicted THz wave transmission of silicon dioxide bi-covered with SWCNTs. (a) Transmission coefficient and (b) normalized time domain waveform.

Figure 3 compares the ADE-FDTD method calculated electromagnetic scattering of 100 μm depth silicon dioxide (SiO_2) [26] whose ε_r=4 bi-covered with SWCNTs, DWCNTs, and H-doped CNTs. The thickness of each CNTs layer is 10 μm. The material parameters for DWCNTs [4] are ε_c=5.76, ω_p=2π×10.5 THz, ω_{p1}=2π×32.2 THz, ω_1=2π×5.5 THz, Γ=2π×24.3 THz, Γ_1=2π×23.3 THz and for H-doped CNTs [5] are ε_c=6.25, ω_p=2π×7.42 THz, Γ=2π×34.29, ω_{p1}=2π×4.69 THz, ω_1=2π×1.53 THz, Γ_1=2π×3.27 THz.

Because the permittivity and conductivity [2] of SWCNTs are larger than those of DWCNTs and H-doped CNTs discussed in this paper, the reflection coefficient of silicon dioxide bi-covered with SWCNTs is larger than those with DWCNTs and H-doped CNTs. Compared to the transmission coefficient of one layer SWCNTs in Fig. 1 (b), the transmission coefficient of SiO_2 bi-covered with SWCNTs in Fig. 3 (b) shows several peaks and dips originating from the silicon dioxide substrate in the Terahertz region.



(a)



(b)

Fig. 3. FDTD predicted Terahertz wave reflection and transmission coefficients of silicon dioxide bi-covered with SWCNTs, DWCNTs, and H-doped CNTs. (a) reflection coefficient and (b) transmission coefficient.

IV. CONCLUSION

In this paper, terahertz wave reflection and transmission of carbon nanotubes slab is investigated with auxiliary differential equation in Finite-Difference Time-Domain method. The extended Drude-Lorentzian model in the frequency domain is used to simulate dispersive carbon nanotubes. The wave and current equations for CNTs are got with the transform relation between frequency domain and time domain and discretized using Yee's scheme. After the validity of method and program, ADE-FDTD method predicted Terahertz wave reflection and transmission of silicon dioxide bi-covered with SWCNTs, DWCNTs and H-doped CNTs are compared. The local resonances of the transmission coefficient associated with the material parameters of silicon dioxide substrate result in some oscillations. The computed results show that impedance mismatch and loss characteristic of SWCNTs make the transmission coefficient of silicon dioxide decrease. The SWCNTs demonstrates good electromagnetic interference shielding effectiveness.

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REFERENCES

[1] M. F. De Volder, S. H. Tawfick, R. H. Baughman, and A. J. Hart, "Carbon nanotubes: present and future commercial applications," *Science*, vol. 339, no. 6119, pp. 535-539, 2013.

[2] X. Y. He and X. N. Fu, "Simulation investigation on optical and electrical properties of carbon nanotube in terahertz region," *Commun. Theor. Phys.*, vol. 51, no. 1, pp. 161-164, 2009.

[3] E. Dadrasnia and H. Lamela, "Optical and electrical characterization of carbon nanotubes by terahertz spectroscopy: comparison between modeling and experimental results," *Proc. of SPIE*, vol. 8096, no. 80963P, pp. 1-6, 2011.

[4] I. Maeng, C. Kang, S. J. Oh, J. H. Sonb, K. H. An, and Y. H. Lee, "Terahertz electrical and optical characteristics of double-walled carbon nanotubes and their comparison with single-walled carbon nanotubes," *Appl. Phys. Lett.*, vol. 90, no. 5, pp. 051914, 1-4, 2007.

[5] C. Kang, I. H. Maeng, S. J. Oh, S. C. Lim, K. H. An, Y. H. Lee, and J. H. Son, "Terahertz optical and electrical properties of hydrogen-functionalized carbon nanotubes," *Phys. Rev. B*, vol. 75, no. 8, pp. 085410, 1-5, 2007.

[6] Z. R. Wu, L. Wang, Y. T. Peng, A. Young, S. Seraphin, and H. Xin, "Terahertz characterization of multi-walled carbon nanotube films," *Journal of Applied Physics*, vol. 103, no. 9, pp. 094324, 1-6, 2008.

[7] J. Lloyd-Hughes and T. Jeon, "A review of the terahertz conductivity of bulk and nano-materials," *Journal of Infrared, Millimeter and Terahertz Waves*, vol. 33, no. 9, pp. 871-925, 2012.

[8] L. Ren, C. L. Pint, A. K. Wójcik, T. Arikawa, Y. Takemoto, K. Takeya, I. Kawayama, A. A. Belyanin, M. Tonouchi, R. H. Hauge, and J. Kono, "Anisotropic terahertz dynamics of highly-aligned single-walled carbon nanotubes," *Terahertz Science and Technology*, vol. 3, no. 1, pp. 26-32, 2010.

[9] J. T. Hong, D. J. Park, J. Y. Moon, S. B. Choi, J. K. Park, F. Rotermund, J. Y. Park, S. Lee, and Y. H. Ahn, "Terahertz wave applications of single-walled carbon nanotube films with high shielding effectiveness," *Applied Physics Express*, vol. 5, no. 1, pp. 015102, 1-3, 2012.

[10] X. J. Feng, W. X. Huang, Y. Luo, J. Zhang, and Y. X. Zhang, "Terahertz spectroscopic investigation of MWNTs and MWNTS/Mica," *Chinese Journal of Sensors and Actuators*, vol. 23, no. 4, pp. 453-457, 2010.

[11] W. Abdelli, X. Mininger, L. Pichon, and H. Trabelsi, "Impact of composite materials on the shielding effectiveness of enclosures," *The Applied Computational Electromagnetics Society*, vol. 27, no. 4, pp. 369-375, 2012.

[12] M. A. Seo, J. H. Yim, Y. H. Ahn, F. Rotermund, D. S. Kim, S. Lee, and H. Lim, "Terahertz electromagnetic interference shielding using single-walled carbon nanotube flexible films," *Applied Physics Letters*, vol. 93, no. 23, pp. 231905, 1-3, 2008.

[13] Y. Huang, N. Li, Y. F. Ma, F. Du, F. F. Li, X. B.

He, X. Lin, H. J. Gao, and Y. S. Chen, "The influence of single-walled carbon nanotube structure on the electromagnetic interference shielding efficiency of its epoxy composites," *Carbon*, vol. 45, no. 8, pp. 1614-1621, 2007.

[14] J. A. Berres and G. W. Hanson, "Multiwall carbon nanotubes at RF-THz frequencies: scattering, shielding, effective conductivity, and power dissipation," *IEEE Transactions on Antennas and Propagation*, vol. 59, no. 8, pp. 3098-3103, 2011.

[15] A. I. Sotiropoulos, I. V. Plegas, S. Koulouridis, and H. T. Anastassiu, "Scattering properties of carbon nanotube arrays," *IEEE Transactions on Electromagnetic Compatibility*, vol. 54, no. 1, pp. 110-117, 2012.

[16] M. Y. Wang, C. W. Qiu, J. Xu, Y. L. Dong, H. Zheng, and H. L. Li, "Mie series for electromagnetic scattering of chiral metamaterials sphere," *Journal of Systems Engineering and Electronics*, vol. 22, no. 6, pp. 885-891, 2011.

[17] M. Y. Wang, G. P. Li, M. Zhou, R. Wang, C. L. Zhong, J. Xu, and H. Zheng, "The effect of media parameters on wave propagation in a chiral metamaterials slab using FDTD," *International Journal of Numerical Modelling: Electronic Networks, Devices and Fields*, vol. 27, no. 1, pp. 109-121, 2014.

[18] L. Hai, M. F. Pantoja, S. G. Garcia, A. R. Bretones, and R. G. Martin, "An FDTD thin-wire model for modeling carbon nanotube dipoles at THz regime," *IEEE Antennas and Wireless Propagation Letters*, vol. 11, pp. 708-711, 2012.

[19] L. Q. Li, Y. X. Shi, F. Wang, and B. Wei, "SO-FDTD method of analyzing the reflection and transmission coefficient of weakly ionized dusty plasma layer," *Acta Phys. Sin.*, vol. 61, no. 12, pp. 125201, 1-5, 2012.

[20] S. G. Zhou, H. L. Li, L. Y. Fu, and M. Y. Wang, "Preliminary study on active modulation of polar mesosphere summer echoes with the radio propagation in layered space dusty plasma," *Plasma Science and Technology*, vol. 18, no. 6, pp. 607-610, 2016.

[21] A. Z. Elsherbeni and V. Demir, *The Finite-Difference Time-Domain Method For Electromagnetics With MATLAB Simulations*. SciTech Publishing, 2009.

[22] M. Y. Wang, H. L. Li, D. L. Gao, L. Gao, J. Xu, and C. W. Qiu, "Radiation pressure of active dispersive chiral slabs," *Opt. Express*, vol. 23, no. 13, pp. 16546-16553, 2015.

[23] K. Han, P. Freeman, H. Y. Han, J. Hamar, and J. F. Stack Jr., "Finite-difference time-domain modeling of ultra-high frequency antennas on and inside the carbon fiber body of a solar-powered electric vehicle," *The Applied Computational Electromagnetics Society*, vol. 29, no. 6, 2014.

[24] D. B. Ge, *Electromagnetic Wave Theory*. Xidian University Press, Xian, 1997.

[25] E. Dadrasnia, S. Puthukodan, and H. Lamela, "Terahertz electrical conductivity and optical characterization of composite nonaligned single- and multiwalled carbon nanotubes," *Journal of Nanophotonics*, vol. 8, no. 1, pp. 083099, 1-10, 2014.

[26] K. S. Lee, T. M. Lu, and X. C. Zhang. "Tera tool terahertz time-domain spectroscopy is a highly sensitive optical tool for dielectric and optical property characterization of thin film at terahertz frequency," *IEEE Circuits & Devices Magazine*, vol. 17, no. 5, pp. 23-28, 2002.

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