Scattering by an array of parallel metallic carbon nanotubes

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The scattering of electromagnetic wave by an array of parallel metallic single-walled carbon nanotubes is investigated based on the boundary-value method. Electronic excitations over each nanotube surface are modeled as an infinitesimally thin cylindrical layer of the free-electron gas. The scattering cross section of both transverse magnetic (TM) and transverse electric (TE) uniform plane waves by the system at normal incidences is obtained.

Keywords: carbon nanotube, scattering, TM mode, TE mode

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The responses of carbon nanotubes (CNTs) to external electromagnetic fields over a broad range of frequencies have been the focus in recent years of many authors.[1–24] In this way, the problem of electromagnetic wave scattering from CNTs was treated using different theoretical methods. Slepyan *et al.*[15] formulated the Leontovich–Levin equation for optical scattering by using an achiral CNT of finite length, based on a quantum-mechanical microscopic model of the conductivity and found that CNTs can be used as optical nanoantennas of both the receiving and transmitting types. Hao and Hanson[16] presented a model for electromagnetic scattering from infinite planar arrays of finite-length metallic CNs, and isolated nanotubes, in the lower IR bands, using a semiclassical formulation based on a periodic Green's function for the array, and a quantum conductance function for the CNs. A microscopic calculation of the Rayleigh (elastic light) scattering spectra for single-walled CNTs (SWCNTs) was presented in Ref. [16]. Mikki and Kishk[18,19] provided a theoretical description of electromagnetic scattering by CNTs based on an effective-boundary condition. Recently, a detailed derivation for the problem of scattering of a plane wave from single- and two-walled CNTs was presented.[20–22] More recently, Wu *et al.*[23] obtained an analytical solution for the electromagnetic scattering from the infinite-length metallic CNT excited by an electric line source. Also, a theoretical investigation of line-source (both the electric and the magnetic) scattering by metallic multi-walled CNTs was presented in Ref. [24].

The present paper is an extension of the previous investigations[7,18–24] to study the electromagnetic scattering from an array of parallel metallic SWCNTs. The analysis begins by representing each field component by an infinite series of cylindrical harmonic functions with unknown coefficients. Then by enforcing the boundary conditions on the surface of each nanotube, an infinite set of equations is obtained which can be written in a matrix form. Although the resulting matrix equation is of infinite size, proper truncation can yield accurate numerical results.[7,25–31]

Assuming that an array of Q parallel metallic SWCNTs with radii $a_1, a_2, \ldots, a_Q$, and the surrounding medium is free space (i.e., vacuum), we use cylindrical coordinate (ρ, ϕ, z) for an arbitrary point in space. Let the system be exposed to an externally impressed electromagnetic field with TM polarization. The normal incident plane wave has E_z^i, H_ρ^i, and H_ϕ^i components. The incident electric field can be written as

$$E_z^i = E_0 \, \mathrm{e}^{\mathrm{j}\beta\rho\cos(\phi-\phi_0)}, \tag{1}$$

where $\beta = \omega/c$ is the free-space wave number, E_0 is a real constant, c is the light speed in vacuum, and ϕ_0 is the angle of incidence of plane wave with respect to the negative x axis, as shown in Fig. 1. In terms of the cylindrical coordinates of the q-th nanotube, whose center is located at (ρ_q', ϕ_q'), from Eq. (1), we find that

$$E_{zq}^i = E_0 \, \mathrm{e}^{\mathrm{j}\beta\rho_q'\cos(\phi_q'-\phi_0)} \sum_{n=-\infty}^{+\infty} \mathrm{j}^n \mathrm{J}_n(\beta\rho_q) \, \mathrm{e}^{\mathrm{j}n(\phi_q-\phi_0)}, \tag{2}$$

where J_n is the Bessel function of the first kind and the time-harmonic excitation $\exp(\mathrm{j}\omega t)$ is implied and suppressed everywhere. The corresponding scattered and transmitted electric field components of the q-th tube are given by

$$E_{zq}^s(\rho_q, \phi_q) = E_0 \sum_{n=-\infty}^{+\infty} \mathrm{j}^n A_q^n \mathrm{H}_n^{(2)}(\beta\rho_q) \, \mathrm{e}^{\mathrm{j}n\phi_q}, \tag{3}$$

$$E_{zq}^t(\rho_q, \phi_q) = E_0 \sum_{n=-\infty}^{+\infty} \mathrm{j}^n B_q^n \mathrm{J}_n(\beta\rho_q) \, \mathrm{e}^{\mathrm{j}n\phi_q}. \tag{4}$$

Here $\mathrm{H}_n^{(2)}$ is the Hankel function of the second kind and A_q^n and B_q^n represent the yet unknown coefficients related to the q-th cylinder, which includes the effect of all interactions between the nanotubes. The corresponding tangential magnetic

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field components can be obtained by using Maxwell's Faraday equation $\boldsymbol{H} = -(\mathrm{j}\omega\mu_0)^{-1}\nabla\times\boldsymbol{E}$.

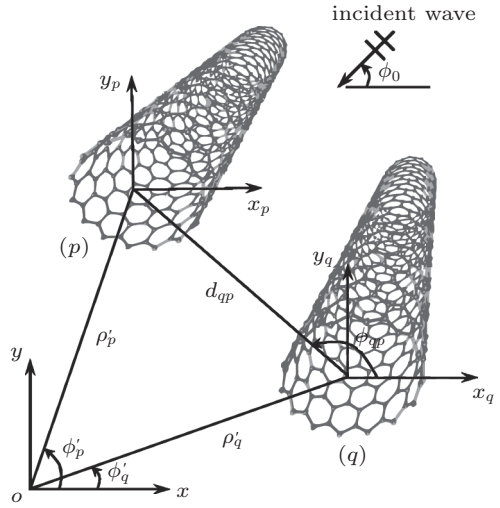


Fig. 1. Geometry of multiple SWCNTs and the coordinate systems.

The unknown amplitude coefficients can be found by applying the appropriate boundary conditions on the surface of the q-th nanotube. In addition to the continuity of the tangential components of the electric field vector at the q-th cylinder interface, as

$$E^i_{zq} + E^s_{zq} + \sum_{p=1;p\neq q}^{Q} E^s_{zp} = E^t_{zq}, \quad (\rho_q = a_q, 0 \le \phi_q \le 2\pi), \tag{5}$$

the second set of boundary conditions must ensure that all tangential magnetic field components experience a jump due to the conductivity $\sigma(\omega) = n_0 e^2/m^*(\gamma + \mathrm{j}\omega)$ associated with the q-th nanotube. Here n_0 is the two-dimensional free-electron density of each CNT, e and m^* are the electron charge and effective mass, respectively, and γ represents a small plasma loss term. This boundary condition can be expressed as

$$\mathrm{H}^i_{\phi q} + \mathrm{H}^s_{\phi q} + \sum_{p=1;p\neq q}^{Q} \mathrm{H}^s_{\phi p} - \mathrm{H}^t_{\phi q} = \sigma(\omega) E^t_{zq},$$
$$(\rho_q = a_q, 0 \le \phi_q \le 2\pi). \tag{6}$$

In this stage, it is necessary to express the scattered field from one tube in terms of the local coordinates of another tube. With the aid of the addition theorem for the Hankel functions, one can write the transformation from the p-th coordinates to the q-th coordinates as:

$$\mathrm{H}^{(2)}_n(\beta\rho_p)\,\mathrm{e}^{\mathrm{j}n\phi_p} = \sum_{n=-\infty}^{+\infty} \mathrm{J}_m(\beta\rho_q)\mathrm{H}^{(2)}_{m-n}(\beta d_{qp})\,\mathrm{e}^{\mathrm{j}m\phi_q}\,\mathrm{e}^{-\mathrm{j}(m-n)\phi_{qp}}, \tag{7}$$

$$d^2_{qp} = \rho'^2_p + \rho^2_q - 2\rho'_p\rho'_q\cos(\phi'_q - \phi'_p), \tag{8}$$

$$\phi_{qp} = \cos^{-1}\left[\frac{\rho'_p\cos\phi'_p - \rho'_q\cos\phi'_q}{d_{qp}}\right]. \tag{9}$$

Substituting Eqs. (2)–(4) [in conjunction with Eq. (9)] into the boundary conditions [Eqs. (5) and (6)] leads to a matrix system of equations for all tubes

$$\begin{bmatrix} [C^{\ell n}_{11}] & \cdots & [C^{\ell n}_{1p}] & \cdots & [C^{\ell n}_{1Q}] \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ [C^{\ell n}_{q1}] & \cdots & [C^{\ell n}_{qp}] & \cdots & [C^{\ell n}_{qQ}] \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ [C^{\ell n}_{Q1}] & \cdots & [C^{\ell n}_{Qp}] & \cdots & [C^{\ell n}_{QQ}] \end{bmatrix} \begin{bmatrix} [A^{\ell}_1] \\ \cdots \\ [A^{\ell}_q] \\ \cdots \\ [A^{\ell}_Q] \end{bmatrix} = \begin{bmatrix} [\Psi^{\ell}_1] \\ \cdots \\ [\Psi^{\ell}_q] \\ \cdots \\ [\Psi^{\ell}_Q] \end{bmatrix}, \tag{10}$$

where the vector $[A]$ represents the unknown expansion coefficients of the scattered field from the Q tubes and the element of the vector Ψ is given by

$$\psi^{\ell}_q = \mathrm{e}^{\mathrm{j}\beta\rho'_q\cos(\phi'_q-\phi_0)}\,\mathrm{e}^{-\mathrm{j}\ell\phi_0}. \tag{11}$$

Also, the element of the submatrices $[C^{\ell n}_{qp}]$ can be written as:

$$C^{\ell n}_{qp} = \begin{cases} 0, & p = q; \ell \neq n, \\ -\dfrac{2/\pi\beta a_q + \eta\sigma(\omega)\mathrm{H}^{(2)}_{\ell}(\beta a_q)\mathrm{J}_{\ell}(\beta a_q)}{\eta\sigma(\omega)\left[\mathrm{J}_{\ell}(\beta a_q)\right]^2}, & p = q; \ell = n, \\ -\mathrm{H}^{(2)}_{\ell-n}(\beta d_{qp})\,\mathrm{e}^{-\mathrm{j}(\ell-n)\phi_{qp}}, & p \neq q. \end{cases} \tag{12}$$

Here, $\eta = \sqrt{\mu_0/\varepsilon_0}$ is the wave impedance and the Wronskian property,

$$\mathrm{J}_m(x)\mathrm{Y}'_m(x) - \mathrm{J}'_m(x)\mathrm{Y}_m(x) = 2/\pi x,$$

has been used. Equation (10) can be solved numerically to retrieve the unknown scattering coefficients. The far scattered electric field can then be computed, after using the large argument approximation of the Hankel function and the far-field approximations $\rho_p \approx \rho - \rho'_p\cos(\phi'_p - \phi)$ and $\phi_p \approx \phi$ as:

$$E^s_z = E_0\sqrt{\frac{2\mathrm{j}}{\pi\beta\rho}}\,\mathrm{e}^{-\mathrm{j}\beta\rho}F(\omega,\phi), \tag{13}$$

where

$$F(\omega,\phi) = \sum_{p=1}^{Q} \mathrm{e}^{\mathrm{j}\beta\rho'_p\cos(\phi'_p-\phi)} \sum_{n=-\infty}^{+\infty} A^n_p \mathrm{j}^n\,\mathrm{e}^{\mathrm{j}n\phi}. \tag{14}$$

The scattering cross section $\sigma_{\rm scat}(\omega)$ of the multiple tube geometry is then given by

$$\sigma_{\rm scat}(\omega,\phi) = \frac{4}{\beta}\,|F(\omega,\phi)|^2. \tag{15}$$

The scattering from an array of parallel CNTs due to an incident plane wave with TE polarization is easily obtained from the above analysis by simply replacing $\mathrm{J}_\ell(\beta a_q)$ and $\mathrm{H}_\ell^{(2)}(\beta a_q)$ in Eq. (12) for $(p=q; n=\ell)$ by $\mathrm{J}'_\ell(\beta a_q)$ and $\mathrm{H}_\ell^{(2)'}(\beta a_q)$, respectively [$\mathrm{J}'_m(x)$ and $\mathrm{H}_m^{(2')}(x)$ denotes the derivative of the Bessel and Hankel function with respect to argument $x=\beta\rho$].

Now, let us present the simulation results of the scattering cross section of an array of SWCNTs for TM and TE waves. As the radius of the system increases, more terms in the infinite series of Eq. (14) are needed to obtain convergence. However for the present system in the optical range, we have $a_q \ll \lambda = 2\pi/\beta$, so, for TM wave the first term in Eq. (14) and for TE wave the first three terms ($n=0, n=\pm 1$) in Eq. (14) are dominant terms and they are sufficient to represent the scattered field.[20] Also, it is easy to find that for the present system for all values of ϕ'_p, ϕ and ϕ_0, $\mathrm{Re}[\mathrm{e}^{\mathrm{j}\beta\rho'_p\cos(\phi'_p-\phi)}] = \mathrm{Re}[\mathrm{e}^{\mathrm{j}\beta\rho'_p\cos(\phi'_p-\phi_0)}] \cong 1$.

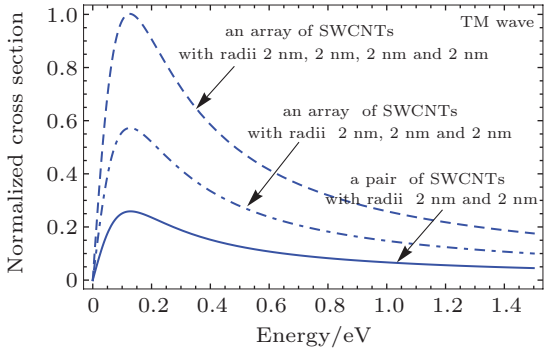


Fig. 2. (color online) Dependence of scattering cross section on the TM wave energy of a pair SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 2$ nm (solid blue line), the array of SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 2$ nm, and $a_3 = 2$ nm (dotted–dashed blue line) and the array of SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 2$ nm, $a_3 = 2$ nm, and $a_4 = 2$ nm (dashed blue line), when the axis-to-axis distance of SWCNTs is 5 nm and $\gamma = 2\times10^{14}$ Hz.

To investigate the geometrical effects of the system on their scattering characteristics, we assume a fixed axis-to-axis distance of SWCNTs and investigate the effect of increasing the number of SWCNTs and radii of the CNTs on the scattering characteristics. In Fig. 2, we show the dependence of scattering cross section on TM wave energy of a pair SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 2$ nm (solid blue line), the array of SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 2$ nm, and $a_3 = 2$ nm (dotted–dashed blue line) and the array of SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 2$ nm, $a_3 = 2$ nm, and $a_4 = 2$ nm (dashed blue line), when the axis-to-axis distance of SWCNTs is 5 nm and $\gamma = 2\times10^{14}$ Hz. The results are normalized to the maximum amplitude of the field. It is easy to find that the maximum scattering cross section coefficients increase with the increase of the number of SWCNTs.

On the other hand, we choose two different values of radii of SWCNTs. Plots of the scattering cross section computed using Eq. (15) are shown in Fig. 3, for TM wave. We consider an SWCNT with the radius $a_1 = 2$ nm and other ones with $a_2 = 4$ nm and 5 nm, when the axis-to-axis distance of SWCNTs is $d_{12} = 8$ nm and $\gamma = 2\times10^{14}$ Hz. It can be seen that the maximum scattering cross section coefficients increase with the increase of the radii of SWCNTs.

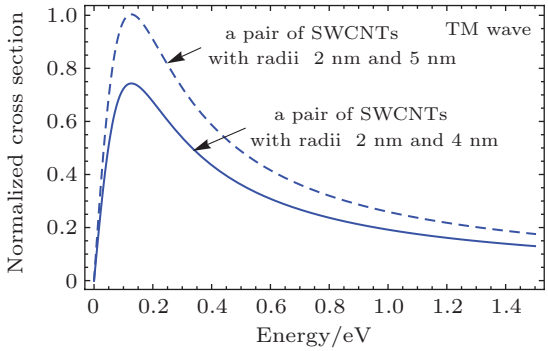


Fig. 3. (color online) Dependence of scattering cross section on the TM wave energy of two pairs of SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 4$ nm (solid blue line) and $a_1 = 2$ nm, $a_2 = 5$ nm (dashed blue line), when the axis-to-axis distance of SWCNTs is 8 nm and $\gamma = 2\times10^{14}$ Hz.

Plots of the scattering cross section computed using Eq. (14) for TE wave are shown in Fig. 4 for different values of two pairs of SWCNTs, when $\gamma = 2\times10^{14}$ Hz and $\phi_0 = 0$. One can see that the normalized scattering cross section coefficient increases with the increase of the radii of the CNTs while its position shifts toward low frequencies.

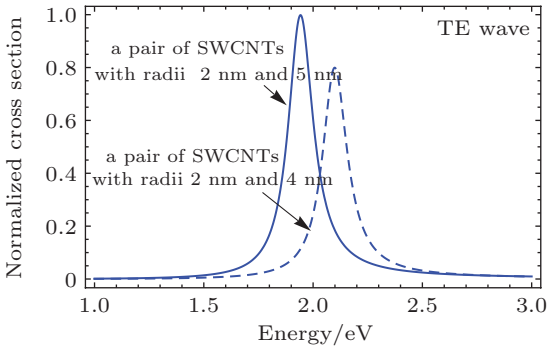


Fig. 4. (color online) Dependence of scattering cross section on TE wave energy of two pairs of SWCNTs with the radii $a_1 = 2$ nm, $a_2 = 4$ nm (solid blue line) and $a_1 = 2$ nm, $a_2 = 5$ nm (dashed blue line), when the axis-to-axis distance of SWCNTs is 8 nm, $\gamma = 2\times10^{14}$ Hz, and $\phi_0 = 0$.

In summary, we have used the modal series expansion of the scattered and transmitted fields in conjunction with appropriate boundary conditions to describe the scattering of the electromagnetic wave by an array of parallel metallic SWCNTs. We have derived general expressions for the radar cross

section per unit length of both TM and TE uniform plane waves by the system at normal incidences, respectively.

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