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Nanotube Devices: A Microscopic Model

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A microscopic model is developed for calculating electrostatic properties of nanotube devices. It is shown that the quantum-mechanical approach yields the same results as the statistical calculation in the limit of a thin tube suspended over a conducting gate at a distance exceeding the nanotube radius. A closed analytic expression is obtained for the atomistic capacitance of a straight nanotube and for a nanotube with a modest curvature. This method allows the fast and exact calculation of device parameters for the nanotube electromechanical systems and nanotube electronic devices. © *2002 MAIK "Nauka/Interperiodica".*

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The high strength of carbon nanotubes, along with low lateral bending stiffness, a size comparable with the scale of modern nanotechnologies, and unique electronic properties provide good prerequisites for their use in nanotube electromechanical systems (NEMS).

The functioning of nanotweezers composed of two multiwall nanotubes with their spacing controlled by an applied voltage was demonstrated experimentally in 2001 [1]. In 2000, it was suggested that a memory cell can be created on the basis of two crossing nanotubes [2].

However, the available models and programs for simulating device characteristics of micron-scale electromechanical systems cannot be used for the calculation of NEMS without substantial modification. At the same time, *ab initio* calculations of nanotube electronic and electromechanical devices seem to be impossible. Therefore, the development of an appropriate physical model is quite topical. Continuum approximations are most promising for modeling such devices, because they provide a high accuracy and minimal computational expenses. In this work, a microscopic model is suggested for the description of electrostatic properties of NEMS, which, in conjunction with the parameterization previously developed for the continuum elasticity of nanotubes [3] and with the continuum theory of van der Waals forces, allows the derivation of basic equations for the analysis of the operation of nanotube devices in nanoelectronics.

In this work, we will apply the electrostatic model to the analysis of equilibrium charge-carrier distribution over the nanotube surface, which is necessary for modeling NEMS operation (Fig. 1). In NEMS, the nanotube shape is determined by the balance between the electrostatic and elastic forces acting on the tube. For weak bending, typical of NEMS, the elastic forces can be considered within the framework of a one-dimensional continuum model [4]. To determine the electrostatic forces, one should calculate the distribution of a charge accumulated on the nanotube under the action of the applied voltage; i.e., one should calculate the distributed capacitance. At present, the conducting nanotubes are described using classical electrostatics of macroscopic conductors, while the quantum-size effects are disregarded. This work fills this gap and gives an estimate for the resulting corrections. The capacitance of a weakly bent nanotube situated over a flat conducting contact (gate) is expressed in terms of the capacitance of a metallic cylinder of the same shape.

Theoretical model. First, we ignore all contact phenomena occurring at the contact–nanotube boundary.[1] Second, we ignore the transverse polarization of the nanotube and assume that the charge density depends, generally, only on the curvilinear coordinate l along the nanotube axis.[2]

The key approximation consists in the use of a local statistical relation between the acting potential and charge density

$$\rho(l) = e\int_0^{E_0(l)} \nu(E)dE, \qquad (1)$$

[1] In our model, the difference $\Delta W = W_M - W_{NT}$ in work functions of an electron in the contact material and the nanotube can be taken into account. In doing so, the relation for E_0 should be replaced by $E_0(l) = \Delta W - e\phi^{\text{act}}(l)$.

[2] The estimate of the relative contribution to the capacitance from the transverse polarization gives $\dfrac{R^2}{4h^2}\dfrac{1}{\log(2h/R)} \ll 1$.

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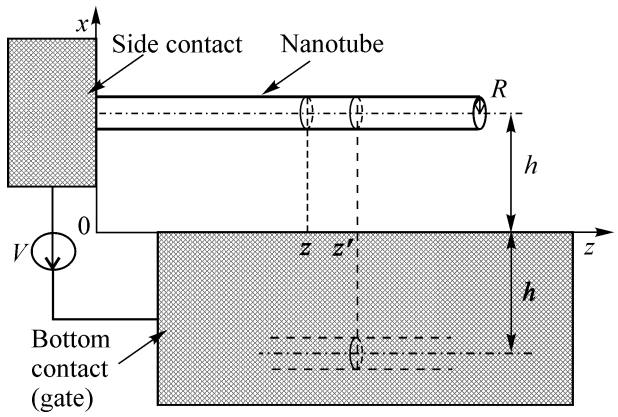

Fig. 1. Scheme of a nanotube electromechanical device. The image charge in the bottom contact (gate) is shown by dashes.

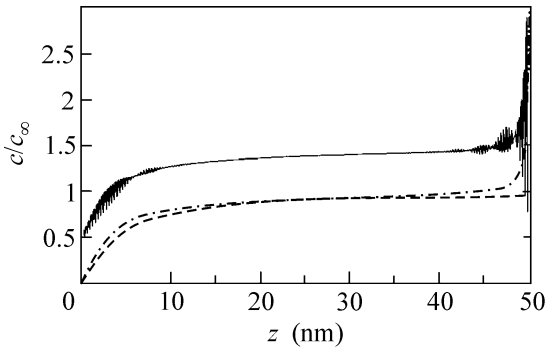

Fig. 2. Linear capacitance of a straight nanotube (in units of c_∞) vs. the distance (in nm) to the side contact. The results of quantum-mechanical calculation (solid curve) are shifted upward, because they coincide with the results of statistical calculation (dot-and-dash curve) to within oscillations (see text). The dashed curve is an approximation (10). The nanotube height is 5 nm, its radius is 0.67 nm, and its length is 50 nm.

where $E_0(l) = -e\phi^{act}(l)$ is the electroneutrality level measured from the Fermi level of the side contact, $\phi^{act}(l)$ is the acting potential on the nanotube axis reckoned from the potential of the side contact, $\nu(E)$ is the density of electronic (hole) states in the nanotube, the energy E is measured from the electroneutrality level; and $e > 0$ is the absolute value of electron charge. This model was proposed by Odintsov and Tokura for considering the Schottky barrier between the contact and the nanotube [5]. Since the density of electron wave functions in the ring direction is constant if the transverse polarization is ignored, by the acting potential in all formulas should be meant its value averaged over the nanotube cross section.

For the conducting nanotubes, the density of states near the electroneutrality level is constant and equals $\nu_M = 8/3\pi b\gamma_0$. Here, $b = 0.14$ nm and $\gamma_0 = 2.7$ eV are the bond length and the hopping integral, respectively. Then, if the condition $e|\phi^{act}| \le \frac{3}{2}\gamma_0(b/R)$, where R is the nanotube radius, is met, the charge density linearly depends on the acting potential

$$\rho(l) = -e^2\nu_M\phi^{act}(l). \qquad (2)$$

The product of the density of states into the squared electron charge $e^2\nu_M = 3.2$ is the dimensionless parameter of our problem.

Expression (1) is written in the zero-temperature limit. However, since the density of states is constant, Eq. (2) also holds for the temperatures at which carrier thermal excitations to the next subband can be ignored.

To test the statistical model, we calculated the charge distribution on a straight armchair nanotube of finite length by solving the Poisson and Schrödinger equations self-consistently. The Schrödinger equation was solved in the tight-binding approximation [6]. The resulting charge density and the corresponding value calculated by the statistical model coincided to within quantum beats due to finiteness of the nanotube length (Fig. 2). Analogous beats were observed experimentally in [7].

Semi-infinite straight nanotube over flat contact. Let us consider a single-wall nanotube arranged parallel to the flat contact at a height h (Fig. 1). The voltage V is applied between the side and bottom contacts. We will reckon the acting potential from the side contact. Then, the potential of the bottom contact is $-V$ and the charge density on the nanotube is positive.

The Green's function $G(\mathbf{r}, \mathbf{r}')$ in the region bounded by two perpendicular planes is the sum of the potentials of a probe unit charge and three image charges. The acting potential can be written as

$$\phi^{act}(\mathbf{r}) = \phi^{ext}(\mathbf{r}) + 4\pi\int G(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')d\mathbf{r}'. \qquad (3)$$

The first term in Eq. (3) is the potential created by two contacts with the voltage V applied to them in the absence of the nanotube. By integrating the Poisson equation for two perpendicular contacts, one obtains this term in the form

$$\phi^{ext}(\mathbf{r}) = \phi^{ext}(x, z) = -V\frac{2}{\pi}\arctan\left(\frac{z}{x}\right). \qquad (4)$$

The second term is the potential created by the nanotube charge and the image charges. Substituting Eq. (3) into Eq. (2) and taking into account that the nanotube

charge density depends only on z, one obtains the integral equation for the linear charge density

$$\frac{\rho(z)}{e^2\nu_M} + \int_0^\infty F(z, z')\rho(z')dz' = -\phi^{\text{ext}}(z) \tag{5}$$

with the one-dimensional Green's function

$$F(z, z') = \frac{1}{4\pi^2} \times \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} 4\pi G((z, R, \alpha), (z', R, \alpha'))d\alpha d\alpha' \tag{6}$$

as a kernel, where α and α' are the angular coordinates of the points $\mathbf{r}$ and $\mathbf{r}'$ in the nanotube-fixed cylindrical system of coordinates. The quantity $F(z, z')$ is the energy of screened Coulomb interaction between two uniformly charged rings representing cross sections of a nanotube of radius R at distances z and z' from the side contact (Fig. 1). In Eq. (6), averaging is done over the angles α and α', because the acting potential in Eq. (2) means its average over the nanotube cross section.

If the distances z and z' to the side contact are much larger than the height h, the contribution from the image charges in the side contact to the one-dimensional Green's function is on the order of $2h^2/(z + z')^3$ and, hence, can be ignored in comparison with the influence of the image charge in the bottom contact. Then, the kernel depends only on the difference $\Delta z = |z - z'|$ and behaves as

$$F(z, z') = \frac{2}{\pi\Delta z}K\left(-\frac{4R^2}{|\Delta z|^2}\right) - \frac{1}{\sqrt{(\Delta z)^2 + 4h^2}} \approx \begin{cases} \frac{1}{\pi R}\log\left(\frac{8R}{\Delta z}\right), & \Delta z \ll R, \\ \frac{1}{\Delta z}, & R \ll \Delta z \ll 2h, \\ \frac{2h^3}{(\Delta z)^3}, & \Delta z \gg 2h, \end{cases} \tag{7}$$

where K is the complete elliptic integral of the first kind. Let us now determine the asymptotic value of the charge density at $z \longrightarrow \infty$. The right-hand side of Eq. (5) becomes equal to the applied voltage V, and the charge density becomes

$$\rho_\infty = -\phi_\infty^{\text{ext}} c_\infty \approx V c_\infty^{\text{met}}(1 - c_\infty^{\text{met}}/e^2\nu_M). \tag{8}$$

In Eq. (8), $c_\infty = (1/e^2\nu_M + 1/c_\infty^{\text{met}})^{-1}$ is the nanotube atomistic capacitance and the notation

$$c_\infty^{\text{met}} = \left(\int_{-\infty}^{\infty} F(\Delta z)d\Delta z\right)^{-1} = \frac{1}{2\log(2h/R)} \tag{9}$$

is introduced for the capacitance of a unit length of an infinite metallic cylinder of radius R situated at a height h parallel to the flat conducting contact. Thus, the relative correction to the classical capacitance is $-c_\infty^{\text{met}}/e^2\nu_M$. For the typical values $h = 5$ nm and $R = 0.67$ nm ([10, 10] armchair nanotube), this amounts to 8%. The correction to the capacitance is inversely proportional to the nanotube density of states, so that it is inversely proportional to the number of layers in multilayer nanotubes. The correction to capacitance weakly (logarithmically) depends on the ratio of the nanotube radius to the distance from the contact.

By analogy with [5], one can analytically calculate the charge-density Fourier component for the straight semi-infinite nanotube (see Appendix). However, for the bent nanotube one fails to obtain a solution in the closed form. Away from the side contact, the charge density changes slowly compared to the one-dimensional Green's function. For this reason, to find an approximate expression for the charge density as a function of the distance to the side contact, one may factor charge density outside the integral sign in Eq. (5). As a result, one arrives at the following approximate expression describing the behavior of the charge density as it approaches its asymptotic value ρ_∞ (see Appendix):

$$\rho(z) \approx -c_\infty\phi^{\text{ext}}(z). \tag{10}$$

To make an estimate for engineering and calculating the characteristics of nanotube electronic and electromechanical devices, we suggest that the finite-length nanotube be divided into three regions: (i) near-contact region, where the screening effect of the image charge in the side contact should be taken into account, (ii) central region, where the charge density is determined by the screening effect of the image charges in the bottom contact (gate), and (iii) end region (only for nanotubes with a free edge), where the charge density is higher than in the central region.

For example, the charge density on the straight single-wall nanotube behaves as follows: it increases linearly on the length of order h near the side contact, asymptotically approaches the value ρ_∞ following the hyperbolic law, and again then increases on the length of order R near the nanotube end (Fig. 2). Correspondingly, the electric field component along the nanotube axis is equal to $c_\infty V/e^2\nu_M h$ in the near-contact region and decreases rapidly as $c_\infty Vh^2/e^2\nu_M hz^2$ in the central region. This approximation allows for the rapid calculation of the Coulomb forces when modeling NEMS.

Bent nanotube of finite length. Let the nanotube axis form be specified by the function $\mathbf{r}(l)$. The specific

charge density on the nanotube is determined by the equation

$$\frac{\rho(l)}{e^2\nu_M} + \int_0^L F(l, l')\rho(l')dl' = -\phi^{\text{ext}}(\mathbf{r}(l)), \quad (11)$$

where L is the nanotube length and, similarly to Eq. (6), the one-dimensional Green's function $F(l, l')$ is equal to the energy of a screened Coulomb interaction of two uniformly charged rings representing cross sections of the nanotube at distances l and l'.

By integrating with respect to dz' and introducing the function $F_1(z, z') = F(l, l')\sqrt{1 + h'(z')^2}$, where $h(z)$ is the x coordinate of a small nanotube element at a distance z from the side contact, one obtains the equation for the charge density in the form analogous to Eq. (5),

$$\frac{\rho(z)}{e^2\nu_M} + \int_0^\infty F_1(z, z')\rho(z')dz' = -\phi^{\text{ext}}(h(z), z). \quad (12)$$

Let us now find the approximate solution to Eq. (12) for a deformed nanotube. Let the nanotube be initially situated at a height h_0 parallel to the bottom contact and bent under the action of electrostatic forces. The nanotube height over the bottom contact, the kernel of Eq. (12), and the charge density can be written as

$$h = h_0 + \delta h, \quad F_1 = F_0 + \delta F, \quad \rho = \rho_0 + \delta\rho, \quad (13)$$

where F_0 and ρ_0 are, respectively, the kernel and the charge density for the straight nanotube at a height h_0. Note that $\delta F < 0$ for downbending, because the screening image charges in the bottom contact become closer to the nanotube in this case. Then, assuming that the nanotube bending is small, one obtains the following equation for the correction $\delta\rho$:

$$\frac{\delta\rho(z)}{e^2\nu_M} + \int_0^\infty F_0(z, z')\delta\rho(z')dz' = -\int_0^\infty \delta F(z, z')\rho_0(z')dz' - \frac{\partial\phi^{\text{ext}}}{\partial h}\delta h. \quad (14)$$

As pointed out above, the charge density in the central region of the straight nanotube increases very slowly and tends to ρ_∞. One can then factor $\rho_0 \approx \rho_\infty$ outside the integral sign on the right-hand side of Eq. (14) for the central region of the nanotube because of a fast decrease in δF. Now, the function $F_0(z, z')$ in the integral on the left-hand side of Eq. (14) has a logarithmic singularity at $z = z'$ and rapidly decreases at $|z - z'| > 2h$ [see Eq. (7)]. Since we assume that the bending is small, while the capacitance logarithmically depends on the height, the charge density is a smooth function of the coordinate z. Then, the charge-density variation can also be factored outside the integral sign on the left-hand side of Eq. (14). Introducing notation $E_x^{\text{ext}} = -\partial\phi^{\text{ext}}/\partial h$, one obtains the following expression for the correction to the charge density:

$$\delta\rho(z) = -Vc_\infty^2\int_0^\infty \delta F(z, z')dz' + c_\infty E_x^{\text{ext}}\delta h. \quad (15)$$

Therefore, the capacitance of the bent nanotube is

$$c(z) = c_\infty - c_\infty^2\int_0^\infty \delta F(z, z')dz' + \frac{1}{V}c_\infty E_x^{\text{ext}}\delta h. \quad (16)$$

As the density of states ν_M tends to infinity, our problem reduces to determining the specific capacitance of a metallic cylinder shaped like a nanotube. After the approximate solution of Eq. (12), for the bent metallic cylinder one has

$$c^{\text{met}}(z) = c_\infty^{\text{met}} - c_\infty^{\text{met}^2}\int_0^\infty \delta F(z, z')dz' + \frac{1}{V}c_\infty^{\text{met}}E_x^{\text{ext}}\delta h. \quad (17)$$

Comparing Eqs. (16) and (17) with the use of Eq. (8) for c_∞ and retaining only the leading term in the correction to the capacitance, one obtains the following relation between the capacitance of the bent nanotube and the capacitance of a bent metallic cylinder:

$$c(z) \approx c^{\text{met}}(z)\left(1 - \frac{c^{\text{met}}(z)}{e^2\nu_M}\right). \quad (18)$$

Equation (18) generalizes Eq. (8).

Thus, we have found a simple relation between the capacitance of a weakly bent nanotube and the capacitance of a metallic cylinder of the same shape.

The results of our calculations allow one to formulate the following principles of modeling the electrostatic properties of electromechanical and electronic nanodevices based on single- and multiwall carbon nanotubes: (1) the equilibrium one-dimensional specific charge density at the tube surface is linearly related to the external potential, with the proportionality coefficient designated below as the nanotube atomistic capacitance; (2) the nanotube atomistic capacitance is determined not only by the intrinsic properties of the nanotube material (density of states at the Fermi level) but also by the geometry of a device (in NEMS, distance from the gate) because of the one-dimensional character of charge screening in the system; (3) the nanotube atomistic capacitance can be expressed analytically through the classical capacitance of a metallic cylinder *of the same* shape and through the density of states in the nanotube; the corresponding expression holds for a single-wall nanotube in the voltage range of a few volts and for modest deformations also having no

effect on the electronic structure of the tube; and (4) the resulting expressions can be used to avoid computational difficulties in calculating the electrostatic forces in NEMS with good accuracy. The further generalization of the theory to the case of nonequilibrium charge density will be helpful in deriving equations for the analysis of the operation of nanotube electronic devices.

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APPENDIX

Closed expression for the charge density on a straight semi-infinite nanotube. Formally, the influence of the image charge in the side contact can be taken into account as follows. Let us continue the charge density ρ and the external potential ϕ^{ext} to the half-space $z < 0$ in an odd way. Then, Eq. (5) can be rewritten as

$$\frac{\rho(z)}{e^2\nu_M} + \int_{-\infty}^{\infty} F_2(z, z')\rho(z')dz' = -\phi^{ext}(z), \tag{19}$$

where the kernel F_2 does not contain terms corresponding to the image charges in the side contact:

$$F_2(z, z') = \frac{2}{\pi|z - z'|}K\left(-\frac{4R^2}{|z - z'|^2}\right) - \frac{1}{\sqrt{(z - z')^2 + 4h^2}}. \tag{20}$$

Since the kernel F_2 for the infinite straight nanotube depends only on the difference $\Delta z = z - z'$, the Fourier transform converts integral equation (19) into an algebraic equation. Then, the exact solution to Eq. (19) in the k space has the form

$$\rho_k = -\frac{\phi_k^{ext}}{1/e^2\nu_M + 2\pi F_{2k}}, \tag{21}$$

where ϕ_k^{ext} and F_{2k} are the Fourier components of the external potential and kernel, respectively:

$$\phi_k^{ext} = -i\frac{e^{-|k|h}}{\pi k}V, \tag{22}$$

$$F_{2k} = \frac{1}{\pi}(I_0(kR)K_0(kR) - K_0(2hk)), \tag{23}$$

where I_0 and K_0 are modified zero-order Bessel functions [8]. The approximation in Eq. (10) is obtained from Eq. (21) by the replacement of the kernel Fourier component F_{2k} by its zero-wave vector value $F_{20} = (1/\pi)\log(2h/R)$. Inasmuch as the Fourier component ϕ_k^{ext} of the external potential rapidly decreases with an increase in the wave vector, the resulting approximation is quite accurate.

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