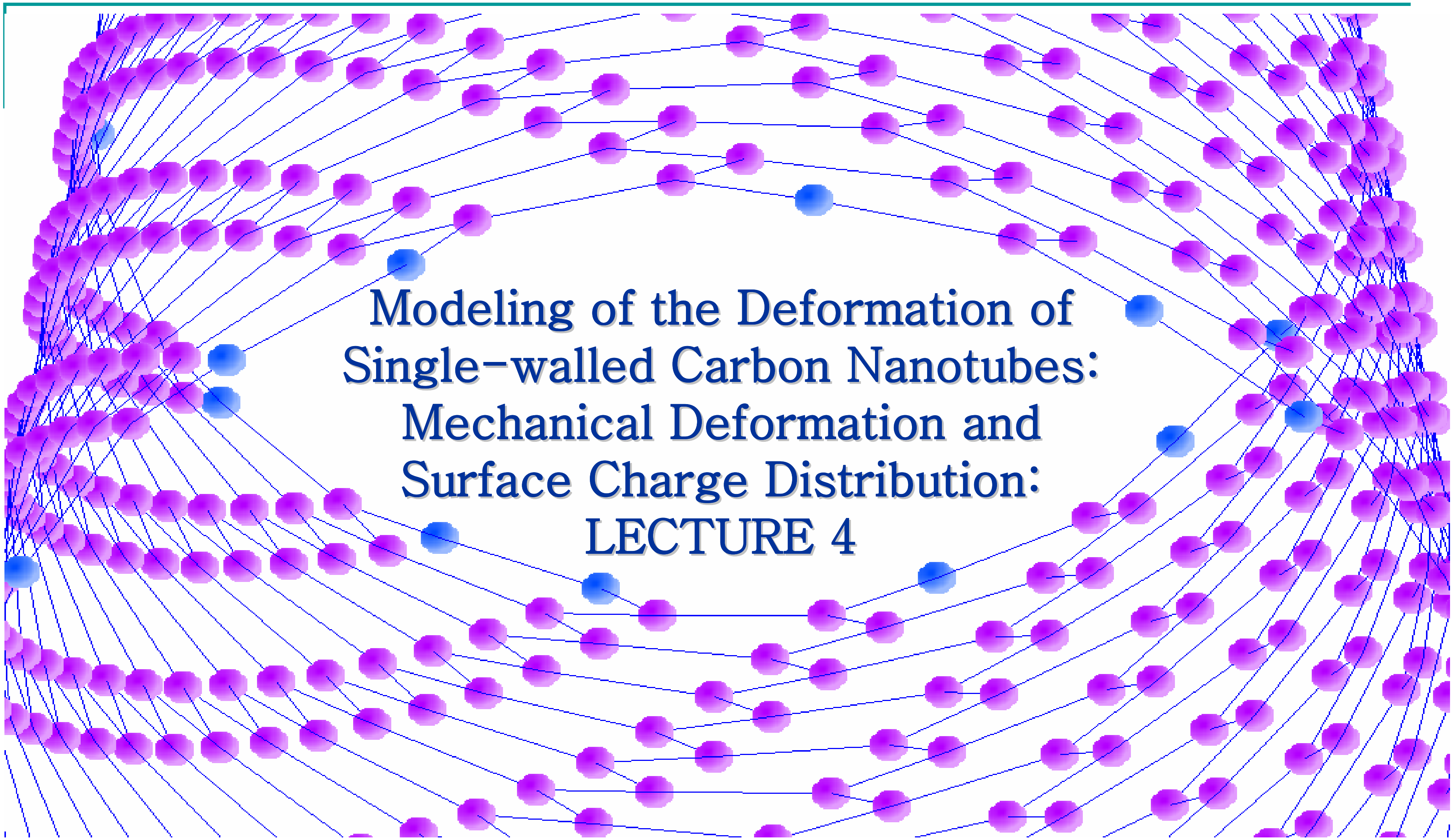

Modeling of the Deformation of Single-walled Carbon Nanotubes: Mechanical Deformation and Surface Charge Distribution: LECTURE 4

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Charge Distribution on Thin Conducting Nanotubes----Reduced 3-D Model

BEM Formulation for Potential Theory

Governing equation (in 2-D or in 3-D):

$$\nabla^2 u(\mathbf{x}) = 0, \quad \forall\, \mathbf{x} \in B \; (1)$$

with given boundary conditions on u or $q = \partial u/\partial n$ on the boundary ∂B.

Green's identity:

$$\int_B [u\nabla^2 v - v\nabla^2 u]dV = \int_{\partial B} \left[u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right] dS \quad (2)$$

Choose *v* to be the (infinite domain) Green's function $G(\mathbf{x}, \mathbf{y})$ that satisfies the equation:

$$\nabla^2 G(\xi, \mathrm{y}) = -\Delta(\xi, \mathrm{y}) \qquad (3)$$

where Δ is the Dirac delta function.

Green's functions that satisfy (3) are:

$$G(\xi, \mathrm{y}) = \frac{1}{2\pi} \ln \left[\frac{1}{r(\xi, \mathrm{y})} \right] \quad \text{in} \quad 2D$$

$$G(\xi, \mathrm{y}) = \frac{1}{4\pi r(\xi, \mathrm{y})} \quad \text{in} \quad 3D \qquad (4)$$

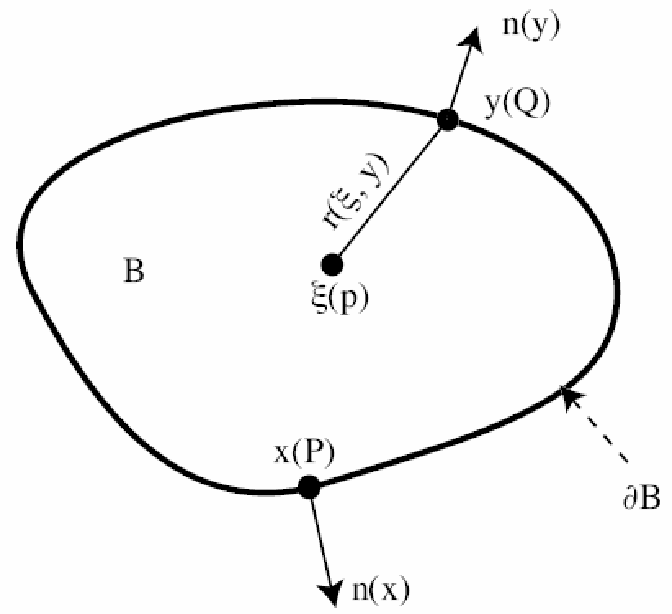


Figure 1:

Substitute (4) into (2) and use (3) to get:

$$u(\boldsymbol{\xi}) = \int_{\partial B} [G(\boldsymbol{\xi}, \mathbf{y}) q(\mathbf{y}) - F(\boldsymbol{\xi}, \mathbf{y}) u(\mathbf{y})] dS(\mathbf{y}) \quad (5)$$

where $$F(\boldsymbol{\xi}, \mathbf{y}) = \frac{\partial G(\boldsymbol{\xi}, \mathbf{y})}{\partial n(\mathbf{y})} \quad (6)$$

Now let $\boldsymbol{\xi} \in B \to \mathbf{x} \in \partial B$ to get the BIE:

$$C(\mathbf{x}) u(\mathbf{x}) = ⨍_{\partial B} [G(\mathbf{x}, \mathbf{y}) q(\mathbf{y}) - F(\mathbf{x}, \mathbf{y}) u(\mathbf{y})] dS(\mathbf{y}) \quad (7)$$

where $C(\mathbf{x}) = \alpha(\mathbf{x})/2\pi$, with $\alpha(\mathbf{x})$ the included angle at $\mathbf{x} \in \partial B$, and ⨍ the CPV of the integral.

Discretization of the BIE (7) - A simple case :

straight constant boundary elements.

$$\alpha u(P^{(i)}) = \sum_{j=1}^{N_E} \int_{\partial B_j} \left[\frac{\partial \ln r(P^{(i)},Q)}{\partial n(Q)} u(Q) - \ln r(P^{(i)},Q) q(Q) \right] dS(Q) \tag{8}$$

$$\alpha u(P^{(i)}) = \sum_{j=1}^{N_E} u(Q^{(j)}) \int_{\partial B_j} \frac{\partial \ln r(P^{(i)},Q)}{\partial n(Q)} dS(Q)$$
$$-q(Q^{(j)}) \int_{\partial B_j} \ln r(P^{(i)},Q) dS(Q)$$

$$\alpha u_i = A_{ij} u_j - B_{ij} q_j \tag{10}$$

$$\alpha I\{u\} = [A]\{u\} - [B]\{q\} \tag{11}$$

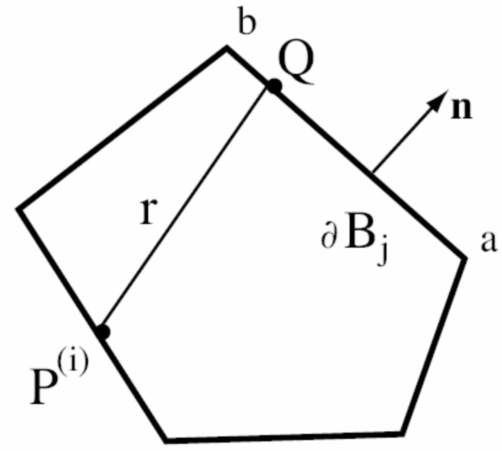


Figure 2:

For convex region B:

$$A_{ij} = \begin{cases} \theta_b - \theta_a & \text{for} \quad D \neq 0 \\ 0 & \text{for} \quad D = 0 \end{cases} \qquad (12)$$

$$B_{ij} = \begin{cases} D\left[\tan(\theta)(\ln(r) - 1) + \theta\right]_a^b & \text{for} \quad D \neq 0 \\ \beta\left[r(\ln(r) - 1\right]_a^b & \text{for} \quad D = 0,\ P^{(i)} \notin \partial B_j \\ r_b(\ln(r_b) - 1) + r_a(\ln(r_a) - 1) & \text{for} \quad D = 0, \\ & P^{(i)} \in \partial B_j \end{cases} \qquad (13)$$

$$\beta = \begin{cases} 1 & \text{for} \quad r_b > r_a \\ -1 & \text{for} \quad r_b < r_a \end{cases} \qquad (14)$$

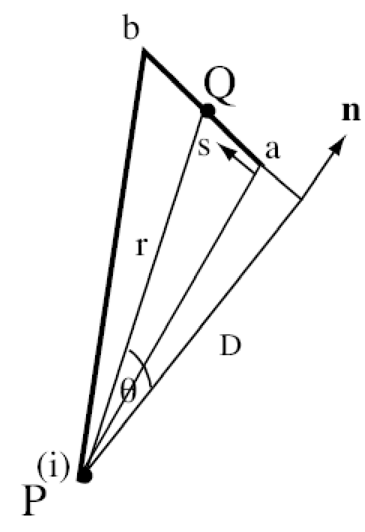


Figure 3:

$$\alpha I\{u\} = [A]\{u\} - [B]\{q\} \qquad (15)$$

Switching columns:

$$[C]\{x\} = [D]\{y\} \equiv \{b\} \qquad (16)$$

where $\{x\}$ contains the unknown and $\{y\}$ the prescribed boundary values.

It is noted that the above procedure requires each node/element to interact with all other nodes/elements directly. Therefore, $\mathcal{O}(N_E)^2$ operations are required to compute the matrices $[C]$ and $[D]$. Storage requirement is also $\mathcal{O}(N_E)^2$.

BEM Formulation for 3-D Potential Theory Outside a Doubly-connected Body

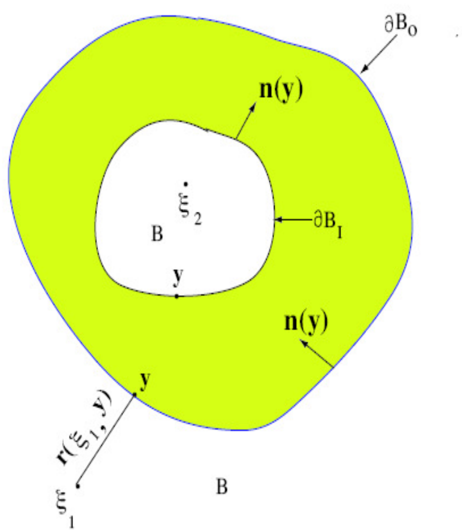
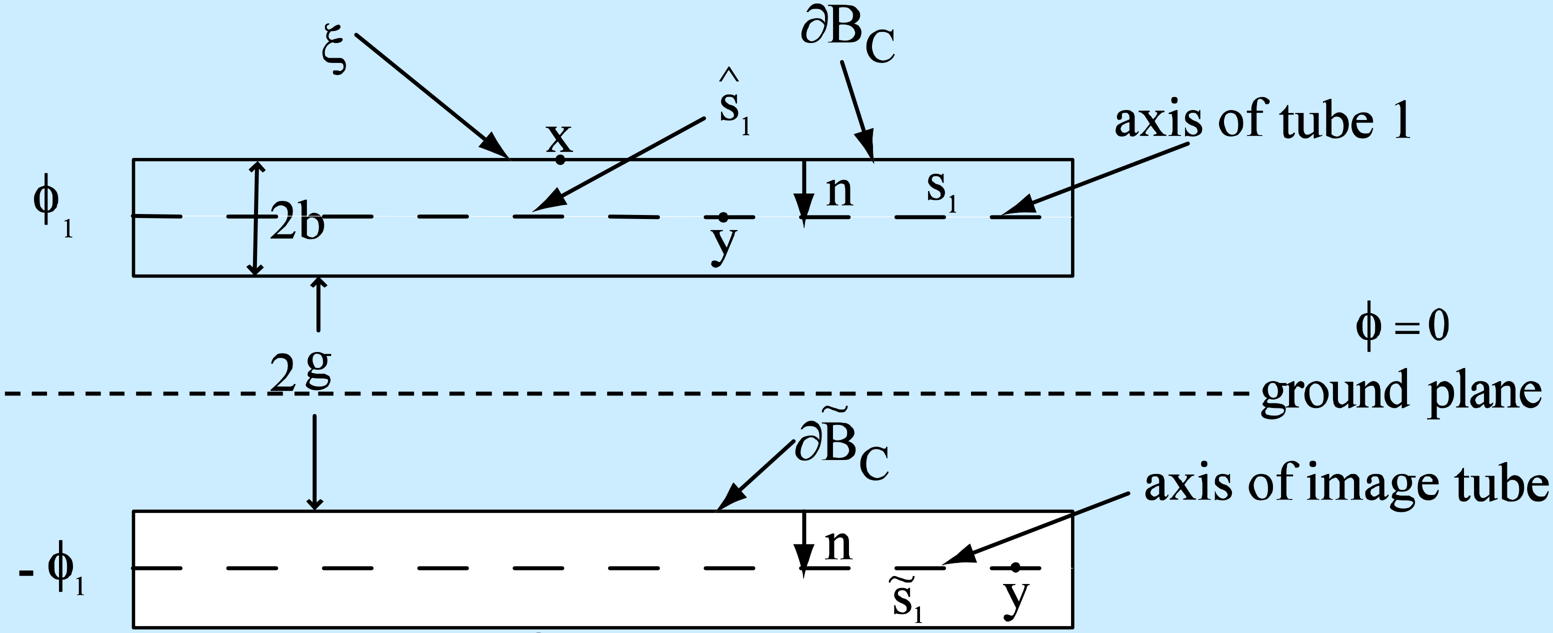


Figure 3: Cross-section of a prismatic doubly-connected conductor

$$
\begin{aligned}
\phi(\boldsymbol{\xi}) = & \int_{\partial B_0} \frac{\sigma(\mathbf{y})}{4\pi\epsilon r(\boldsymbol{\xi},\mathbf{y})} ds(\mathbf{y}) + \int_{\partial B_I} \frac{\sigma(\mathbf{y})}{4\pi\epsilon r(\boldsymbol{\xi},\mathbf{y})} ds(\mathbf{y}) \\
& + \int_{\partial B_0} \frac{\mathbf{r}(\boldsymbol{\xi},\mathbf{y}) \cdot \mathbf{n}(\mathbf{y})\phi(\mathbf{y})}{4\pi r^3(\boldsymbol{\xi},\mathbf{y})} ds(\mathbf{y}) \\
& + \int_{\partial B_I} \frac{\mathbf{r}(\boldsymbol{\xi},\mathbf{y}) \cdot \mathbf{n}(\mathbf{y})\phi(\mathbf{y})}{4\pi r^3(\boldsymbol{\xi},\mathbf{y})} ds(\mathbf{y}) + C \\
& + \int_{\partial B_E} \frac{\sigma(\mathbf{y})}{4\pi\epsilon r(\boldsymbol{\xi},\mathbf{y})} ds(\mathbf{y}) \\
& + \int_{\partial B_E} \frac{\mathbf{r}(\boldsymbol{\xi},\mathbf{y}) \cdot \mathbf{n}(\mathbf{y})\phi(\mathbf{y})}{4\pi r^3(\boldsymbol{\xi},\mathbf{y})} ds(\mathbf{y}), \qquad \boldsymbol{\xi} \in B \qquad (17)
\end{aligned}
$$

Only the first integral survives for a thin conductor with $\phi = A$.

BIEs for CNT

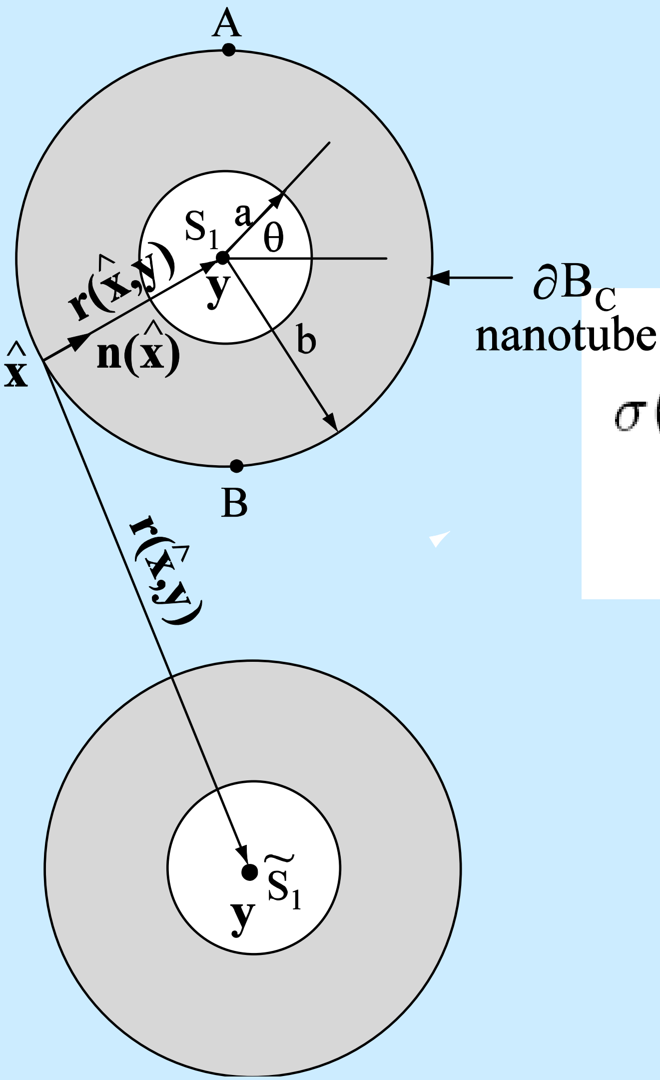


For $\mathbf{x} \in \partial Bc$:

$$\phi(x) = \int_{s_1} \frac{q(y)}{4\pi\varepsilon r(x,y)} dl(y) + \int_{\tilde{s}_1} \frac{q(y)}{4\pi\varepsilon r(x,y)} dl(y) + C \qquad (18)$$

$$q(y) = \int_0^{2\pi} \sigma(y_3, b, \theta) b d\theta \qquad y_3 \in s_1 \ or \ \tilde{s}_1 \qquad (19)$$

Gradient BIE - Source Point Approaching the Nanotube Surface



$$\sigma(\mathrm{x}) = \epsilon \frac{\partial \phi}{\partial n}(\mathrm{x}) = \epsilon \mathbf{n}(\mathrm{x}) \cdot [\nabla_{\xi} \phi(\boldsymbol{\xi})]_{\xi=\mathrm{x}} \qquad (20)$$

$$\sigma(\hat{\mathrm{x}}) = \int_{s_1 \cup \tilde{s}_1} \frac{\mathbf{r}(\hat{\mathrm{x}}, \mathrm{y}) \cdot \mathbf{n}(\hat{\mathrm{x}}) q(\mathrm{y})}{4\pi r^3(\hat{\mathrm{x}}, \mathrm{y})} d\ell(\mathrm{y}), \qquad \hat{\mathrm{x}} \in \partial B_C \qquad (21)$$

This is a post-processing step.

Charge density q as a function of length

$l_N\,(nm)$	$q_0\,(pC/m)$ computed	$q_0 = \frac{2\pi\varepsilon\phi}{\operatorname{arccosh}(1+g/b)}\,(pC/m)$ exact for $l_N \to \infty$	difference(%)
1000	8.59	8.051	6.65
1500	8.35		3.71
2000	8.24		2.34
3000	8.15		1.23

table 1 varying length of nanotube

Two nanotube models with $\phi_1 = 1$ volt, $\tilde{\phi}_1 = -1$ volt $\varepsilon = 8.854 \times 10^{-12}$F/m.
$b = 1$ nm and $g = 500$ nm.

Charge density q as a function of outer radius

$b(nm)$	$q_0(pC/m)$ computed	$q_0 = \frac{2\pi\varepsilon\varphi}{\operatorname{arccos}h(1+g/b)}(pC/m)$ exact for $l_N \to \infty$	difference(%)
20	14.37	14.08	2.06
7.5	11.53	11.34	1.68
3	9.70	9.57	1.36
1	8.15	8.051	1.23

table 2 varying outer radius of nanotube

Two nanotube models with $\phi_1 = 1$ volt, $\tilde{\phi}_1 = -1$ volt $\ell_N = 3000$ nm and $g = 500$ nm.
$\varepsilon = 8.854 \times 10^{-12}$ F/m.

Performs well for $\ell_N/(2b) \geq 500$

$L/b \geq 500$

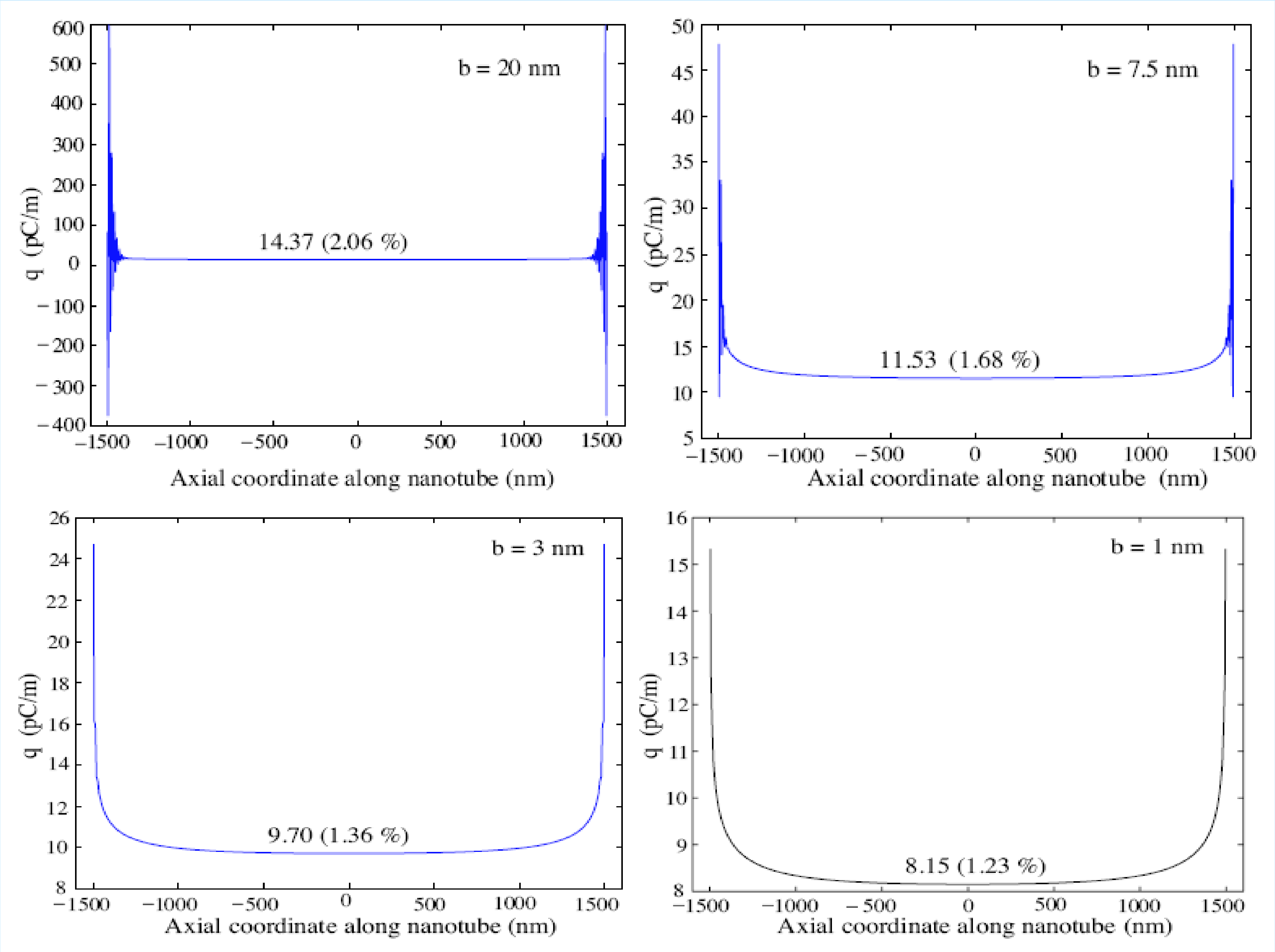


Figure 9 Charge density q along nanotube for different values of b

Charge density q as a function of gap

$g(nm)$	$q_0(pC/m)$ computed	$q_0 = \frac{2\pi\varepsilon\varphi}{\text{arccos}\,h(1+g/b)}(pC/m)$ exact for $l_N \to \infty$	difference(%)
500	8.15	8.051	1.23
100	10.49	10.48	0.1
25	14.08	14.08	0
5	22.38	22.45	0.31

table 3 varying gap between nanotube and ground

Two nanotube models with $\phi_1 = 1$ volt, $\tilde{\phi}_1 = -1$ volt $\ell_N = 3000$ nm and $g = 500$ nm.
$\varepsilon = 8.854 \times 10^{-12}$ F/m b=1nm.

Performs well for $g/(2b) \geq 2.5$

Charge density q as a function of number of elements

number of elements	q_0 at center (pC/m)
11	8.1526
25	8.1523
51	8.1521
101	8.1520
201	8.1519

table 4 convergence test—varying number of elements (8.051)

Two nanotube models with $\phi_1 = 1$ volt, $\tilde{\phi}_1 = -1$ volt $\ell_N = 3000$ nm and $g = 500$ nm
$\varepsilon = 8.854 \times 10^{-12}$ F/m.

Gradient BIEs for a CNT with image

$$\sigma(x) = \varepsilon \frac{\partial \phi}{\partial n}(x) = \varepsilon\, n(x) \cdot [\nabla_{\xi} \phi(\xi)]_{\xi = x}$$

$$\sigma(x_3, b, \pi/2) = \int_{s_1^+ \cup s_2^+} \frac{q(y)\, r(x^+, y) \cdot n(x^+)}{4\pi r^3(x^+, y)}\, dl(y)$$

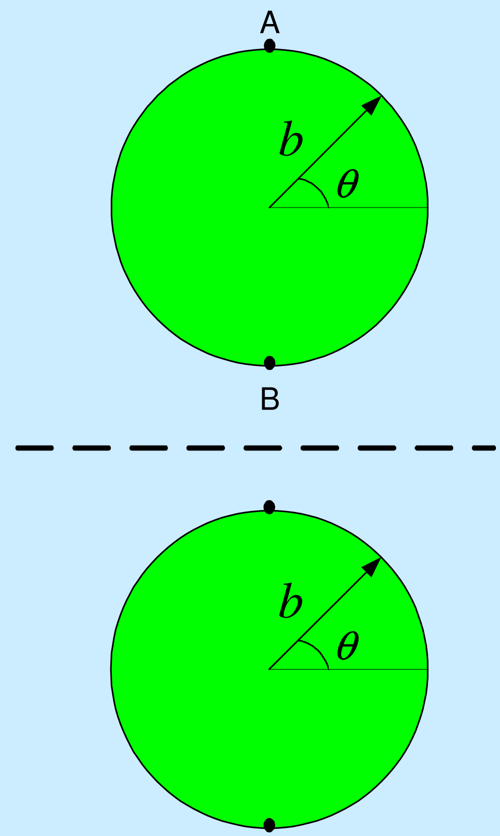


Figure 10 2 Cross section model

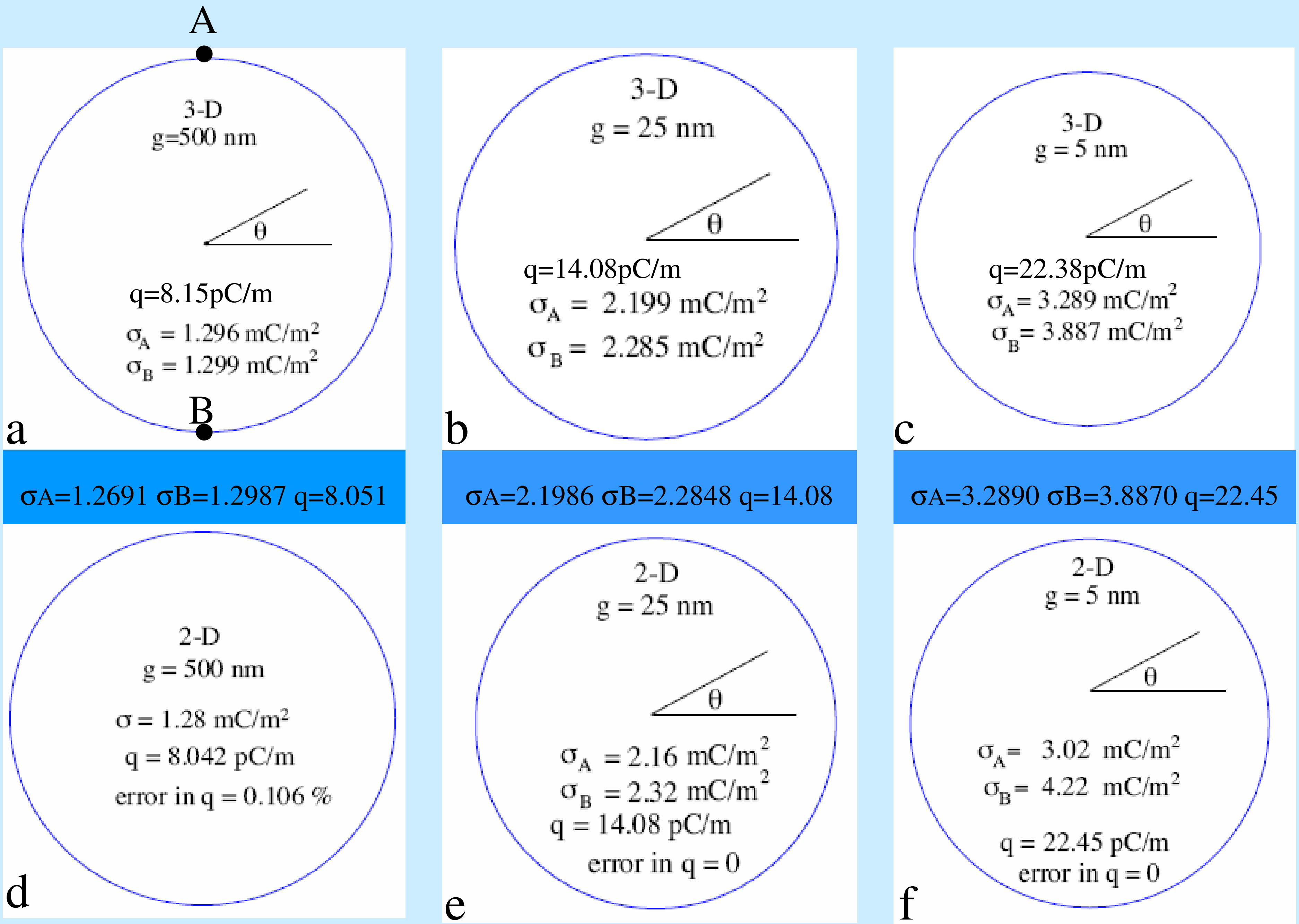
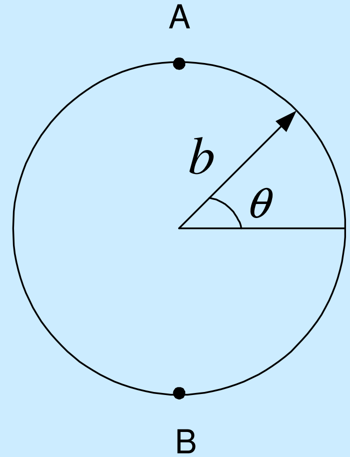


Figure 11 Polar plots of σ for different values of g 3 Deduced model (a)g=500nm (b)g=25nm (c)g=5nm
2 Dross section model (d)g=500nm (e)g=25nm (f)g=5nm

		3D	2D	Analytical soln
g=500	σ_A	1.2963	1.28	1.2961
	σ_B	1.2985	1.28	1.2987
g=25	σ_A	2.1987	2.16	2.1986
	σ_B	2.2849	2.32	2.2848
g=5	σ_A	3.2890	3.02	3.2890
	σ_B	3.8870	4.22	3.8870

table 5 charge density on two points A & B



$$\sigma(A) = \frac{q}{\pi b}\left[\frac{g+b}{2g+3b}\right]$$

$$\sigma(B) = \frac{q}{\pi b}\left[\frac{g+b}{2g+b}\right]$$

Two nanotube models with $\phi_1 = 1$ volt, $\tilde{\phi}_1 = -1$ volt $\ell_N = 3000$ nm and $g = 500$ nm.
$\varepsilon = 8.854 \times 10^{-12}$ F/m b=1nm

Three Nanotubes with three imaginary tubes

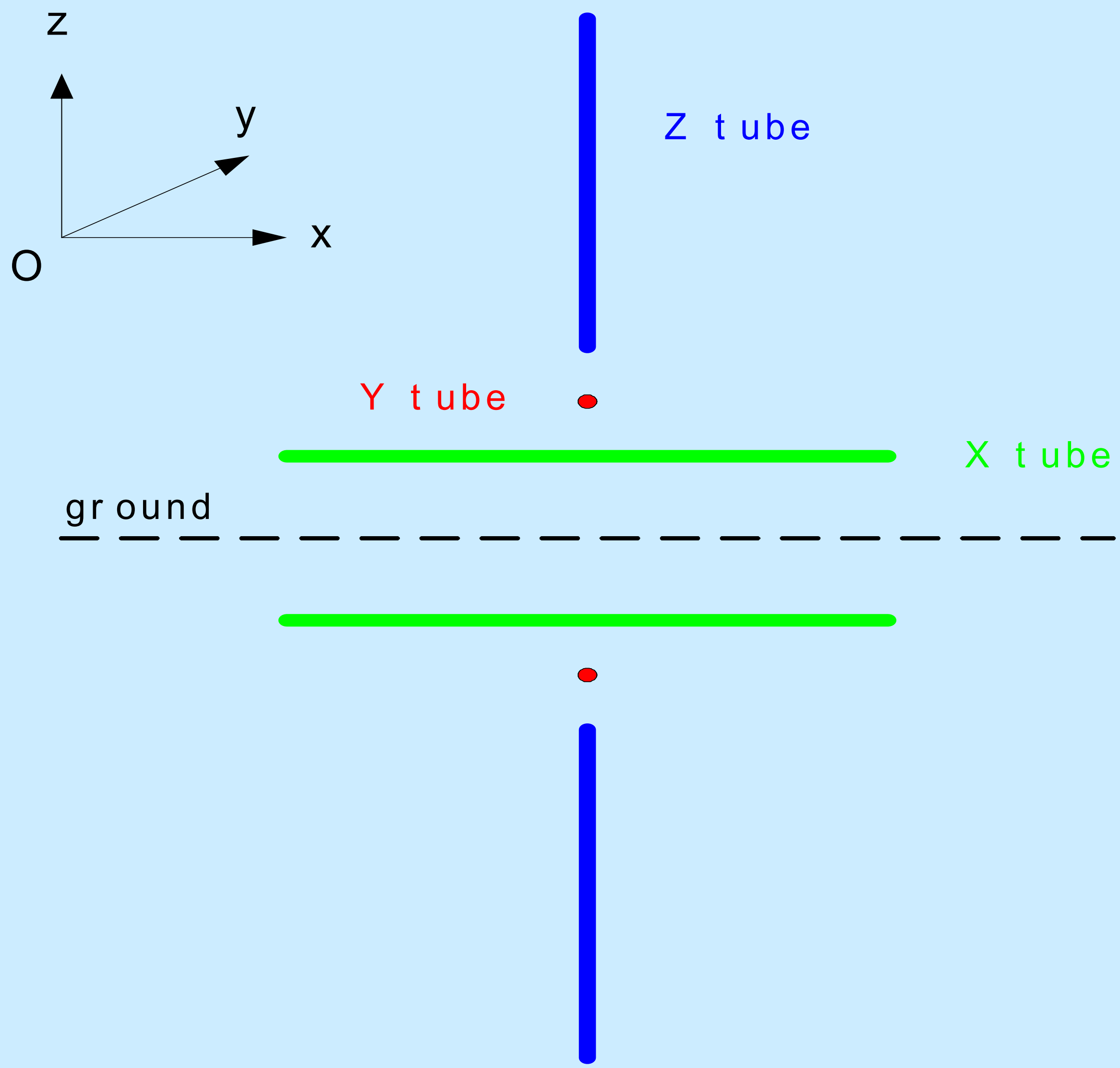
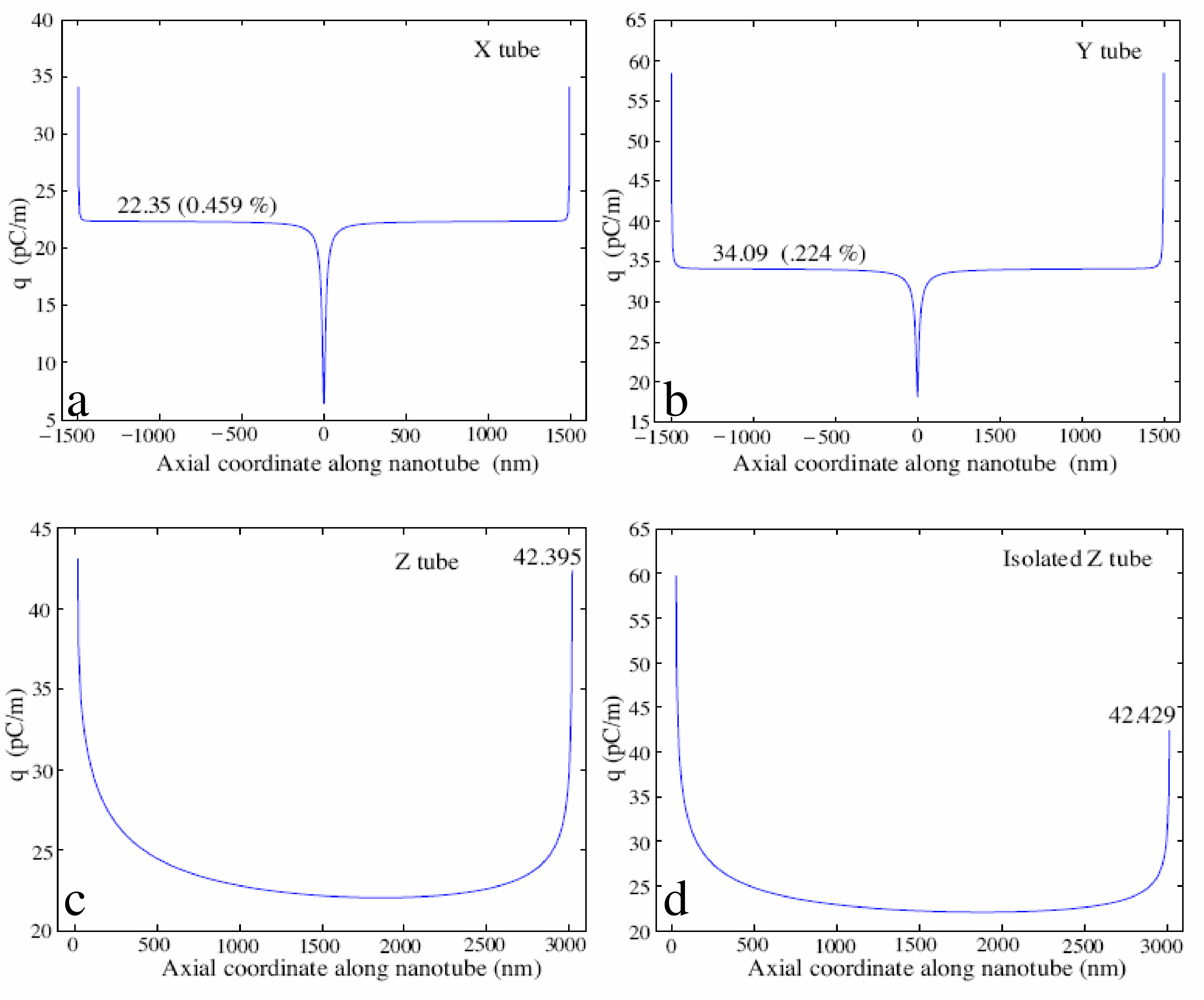


Figure 12 Configuration with three tubes



$\ell_{N1} = \ell_{N2} = \ell_{N3} = 3000nm,\ g_1 = g_2 = g_3 = 5nm \quad \phi_1 = 1, \phi_2 = 2, \phi_3 = 3 \quad b = 1nm \quad \varepsilon = 8.854\times10^{-12} F/m$

Figure 13 q along (a) tube X (b)tube Y (c) tube Z (d) isolated Z tube

H. Chen and S. Mukherjee, Charge distribution on thin conducting nanotubes. International Journal for Numerical Methods in Engineering. 2006. In press.

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