Supporting Information: Calculation of the near electric field distribution for an TMD coated GNS

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Here, we intend to calculate the spatial distribution of electric field for an TMD coated gold nanoshell in the presence of an incident electric field with x-polarized plane wave as $\mathbf{E}_i = E_0 \exp[ikr\cos\theta]\hat{\mathbf{x}}$ with a time dependence of $\exp(-i\omega t)$. This nanopartice has three layers so that each of them is characterized by a size parameter as $x_l = 2\pi n_m r_l/\lambda = kr_l$ and a relative refractive index as $m_l = N_l/N_m, l = 1,2,3$, where λ is the wavelength of the incident light in vaccum, r_l is the outer radius of the lth layer, N_m and N_l are the refractive indices of the medium (i.e., $N_m = \sqrt{\varepsilon_m}$) and its lth layer, respectively. The electric field in lth layer is expressed as the superposition of the complex vector harmonic functions including $\mathbf{M}^{(j)}_{oln}$ and $\mathbf{N}^{(j)}_{eln}$ ($j = 1,3$) as[1]

$$\mathbf{E}_l = \sum_{n=1}^{\infty} E_n \left[c_n^{(l)} \mathbf{M}^{(1)}_{oln} - i d_n^{(l)} \mathbf{N}^{(1)}_{eln} + i a_n^{(l)} \mathbf{N}^{(3)}_{eln} - b_n^{(l)} \mathbf{M}^{(3)}_{oln} \right], \tag{1}$$

where superscripts $j = 1$ and $j = 3$ denote the first kind of spherical Bessel and Henkel functions, respectively. These vector spherical harmonics in terms of the Ricaati-Bessel functions are written as[2]

$$\mathbf{M}^{(j)}_{oln} = \cos\phi\,\pi_n(\cos\theta)\frac{r_n^{(j)}(\rho)}{\rho}\hat{\mathbf{e}}_\theta - \sin\phi\,\tau_n(\cos\theta)\frac{r_n^{(j)}(\rho)}{\rho}\hat{\mathbf{e}}_\phi$$

$$\mathbf{N}^{(j)}_{eln} = \cos\phi\, n(n+1)\sin\theta\,\pi_n(\cos\theta)\frac{r_n^{(j)}(\rho)}{\rho^2}\hat{\mathbf{e}}_r + \cos\phi\,\tau_n(\cos\theta)\frac{D_n^{(j)}(\rho) r_n^{(j)}(\rho)}{\rho}\hat{\mathbf{e}}_\theta$$

$$-\sin\phi\,\pi_n(\cos\theta)\frac{D_n^{(j)}(\rho) r_n^{(j)}(\rho)}{\rho}\hat{\mathbf{e}}_\phi \tag{2}$$

where $\rho = km_l r$, $E_n = i^n E_0 (2n+1)/(n(n+1))$ and $r_n^{(j)}(\rho)$ for $j = 1$ and $j = 3$ indicates the Riccati-Bessel functions ψ_n and ζ_n, respectively. These functions are related to the spherical Bessel and Hankel functions as

$$j_n(\rho) = \frac{\psi_n(\rho)}{\rho}, \qquad h_n^{(1)} = \frac{\zeta_n(\rho)}{\rho} \tag{3}$$

and their logarithmic derivatives are defined as $D_n^{(1)} = \psi_n'/\psi_n$ and $D_n^{(3)} = \zeta_n'/\zeta_n$. The angular distribution functions π_n and τ_n can be calculated from the following recurrence relations[3] :

$$\pi_0(\cos\theta) = 0, \quad \pi_1(\cos\theta) = 1,$$

$$\pi_n(\cos\theta) = \frac{2n-1}{n-1}\cos(\theta)\pi_{n-1}(\theta) - \frac{n}{n-1}\pi_{n-2}(\theta) \quad (n \geq 2),$$

$$\tau_n(\cos\theta) = n\cos\theta\,\pi_n(\cos\theta) - (n+1)\pi_{n-1}(\cos\theta) \quad (n \geq 1). \tag{4}$$

Here, the expansion coefficients ($a_n^{(l)}$, $b_n^{(l)}$, $c_n^{(l)}$ and $d_n^{(l)}$) are calculated via using the procedure of Bohren and Huffman's[4]. For this purpose, the boundary conditions at all the interfaces due to maching the tangential components of electric field at each layer and the orthogonality condition for vector harmonics yield four independent linear equations for a given n[5]. Solving these equations, the expansion coefficients obtain as

$$a_n^{(l)} = \frac{D_n^{(1)}(m_l x_l)\Gamma_1(m_{l+1}, x_l) + \Gamma_3(m_{l+1}, x_l)\frac{m_l}{m_{l+1}}}{\zeta_n(m_l x_l)\mathscr{D}(m_l x_l)}$$

$$b_n^{(l)} = \frac{D_n^{(1)}(m_l x_l)\Gamma_2(m_{l+1}, x_l)\frac{m_l}{m_{l+1}} + \Gamma_4(m_{l+1}, x_l)}{\zeta_n(m_l x_l)\mathscr{D}(m_l x_l)} \tag{5}$$

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$$c_n^{(l)} = \frac{D_n^{(3)}(m_l x_l)\Gamma_2(m_{l+1}, x_l)\frac{m_l}{m_{l+1}} + \Gamma_4(m_{l+1}, x_l)}{\psi_n(m_l x_l)\mathscr{D}(m_l x_l)}$$

$$d_n^{(l)} = \frac{D_n^{(3)}(m_l x_l)\Gamma_1(m_{l+1}, x_l) + \Gamma_3(m_{l+1}, x_l)\frac{m_l}{m_{l+1}}}{\psi_n(m_l x_l)\mathscr{D}(m_l x_l)} \tag{6}$$

where

$$\mathscr{D}(z) = D_n^{(1)}(z) - D_n^{(3)}(z)$$

$$\Gamma_1(z) = a_n^{(l+1)}\zeta_n(z) - d_n^{(l+1)}\psi_n(z)$$

$$\Gamma_2(z) = b_n^{(l+1)}\zeta_n(z) - c_n^{(l+1)}\psi_n(z)$$

$$\Gamma_3(z) = d_n^{(l+1)}D_n^{(1)}(z)\psi_n(z) - a_n^{(l+1)}D_n^{(3)}(z)\zeta_n(z)$$

$$\Gamma_4(z) = c_n^{(l+1)}D_n^{(1)}(z)\psi_n(z) - b_n^{(l+1)}D_n^{(3)}(z)\zeta_n(z) \tag{7}$$

Since the electric field is finite at the origin, there are no outward waves in the first layer and it leads to an additional condition as $a_n^{(1)} = b_n^{(1)} = 0$. Moreover, the inward waves outside the particle must be equal to the incident electric field, so $c_n^{(4)} = d_n^{(4)} = 1$, $a_n^{(4)} = a_n$ and $b_n^{(4)} = b_n$, where a_n and b_n are the scattering coefficients. In order to obtain the coefficiencts a_n and b_n, one can apply a recursion algorithm with considering new coefficients A_n and B_n [5]. In this way:

$$A_n^{(1)} = 0, \quad H_n^a(m_1 x_1) = D_n^{(1)}(m_1 x_1),$$

$$H_n^a(m_l x_l) = \frac{R_n(m_l x_l)D_n^{(1)}(m_l x_l) - A_n^l D_n^{(3)}(m_l x_l)}{R_n(m_l x_l) - A_n^{(l)}}$$

$$A_n^{(l+1)} = R_n(m_{l+1}x_l)\frac{m_{l+1}H_n^a(m_l x_l) - m_l D_n^{(1)}(m_{l+1}x_1)}{m_{l+1}H_n^a(m_l x_l) - m_l D_n^{(3)}(m_{l+1}x_1)} \tag{8}$$

and

$$B_n^{(1)} = 0, \quad H_n^a(m_1 x_1) = D_n^{(1)}(m_1 x_1),$$

$$H_n^b(m_l x_l) = \frac{R_n(m_l x_l)D_n^{(1)}(m_l x_l) - B_n^l D_n^{(3)}(m_l x_l)}{R_n(m_l x_l) - B_n^{(l)}}$$

$$B_n^{(l+1)} = R_n(m_{l+1}x_l)\frac{m_l H_n^b(m_l x_l) - m_{l+1} D_n^{(1)}(m_{l+1}x_1)}{m_l H_n^b(m_l x_l) - m_{l+1} D_n^{(3)}(m_{l+1}x_1)} \tag{9}$$

where $R_n(z) = \psi_n(z)/\zeta_n(z)$. In this case, the calculation starts from $l = 1$ for $A_n^{(l)}$ and $B_n^{(l)}$, which results $A_n^{(1)} = B_n^{(1)} = 0$ according to the initial conditions inside the core. In the continuation of this method, from the known values of $A_n^{(1)}$ and $B_n^{(1)}$, the values $A_n^{(2)}$ and $B_n^{(2)}$ are calculated so that the final coefficients in these series determines the scattering coefficients a_n and b_n as $a_n = A_n^{(4)}$ and $b_n = B_n^{(4)}$. After calculating the scattering coefficients, we can obtain the expansion coefficients and eventually using 1 will be determined the electric field spatial distribution in the all layers.

Notes and references

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