Electromagnetic scattering of the carbon nanotubes excited by an electric line source*

Wang Yue(王 玥)[a)b)c)], Wu Qun(吴 群)[b)c)†], Wu Yu-Ming(吴昱明)[d)], He Xun-Jun(贺训军)[a)], and Li Le-Wei(李乐伟)[e)]

[a)] *Department of Electrical Science and Technology, Harbin University of Science and Technology, Harbin* 150080, *China*

[b)] *School of Electronics and Information Technology, Harbin Institute of Technology, Harbin* 150001, *China*

[c)] *State Key Laboratory of Millimeter Wave, Southeast University, Nanjing* 210096, *China*

[d)] *School of Electrical & Electronic Engineering, Nanyang Technological University,* 639798, *Singapore*

[e)] *Department of Electrical and Computer Engineering, National University of Singapore, 10 Kent Ridge Crescent* 119260, *Singapore*

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An analytical solution is presented for the electromagnetic scattering from an infinite-length metallic carbon nanotube and a carbon nanotube bundle. The scattering field and scattering cross section are predicted using a modal technique based on a Bessel and Hankel function for the electric line source and a quantum conductance function for the carbon nanotube. For the particular case of an isolated armchair (10, 10) carbon nanotube, the scattered field predicted from this technique is in excellent agreement with the measured result. Furthermore, the analysis indicates that the scattering pattern of an isolated carbon nanotube differs from that of the carbon nanotube bundle of identical index (m, n) metallic carbon nanotubes.

Keywords: scattering, carbon nanotubes, terahertz

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1. Introduction

Single-walled carbon nanotubes (SWNTs) comprise a family of more than several hundred structures characterized by different diameters and helicity, which determine their electronic structure and optical properties.[1,2] They can be either metallic or semiconducting, sensitively dependent on the atomic structure. This richness and diversity makes carbon nanotubes so promising for various applications. In this paper, we consider electromagnetic scattering from infinite-length metallic single-walled carbon nanotubes and a carbon nanotube bundle.[3] The diameter and helicity of an SWNT are uniquely characterized by the vector $\boldsymbol{C}_{\rm h} = n\boldsymbol{a}_1 + m\boldsymbol{a}_2$, where n, m are integers and $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ are lattice basis vectors. The (n, m) indices determine the metallic or semiconducting behaviour of SWNTs. Armchair ($m = n$) SWNTs are metallic, with cross-section radius $a = 3mb/(2\pi)$, where b is the inter-atomic distance in grapheme. The homogeneous carbon nanotube bundle under considered is composed of identical index (m, m) armchair nanotubes. The model utilized here combines an effective boundary condition to describe the wave propagation around carbon nanotubes, together with the quantum conductance function for the carbon nanotubes.[4]

During the past years, different theoretical models have been used to describe electromagnetic wave scattering by carbon nanotubes and other scattering configurations.[5−9] Recent studies on the Rayleigh scattering spectra of SWNTs provide spectroscopic information about the system through the scattering resonant enhancement when the photon energy matches that of an electronic transition. These data permit us to test key theoretical constructs concerning the scattering properties of carbon nanotubes.[10,11]

This paper presents an exact analytical solution of the scattering of cylindrical waves from infinitely

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†Corresponding author. E-mail: qwu@hit.edu.cn

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long metallic SWNTs and bundles excited by an electric line source. The analysis shows that the scattering intensity peak shifts and narrows the line shape in bundle in comparison with the SWNT case. The nanotube bundle radius plays a critical role in governing the scattering characteristics. It also shows that a relatively large amplitude scattered field can be obtained from a carbon nanotube bundle.

2. Analytic development

The SWNTs illuminated by an electric line source with a constant electric current $I_{\rm e}$ placed parallel to the nanotube is depicted in Fig. 1. The carbon nanotube is located in the cylindrical coordinate system with the associated Cartesian coordinate system as shown in the figure. It is of infinite extent in the z-direction, has a radius of a, and is centered at the origin of the coordinate systems. The ambient medium is free space. The position vector of a given observation point is $\boldsymbol{\rho}_{\rm o}$, while the position vector of the electric line source is $\boldsymbol{\rho}_{\rm s}$. The bundle is modeled by N metallic CNTs closely packed together with infinite length. Thus, the bundle can be modeled as a multishell structure comprising p concentric shells. The total number of CNTs within the bundle is $N = 3p^2 - 3p + 1$. The cross sectional radius R, determined by the radius of SWNT and the distance between two parallel SWNT, is given by $R = (2p-1) \times a + (p-1) \times 0.34$.

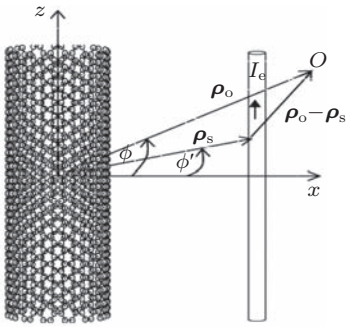


Fig. 1. A carbon nanotube illuminated by an electric line source located in free space.

The incident field generated by the source is given by[12]

$$E_z^{\rm i} = -\frac{\omega\mu_0 I_{\rm e}}{4}\sum_{m=-\infty}^{\infty}\begin{pmatrix} {\rm J}_m(k_0\rho_{\rm o})H_m^{(2)}(k_0\rho_{\rm s})\,{\rm e}^{{\rm j}m(\phi-\phi')} & \text{for } (\rho_{\rm o}<\rho_{\rm s}) \\ {\rm J}_m(k_0\rho_{\rm s})H_m^{(2)}(k_0\rho_{\rm o})\,{\rm e}^{{\rm j}m(\phi-\phi')} & \text{for } (\rho_{\rm o}>\rho_{\rm s}) \end{pmatrix}, \tag{1}$$

$$E_\phi^{\rm i} = E_\rho^{\rm i} = 0, \tag{2}$$

where the function ${\rm J}_m(x)$ is the Bessel function of the first kind, while $H_m^{(2)}(x)$ is the m-order Hankel function of the second kind. The scattering electric field $E_z^{\rm s}$ and the transmitting field $E_z^{\rm t}$ due to the existence of the SWNT can then be written as

$$E_z^{\rm s} = -\frac{\omega\mu_0 I_{\rm e}}{4}\sum_{m=-\infty}^{\infty} S_m H_m^{(2)}(k_0\rho_{\rm o})\,{\rm e}^{{\rm j}m(\phi-\phi')}, \tag{3}$$

$$E_z^{\rm t} = -\frac{\omega\mu_0 I_{\rm e}}{4}\sum_{m=-\infty}^{\infty} T_m {\rm J}_m^{(}k_0\rho_{\rm o})\,{\rm e}^{{\rm j}m(\phi-\phi')}, \tag{4}$$

where S_m and T_m are the unknown coefficients, and Hankel function of the second kind is also selected to indicate that the scattering field is a wave traveling in the outward radial direction. It is remarkable that the field inside the SWNT is not exactly zero or even decaying, where the modified Bessel function simply does not satisfy the wave equation of the problem. The effective boundary conditions are then applied at the carbon nanotube surface in order to determine S_m and T_m, and the final result is

$$S_m = \frac{-\eta\sigma_{\rm cn}(\omega)[{\rm J}_m(k_0a)]^2 H_m^{(2)}(k_0\rho_{\rm s})}{2/(\pi k_0 a) + \eta\sigma_{\rm cn}(\omega){\rm J}_m(k_0a)H_m^{(2)}(k_0a)}, \tag{5}$$

$$T_m = \frac{2/(\pi k_0 a)H_m^{(2)}(k_0\rho_{\rm s})}{2/(\pi k_0 a) + \eta\sigma_{\rm cn}(\omega){\rm J}_m(k_0a)H_m^{(2)}(k_0a)}, \tag{6}$$

where the quantum conductivity $\sigma_{\rm cn}(\omega)$ of the carbon nanotube is given by

$$\sigma_{\rm cn}(\omega) = \frac{{\rm J}\,{\rm e}^2\omega}{\pi^2\hbar a}\left\{\frac{1}{\omega(\omega-{\rm J}\nu)}\sum_{s=1}^{m}\int\frac{\partial F_{\rm c}}{\partial p_z}\frac{\partial\varepsilon_{\rm c}}{\partial p_z} - 2\sum_{s=1}^{m}\int {\rm d}p_z\varepsilon_{\rm c}|R_{\rm vc}|^2\frac{F_{\rm c}-F_{\rm v}}{\hbar^2\omega(\omega-{\rm J}\nu)-4\varepsilon_{\rm c}^2}\right\}, \tag{7}$$

where e is the charge of an electron, $\nu = 1/\tau$ is the phenomenological relaxation frequency with τ being the relaxation time, $\hbar$ is the reduced Planck's constant, $F_{\rm c,v}$ and $\varepsilon_{\rm c,v}$ are the equilibrium Fermi distribution function and electron dispersion relation in the

conduction or valance bands, respectively, and $R_{\mathrm{v,c}}$ is the matrix element for the tube. Details of the expressions for these quantities have been omitted and can be obtained in Ref. [4]. The effective surface conductivity of the bundle is given by $\sigma_{\mathrm{eff}} = D\sigma_{\mathrm{cn}}(\omega)/2\pi R$, where D is the number of SWNT of the pth shell in bundle.[13] The current induced on the surface of the SWNT can be written as

$$J_z = -\frac{\omega\mu_0 I_{\mathrm{e}}\sigma_{\mathrm{cn}}(\omega)}{4} \times \sum_{m=-\infty}^{\infty}\left[\frac{2/(\pi k_0 a)H_m^{(2)}(k_0\rho_{\mathrm{s}})\mathrm{J}_m(k_0 a)}{2/(\pi k_0 a)+\eta\sigma_{\mathrm{cn}}(\omega)\mathrm{J}_m(k_0 a)H_m^{(2)}(k_0 a)} \times \mathrm{e}^{\mathrm{J}m(\phi-\phi')}\right]. \quad (8)$$

One of the most important parameters in scattering is the scattering cross section obtained by knowing the scattering field in the far zone. From Eqs. (1), (3), and (5), the scattering width is given by

$$\sigma_{\mathrm{2D}} = \lim_{\rho_{\mathrm{o}}\to\infty}\left(2\pi\rho_{\mathrm{o}}\frac{\left|-\frac{\omega\mu_0 I_{\mathrm{e}}}{4}\sqrt{\frac{2\mathrm{J}}{\pi k_0\rho_{\mathrm{o}}}}\,\mathrm{e}^{\mathrm{J}k_0\rho_{\mathrm{o}}}\sum_{m=-\infty}^{\infty}\mathrm{J}^m S_m\,\mathrm{e}^{\mathrm{J}m(\phi-\phi')}\right|^2}{\left|-\frac{\omega\mu_0 I_{\mathrm{e}}}{4}H_0^{(2)}(k_0\,|\rho_{\mathrm{o}}-\rho_{\mathrm{s}}|)\right|^2}\right) = \frac{4}{k_0}\frac{\left|\sum_{m=-\infty}^{\infty}\mathrm{J}^m S_m\,\mathrm{e}^{\mathrm{J}m(\phi-\phi')}\right|^2}{\left|H_0^{(2)}(k_0\,|\rho_{\mathrm{o}}-\rho_{\mathrm{s}}|)\right|^2}, \quad (9)$$

which is dependent on ϕ even for small radius nanotubes.

3. Results and discussion

To test the validity of our solution, the metallic armchair (10, 10) carbon nanotube under consideration is compared with the exact Rayleigh spectroscopy experiments in Ref. [10]. Figure 2 shows that the scattering cross section predicted from Eq. (9) is in excellent agreement with the measured result in the range of 1.7–2.6 eV. The Rayleigh spectrum of (10, 10) carbon nanotube exhibits a well-defined resonant characteristic and line shape, which are perfectly represented by our analyses.

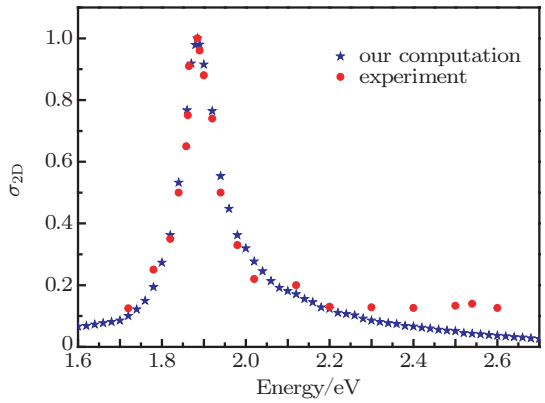


Fig. 2. (colour online) Comparison of the scattering width between measurement and theory.

The quantum conductance function in Eq. (7) is based on the tight binding model including optical transitions.[14,15] The energy of optical transition in metallic SWNTs is labeled by $E_{ii} = 3sb\gamma_0/a$, where $s = 1, 2, 3, \ldots$, and γ_0 is the overlap integral ($\gamma_0 = 3.03$ eV). In Ref. [10], the Rayleigh spectrum of the (10, 10) armchair nanotube exhibits a well-defined single E_{11} resonance feature, and the peak is lied in $E_{11} = 1.88$ eV, which agrees with our computational value of 1.89 eV and the theoretical prediction $E_{11} = 1.903$ eV based on the tight binding model.

The validity of this prediction is important not only for fundamental understanding of the scattering properties of SWNTs but also for its critical role in nano antenna in lower infrared and THz bands.

The following two figures deal with the current density induced over the surface of an SWNT at $\phi = \pi/3$. Figures 3 and 4 show the real and imaginary parts of the current density for the armchair carbon nanotube (m=10, 40, and 60), respectively. It can be seen that the value of J_z decreases with the increasing radius of the nanotube, which is apparent from Eq. (8).

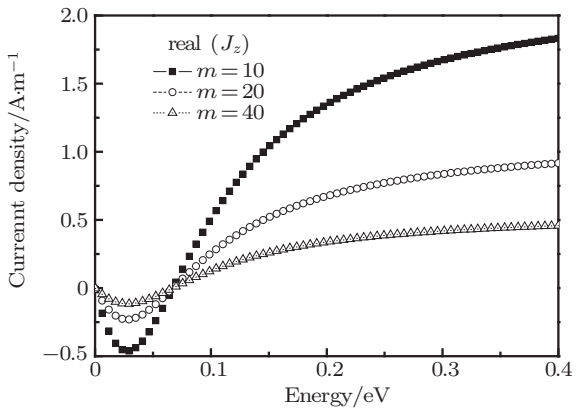


Fig. 3. The real part of the current density over the surface of an SWNT. Results correspond to $a = 0.678$ nm (solid line), $a = 1.356$ nm (dashed line), and $a = 2.712$nm (dotted line).

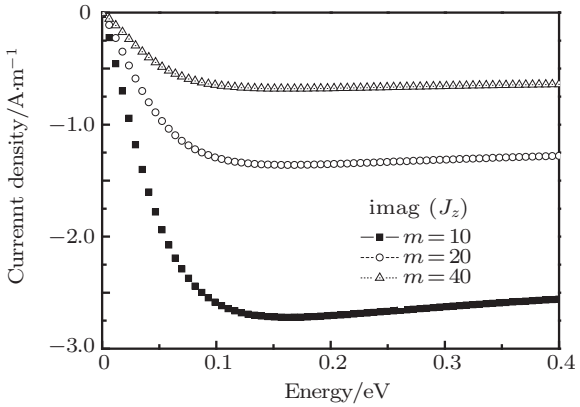


Fig. 4. The imaginary part of the current density over the surface of an SWNT. Results correspond to $a = 0.678$ nm (solid line), $a = 1.356$ nm (dashed line), and $a = 2.712$ nm (dotted line).

For the present system in the optical band and lower band, the radius a of the SWNT is much less than the wavelength ($a \ll \lambda$). From Eq. (9), the first term in the infinite series dominates and it is sufficient to represent the scattering cross section. In this case, the Bessel function of the first kind and the Hankel function of the second kind for zeroth-order can be approximated as $\mathrm{J}_0(k_0 a) \approx 1$ and $H_0^{(2)}(k_0 a) \approx -\mathrm{J}2/[\pi \ln(0.89 k_0 a)]$.

Although the scattering cross section increases with the increasing radius of the nanotube, the magnitude of the scattering cross section increases by only 0.02% when the radius of the nanotube is changed from 0.678 nm to 2.712 nm. As can be seen from Fig. 5, the scattering pattern for an armchair SWNT ($m = 10$, $a = 0.768$ nm) is almost identical to that of the case of an SWNT ($m = 40$, $a = 2.712$ nm). On the other hand, the scattering pattern of an SWNT is significantly different from that of a bundle.

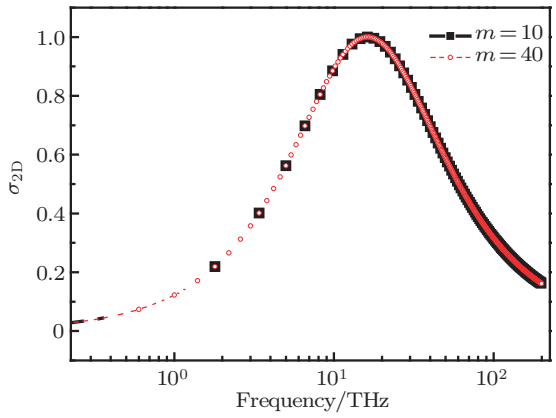


Fig. 5. (colour online) Normalized scattering cross section of an SWNT for $m = 10$ and $m = 40$.

Figures 6 and 7 show the normalized scattering cross section of an armchair (40, 40) SWNT and a bundle for $\phi' = 0°$ and $\phi \in [90°, 94°]$, respectively. In both the cases, the scattering width is dependant on ϕ, and when $\phi = 92°$, σ_{2D} approaches its maximum.

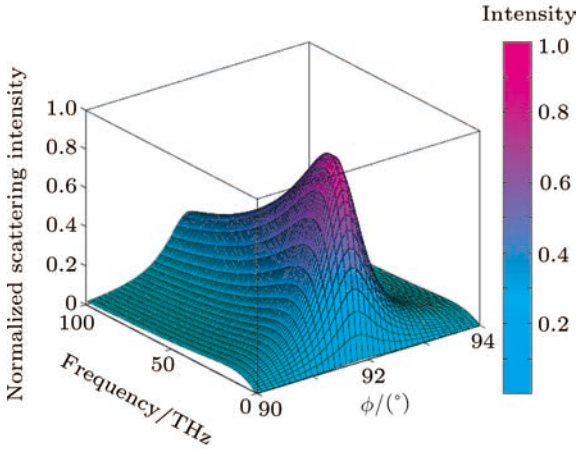


Fig. 6. (colour online) Scattering feature of armchair carbon nanotube with $a = 2.712$ nm.

From Figs. 6 and 7, it can be observed that compared with the SWNT case, the scattering intensity peak shifts to a lower frequency and narrows the line shape in the bundle, which is determined by the quantum conductance of the SWNT and the effective surface conductivity of the bundle.

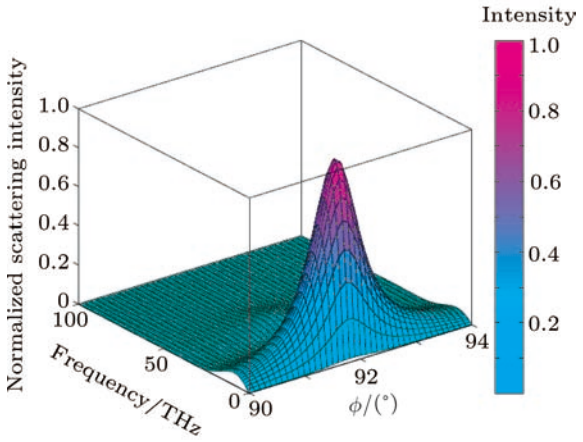


Fig. 7. (colour online) Scattering feature of a nanotube bundle with $R = 2.7$ μm.

4. Conclusion

The analytical solution for the electromagnetic scattering from the carbon nanotube exited by an electric line source has been presented. It is shown that the scattering pattern from an SWNT is significantly different from the bundle case when the bundle contains the identical armchair SWNT. It has been found that the maximum scattering cross section coefficient increases with the increasing nanotube radius, and

that the scattering cross section peak increases and its position shifts toward low frequencies in the bundle case.

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