Quantitative evaluation of Coulombic interaction in the oriented-attachment growth of nanotubes

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Derivation of CI between a growing NT and two attaching NPs

The derivation as follows is based on the configuration demonstration in Figure 1. Coulomb's law is employed to derive the CI between the attaching nanoparticles and the growing nanotube, which is expressed in Eq. 1,

$$E = \frac{1}{4\pi\varepsilon}\frac{Q_1 Q_2}{r} \tag{1}$$

where Q_1 and Q_2 represent the charges of two random points, r is the separation between the two points, and ε is the dielectric constant of the medium, respectively. In the derivation of CI between an attaching NP and a growing NT, the CI between the NP and a point in the cylindrical side of the NT is expressed in Eq. 2,

$$E_{1,P} = \frac{1}{4\pi\varepsilon}\frac{q_0 q_P}{r} \tag{2}$$

where q_0 $(= \sigma_0 * 4\pi{r_0}^2)$ represents the charge of the nanoparticle, r_0 represents the radius of NP, and q_p represents the charge of a random point in the cylindrical surface. The CIs between the two (outer and inner) cylindrical sides of the NT and the NP are expressed in Eq. 3 and Eq. 4,

$$E_{1,1} = \frac{1}{4\pi\varepsilon}\int_{c-\frac{l}{2}}^{c+\frac{l}{2}}\frac{q_0\sigma_1 2\pi r_1 dx}{r} = \frac{q_0 q_1}{4\pi\varepsilon l}\int_{c-\frac{l}{2}}^{c+\frac{l}{2}}\frac{dx}{\sqrt{x^2+r_1^2}} \tag{3}$$

$$E_{1,2} = \frac{1}{4\pi\varepsilon}\int_{c-\frac{l}{2}}^{c+\frac{l}{2}}\frac{q_0\sigma_1 2\pi r_2 dx}{r} = \frac{q_0 q_2}{4\pi\varepsilon l}\int_{c-\frac{l}{2}}^{c+\frac{l}{2}}\frac{dx}{\sqrt{x^2+r_2^2}} \tag{4}$$

where σ_1 represents the charge density on the cylindrical side of the NT, r_1 and r_2 are the radii of the outer and the inner cylindrical sides of the NT, c is the center-to-center separation between the nanoparticle and the nanotube, l is the length of the NT, $q_1 (= \sigma_1 * 2\pi r_1)$ is the surface charge of the outer cylindrical side of the NT, and $q_2 (= \sigma_1 * 2\pi r_2)$ is the surface charge of the inner cylindrical side of the NT. Eq. 5 shows the CI

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between the NP and the two cylindrical sides of the NT.

$$E_1 = E_{1,1} + E_{1,2}$$
$$= \frac{q_0 q_1}{4\pi\varepsilon l}\left[ln\left(c + \frac{l}{2} + \sqrt{\left(c + \frac{l}{2}\right)^2 + r_1^2}\right) - ln\left(c - \frac{l}{2} + \sqrt{\left(c - \frac{l}{2}\right)^2 + r_1^2}\right)\right]$$
$$+ \frac{q_0 q_2}{4\pi\varepsilon l}\left[ln\left(c + \frac{l}{2} + \sqrt{\left(c + \frac{l}{2}\right)^2 + r_2^2}\right) - ln\left(c - \frac{l}{2} + \sqrt{\left(c - \frac{l}{2}\right)^2 + r_2^2}\right)\right] \quad (5)$$

The expression of the CI between the NP and one end side of the NT is shown as Eq. 6,

$$E_2 = \frac{1}{4\pi\varepsilon}\frac{q_0 \sigma_2 2\pi x}{r}dx \quad (6)$$

where σ_2 is the surface charge density of the end side of the NT, and x represents the distance from the center point of the end side of the NT to a random point of the end side of the NT. Integration of Eq. 6 over x from 0 to r_1 yields the equation of CI between the NP and the two end sides of the NT, the diameters of which are equal to the outer diameter of the NT, as shown in Eq. 7,

$$E_{2,1} = \frac{1}{4\pi\varepsilon}\int_0^{r_1}\frac{q_0 \sigma_2 2\pi x dx}{r}$$
$$= \frac{q_0 q_3}{2\pi\varepsilon r_1^2}\int_0^{r_1}\frac{x dx}{\sqrt{x^2 + \left(c + \frac{l}{2}\right)^2}} + \frac{q_0 q_3}{2\pi\varepsilon r_1^2}\int_0^{r_1}\frac{x dx}{\sqrt{x^2 + \left(c - \frac{l}{2}\right)^2}} \quad (7)$$

where q_3 $(= \sigma_2 * \pi {r_1}^2)$ is the total surface charge of the circular end side of the NT, the diameter of which equals the outer diameter of the NT. Integration of Eq. 6 over x from 0 to r_2 leads to the equation of CI between the NP and the two end sides of the NT, the diameters of which are equal to the inner diameter of the NT, as shown in Eq. 8,

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$$E_{2,2} = \frac{1}{4\pi\varepsilon}\int_0^{r_2}\frac{q_0\sigma_2 2\pi x dx}{r}$$
$$= \frac{q_0 q_4}{2\pi\varepsilon r_2^2}\int_0^{r_2}\frac{xdx}{\sqrt{x^2+\left(c+\frac{l}{2}\right)^2}}$$
$$+\frac{q_0 q_4}{2\pi\varepsilon r_2^2}\int_0^{r_2}\frac{xdx}{\sqrt{x^2+\left(c-\frac{l}{2}\right)^2}} \quad (8)$$

where q_4 $(=\sigma_2 * \pi r_2{}^2)$ is the surface charge of the circular end side, the diameter of which equals the inner diameter of the NT. Then the CI between the NP and the two end sides of the NT can be expressed in Eq. 9.

$$E_2 = E_{2,1} - E_{2,2} = \frac{1}{4\pi\varepsilon}\int_0^{r_1}\frac{q_0\sigma_2 2\pi x dx}{r} - \frac{1}{4\pi\varepsilon}\int_0^{r_2}\frac{q_0\sigma_2 2\pi x dx}{r}$$
$$= \frac{q_0 q_3}{2\pi\varepsilon r_1^2}\int_0^{r_1}\frac{xdx}{\sqrt{x^2+\left(c+\frac{l}{2}\right)^2}} + \frac{q_0 q_3}{2\pi\varepsilon r_1^2}\int_0^{r_1}\frac{xdx}{\sqrt{x^2+\left(c-\frac{l}{2}\right)^2}}$$
$$- \frac{q_0 q_4}{2\pi\varepsilon r_2^2}\int_0^{r_2}\frac{xdx}{\sqrt{x^2+\left(c+\frac{l}{2}\right)^2}}$$
$$- \frac{q_0 q_4}{2\pi\varepsilon r_2^2}\int_0^{r_2}\frac{xdx}{\sqrt{x^2+\left(c-\frac{l}{2}\right)^2}} \quad (9)$$

Solution of Eq. 9 leads to Eq. 10.

$$E_2 = \frac{q_0 q_3}{2\pi\varepsilon r_1^2}\left[\sqrt{r_1^2+\left(c+\frac{l}{2}\right)^2} + \sqrt{r_1^2+\left(c-\frac{l}{2}\right)^2} - 2c\right] - \frac{q_0 q_4}{2\pi\varepsilon r_2^2}\left[\sqrt{r_2^2+\left(c+\frac{l}{2}\right)^2} + \sqrt{r_2^2+\left(c-\frac{l}{2}\right)^2} - 2c\right] \quad (10)$$

Assuming that the charge densities of the NR and the NP are identical ($\sigma_0 = \sigma_1 = \sigma_2 = \sigma$), based on Eqs. 5 and 10 the total CI between the NP and the NT can thus be expressed by Eq. 11,

$$E_{CI} = \frac{2}{\pi\varepsilon}\pi^2\sigma^2 r_0^2\left[r_1\left(ln\frac{a+c+\frac{l}{2}}{b+c-\frac{l}{2}}\right) + r_2\left(ln\frac{g+c+\frac{l}{2}}{f+c-\frac{l}{2}}\right) + (a+b-g-f)\right] \quad (11)$$

where $a = \sqrt{\left(c+\frac{l}{2}\right)^2 + r_1^2}$, $b = \sqrt{\left(c-\frac{l}{2}\right)^2 + r_1^2}$, $g = \sqrt{\left(c+\frac{l}{2}\right)^2 + r_2^2}$, $f = \sqrt{\left(c-\frac{l}{2}\right)^2 + r_2^2}$.

Since our analysis focuses on the CI between two attaching nanoparticles and a nanotube, we multiply Eq. 11 by a factor of 2 to obtain the final analytical expression of the CI between the growing NT and the two attaching NPs, as shown in Eq. 12.

$$E_{CI}{}' = \frac{4}{\pi\varepsilon}\pi^2\sigma^2 r_0^2\left[r_1\left(ln\frac{a+c+\frac{l}{2}}{b+c-\frac{l}{2}}\right) + r_2\left(ln\frac{g+c+\frac{l}{2}}{f+c-\frac{l}{2}}\right) + (a+b-g-f)\right] \quad (12)$$

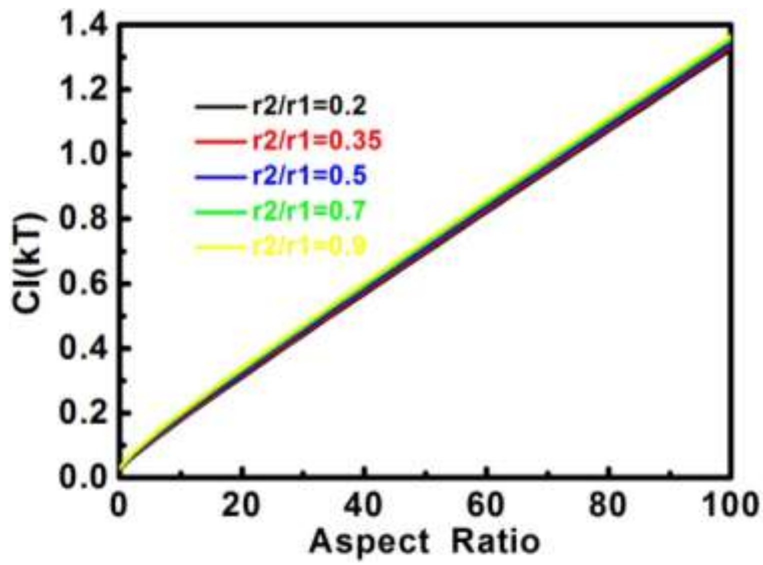

Figure S1. Plots of CI *versus* AR between NPs and NTs of different ratios of r_2 to r_1, assuming $r_0=r_1=50$ nm, and l=AR r_1+r_0.