Theory of Nanotube Opto–electromechanical Device

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Abstract— Theory of a novel carbon nanotube opto–electronic switch is presented. Current control is realized at the molecular level by applying field of an atomic charge or atomic dipole across the nanotube channel, which can work as a local gate. In the case of a unit (1 e) point charge, close to the surface, a scattering potential strength is ~ 2 eV if neglecting the screening. Thus, the screened potential has to be used and it is ~ 0.1 eV for a SWNT with typical parameters. In case of the dipole scatterer, the potential is approximately 10 times weaker. The change of the dipole orientation with respect to the channel axis modulates the potential shape from a single barrier/well to a coupled triangular barrier and well. A possibility for creating a light-controlled electronic device is discussed.

I. INTRODUCTION

Recently demonstrated single wall nanotube (SWNT) field effect transistors (FET) [1], [2] give a beautiful example of an electronic device, which can be controlled by applying a voltage and may scale down to several tens of nanometers. However, creating gates to a SWNT device at this and smaller (atomic) scales may become a hard problem for technology. Electrochemical and/or chemical analogues of nanotube FETs [3], [4] could be promising as the gate acts at the molecular scale, but the chemical gating is not applicable for modern electronics due to its slow response. We proposed a SWNT–organic molecule complex to be used as a novel molecular electronic device: Nanotube Light-Controlled Switch in [5]. The device consists of a carbon nanotube and a switching molecule attached to its surface. We refer a reader to original articles [5], [6] for details of the molecular complex structure.

The switching molecule may consist of two parts: an "anchor" connected to the nanotube sidewall and a (dipole) charged "tail". A fast nanomechanical motion of the charged "tail" of the molecule, which is caused by a photon absorption and subsequent "cis–trans" isomerization, produces an electro-static potential modulation, *i.e.*, results in a local electrostatic gating. The variation of the potential of this molecular gate is predicted to lock/unlock the current through the nanotube [5]. The switching molecule charge creates an electrostatic barrier for the nanotube charge carrier motion that causes their scattering and decreases the conductance. We showed earlier that the current modulation for a single switch can be as large as 40–50%. Certainly, for robust operation of the Mol–FET, the switching molecule must have two well defined minima: ON and OFF states, with a barrier between states being at least larger than the operation temperature. Not only the proposed cis–trans isomerization mechanism [5] can satisfy this condition, but we do not go into details here. For the rest of the paper, it is important that there are examples of optically driven chemical/biological "motors" that can realize an opto–electromechanical action and switch the potential at the surface of the nanotube channel. The study of a charge carrier scattering by the potential is in the focus of this work.

In the paper we consider a scattering potential of a point charge as well as a point dipole. The latter can be represented at the molecular level by a strongly polarized bond placed/adsorbed at the SWNT surface. We calculate the self-consistent potential of this charge/dipole and of the conduction electrons of the nanotube. The response of the latter to the external potential results in an effective screening of the external potential. Simple analytical expressions for the potentials will be obtained where possible. It gives a clear understanding of physics of a SWNT bandstructure modulation due to atomic fields in the molecular complexes. A quantum mechanical calculation of the transmission probability will be presented. Then, the Landauer formula can be used to estimate the conductance of the Mol–FET.

II. SELFCONSISTENT POTENTIAL OF THE POINT CHARGE

The electrostatic potential of the charge near the nanotube surface depends on its position relative to the tube axis [7]. For several charged moieties a radial distance to the axis of the SWNT, ρ, has been obtained with a quantum chemical calculation in [5] and constitutes ~ 1.2 nm. We have demonstrated earlier [5] that the potential created by the charged molecule at the SWNT surface has a short (longitudinal) range of several nanometers, and long weak tails, which decay as $1/z^3$. As long as the charge is at the distance of tens of nanometers from the side contacts, the influence of leads on the potential is negligible. Thus, we ignore all contact phenomena which may appear at the leads.

In cylindrical coordinates, the effective potential of the charge on the surface of the SWNT reads as follows:

$$\phi^{xt}(z, \beta, \rho) = \frac{q}{\sqrt{R^2 + \rho^2 + z^2 - 2R\rho\cos\beta}}, \qquad (1)$$

where ρ is the cylindrical coordinate of the charge q, z, R and β are the coordinates of the electron (the longitudinal distance to the charge, the nanotube radius and the angular coordinate).

The local band bending is due to the local shift of the band-structure of the SWNT by the electrical potential. The quantum mechanical description of this mechanism is presented elsewhere [8]. In neglecting the mixing between subbands [9], which means a conservation of an angular momentum, m, only the component of the electric potential with the full axial symmetry is considered. Thus, the above expression has to be integrated over the β. The amplitude of the potential is given by a prefactor q/R, which has to be multiplied by a dimensionless integral:

$$\int_0^{2\pi} \frac{d\beta}{\sqrt{(z/R)^2 + 1 + (\rho/R)^2 - 2\cos\beta\,\rho/R}} =$$

$$\frac{4}{\sqrt{(z/R)^2 + (\rho/R - 1)^2}} K\left(-\frac{4\rho R}{z^2 + (\rho - R)^2}\right), \quad (2)$$

where K is a complete elliptic integral of the first kind [10]. The integral depends on the longitudinal distance to the charge, z, and on the ratio of the radial coordinates of the charge and the electron, ρ/R, as a parameter. The latter is about 1.7 for a typical adsorbate.

An expansion of the potential in series in z near the maximum gives only even powers of the distance, thus, at small distances it is a parabolic potential barrier or well, depending on the signs of the external charge, q, and of the major charge carriers in the nanotube, e.

Here we present an analytical expression for the potential barrier of the charge q when the distance to the nanotube sidewall is much smaller than the tube radius: $\rho - R \ll R$. This approximation gives a reasonable accuracy in wide range of substances absorbed at the surface of a nanotube of large radius, $R > 2$ nm. Then we can keep only leading terms in expansion in $\delta = \rho/R - 1$:

$$\varphi_{xt} \simeq \frac{q}{R}\left((2-\delta)\ln\frac{8}{\delta} + \delta + \ldots - \frac{z^2}{2R^2}\left(\frac{3 + 2\ln\frac{8}{\delta}}{8} + \right.\right.$$

$$\left.\left. \frac{2-\delta}{\delta^2} + \frac{1 - 6\ln\frac{8}{\delta}}{16} + \ldots\right)\right) \simeq \frac{q}{R}\left(F_0 - z^2 F_2\right). \quad (3)$$

This expression gives a potential ~ 2 eV at the origin, $z = 0$, for a single (electron) charge of the molecule $q = e$ and $\delta = 0.7$. However, this is not the potential seen by the charge carriers in the channel because of the depolarization of the external potential by the valence electrons of the tube. The expression for this depolarization can be obtained in a selfconsistent way by taking into account a Coulomb interaction between electrons with a Random Phase Approximation (RPA). Here, for clarity, we use a simpler argument. The correction is proportional to the dimensionless strength of the Coulomb potential in the nanotube. For a SWNT this parameter is given by a ratio of a geometrical capacitance of the tube to its quantum capacitance introduced in [11]. For a free (suspended) tube the geometrical capacitance depends logarithmically on its length, while for the tube on the substrate it depends on a characteristic screening length of the substrate (for example,
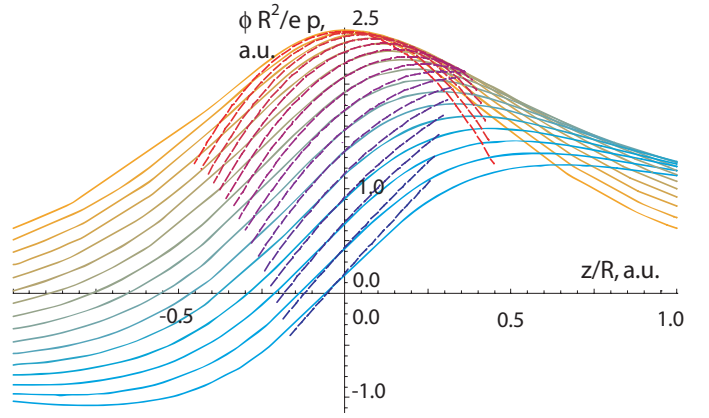

Figure 1. Selfconsistent solution for the one–dimensional electric potential (created by a dipole impurity) absorbed on the SWNT surface. The color of each curve (from red to blue) corresponds to the angle of the dipole to the tube axis. Dashed light color curves correspond to an analytical approximation as described in the text and represent well the potential at small distances.

the backgate distance). Considering that this dependence is weak, we substitute typical parameters that yield the depolarization as $C_g/C_Q \sim 1/\left(3.2 \times 2\log\left(\frac{L}{R}\right)\right) \simeq 1/30 - 1/50$. The characteristic length L is given by the working length of the SWNT device, estimated as the distance between the side electrodes, or by the distance to the backgate, whichever is smaller.

Finally, the band bending as a function of the coordinate along the nanotube is given by the equation:

$$U(z) = \frac{C_Q^{-1}}{C_g^{-1}} \frac{eq}{R}\left(F_0[\rho/R] - z^2 F_2[\rho/R] + \ldots\right), \quad (4)$$

where the functions F_0 and F_2 are given by Eq.(3).

III. POINT DIPOLE ON THE SWNT: SCATTERING POTENTIAL

In this section we consider a scattering potential as created by a single point dipole at the surface of the SWNT. In contrast to the case of a (monopole) charge, the dipole field depends substantially on the orientation of the dipole with respect to the axis of the nanotube. In the paper we consider the only intra–subband scattering of the charge carriers, then, only the longitudinal component of the potential is important as changing the longitudinal component of momentum of the charge. For simplicity we do not consider here the dipole which has all three non–zero components in the coordinate system of z axis pointed along the tube. One perpendicular component of the dipole p_y is taken to be zero, which corresponds to the vector of the dipole, $\vec{p}$, staying in the plane with $\vec{z}$. Then, the dipole orientation is given by one variable, α, the angle between the dipole direction and its radial axis, which is chosen as axis x in this article. Then, the dipole–electron interaction energy reads as follows:

$$e\varphi_{\text{dip}}(z, \beta, \alpha, \rho) = \frac{ep\left((\rho - R\cos\beta)\cos\alpha + z\sin\alpha\right)}{(R^2 + \rho^2 + z^2 - 2R\rho\cos\beta)^{3/2}}, \quad (5)$$
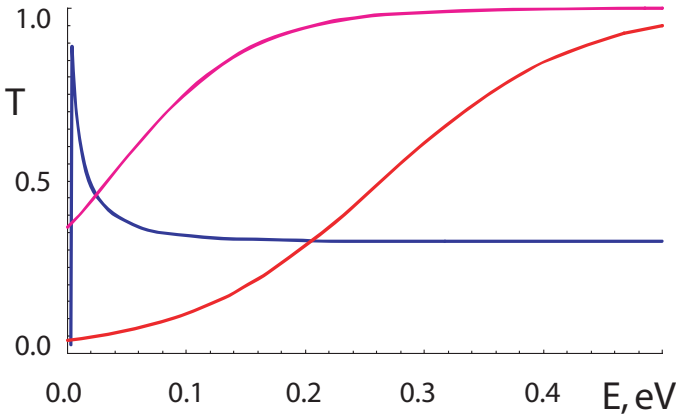
Figure 2. Transmission probabilities for charge carrier in a semiconductor SWNT scattered by a charge absorbed on the tube surface (red/middle), a dipole impurity (pink and blue, top and bottom, for the direction of the dipole perpendicular and along the tube).

where R, ρ, β and z have the same definition as in Eq.(1) and $(\pi/2 - \alpha)$ is the angle between the dipole, p, and the tube axis. For the intra–subband scattering problem, the potential has to be averaged over the electron positions on the tube surface. As before, we express the resulting 1D potential energy of the electron as the product of the amplitude, ep/R^2, depending on the SWNT radius and the dipole strength, and the dimensionless integral, bearing the angular dependence:

$$U_d(z) = \frac{C_Q^{-1}}{C_g^{-1}} \frac{ep}{R^2} \Big(G_0[\rho/R] \cos\alpha + z G_1[\rho/R] \sin\alpha$$

$$-z^2 G_2[\rho/R] \cos\alpha + \dots \Big), \quad (6)$$

here functions G_i are combinations of elliptic integrals. Their expansions at small δ are as follows: $G_0 \sim \ln(8/\delta)/2 + 1/\delta - 1 + o(\delta)$, $G_1 \sim (3 + 2\ln(8/\delta))/16 + 2/\delta^2 - 1/\delta + o(\delta)$, $G_2 \sim (7 - 6\ln(8/\delta))/32 - 2/\delta^3 + 1/2\delta^2 - 1/8\delta + o(\delta)$. The Figure 1 shows the full potential and these analytical asymptotes. The color from red to blue corresponds to the angle α from 0 to $\pi/2$.

The potential of the dipole directed toward/outward the nanotube surface ($\alpha = 0, \pi$) has the shape of a harmonic ($\sim z^2$) barrier/well with weak tails. As far as the Fermi level is comparable with the potential amplitude, the main scattering is at the central region of the potential, which is about several R in length. When the dipole is oriented along the nanotube ($\alpha = \pm\pi/2$), the potential is the odd function of z and there is a region of strong built–in electric field at the origin $z = 0$ and "weak" field regions extended up to $3 - 4R$ to the left and to the right.

IV. TRANSMISSION PROBABILITY

We model now the ballistic transport through the potential barriers given by expressions Eqs.(4,6). We focus first on the scattering at the external charge.

By expanding the acting potential near the maximum and using a semiclassical (WKB) probability for the reflection

from the harmonic potential barrier [12] we obtain the transmission coefficient for a single molecular gate as follows:

$$\mathcal{T}_c(E) = \frac{1}{1 + \exp[-2\pi \frac{E-F_0}{\hbar}\sqrt{\frac{m^*}{F_2}}]}, \quad (7)$$

where m^* is an effective mass at the band edge, which is given by expression

$$m^* = \hbar^2 \frac{\partial^2 k}{\partial E^2} = 4.5bR\gamma, \quad (8)$$

for the SWNT of the radius R and is about 0.06 of the free electron mass for $R \simeq 0.7$ nm. Here $\gamma \simeq 2.7$ eV is a hopping integral and $b \simeq 0.14$ nm is a SWNT bond length.

The transmission probability for a typical semiconductor SWNT ($R \simeq 0.7$ nm), $\delta \simeq 0.7$ and $q = e$ is given in Figure 2 in red color (middle curve). On the same graph we present the result of calculation for the dipole scattering. In this case the transmission coefficient is given by a similar equation:

$$\mathcal{T}_p(E) = \frac{1}{1 + \exp[-2\pi \frac{E-G_0}{\hbar}\sqrt{\frac{m^*}{G_2}}]}, \quad (9)$$

where we changed functions F with G which are smaller at the same parameters R, and δ by the ratio $qR/p \sim 10$.

In a ballistic regime, the conductance of the semiconductor SWNT at low voltage can be approximated as:

$$G = 2G_o\mathcal{T}(E_F) \quad (10)$$

here $2G_o = 2e^2/h$ is four times of the quantum of conductance (because of two spin × two channels of the SWNT). Considering the low voltage (linear) regime, the current modulation is given by the modulation of the conductance as in Eq.(10). We present a typical room temperature IV curve of a Mol–FET with a semiconductor tube of radius ~ 0.7 nm and a gap ~ 0.6 eV, degenerately doped (or shifted to this degeneracy by applying the external gate voltage). The IV curves in Figure 3 correspond to the Fermi levels from 0.01 eV (red) to 0.21 eV (blue) from the bottom of the conduction band. For given parameters the amplitude of the barrier, created by the unit charge on the SWNT surface, is ~ 0.26 eV. The IVC has only slight dependence on temperature.

We note that the transmission probability $\mathcal{T}$, and hence, the Mol–FET conductance is an exponential function of the charge–nanotube distance, ρ. Thus, changing the molecule conformation and the radial coordinate of the charge, one can modulate the current. The conformational changes are known to be forced by a resonant absorbtion of a photon of certain wavelength in molecules like the azobenzene. Similarly, the dipole reorientation can follow the photon absorption, thus providing the nano–opto–electromechanical mechanism of local gating of the nanotube FET.

At the large bias potential $V \gg E_F + F_0, G_0$, most of electrons, which were injected from the source, will reach the drain without scattering because the transmission coefficient saturates for the hot electrons. Thus, the saturation current of $2G_0V$ has to be observed if no voltage drops at the contact region.
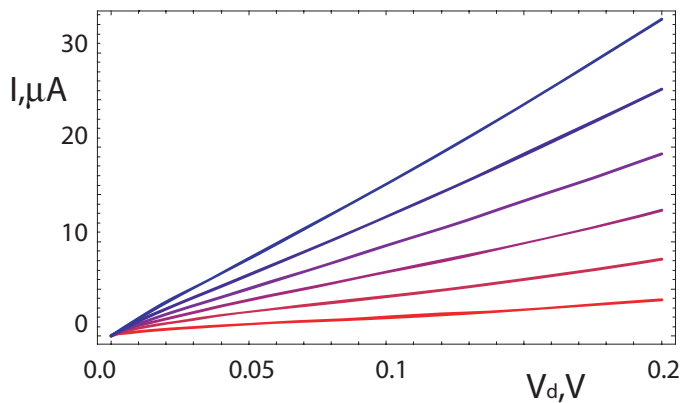
Figure 3. IV curve for a charge scattering. The color of each curve (from red to blue, bottom to top) corresponds to increasing Fermi level from 0.01 to 0.21 eV from the band edge. Parameters of the model are described in the text.

V. CONCLUSION

We studied a light–controlled molecular electromechanical switch which is a molecular field effect transistor, where a special molecule plays the role of a local gate to a SWNT channel. This molecule can change its conformation by resonant absorbtion of a photon [5]. Since the molecule is charged (by design) or obtains a dipole, it creates a potential barrier/well for the charges moving in the SWNT channel. We calculated scattering of the charge carriers in the potential of a single charge and a single dipole placed on the surface of a semiconductor nanotube. Analytical expressions for the one–dimensional potential of the charge/dipole are obtained and used to model the scattering within semiclassical (WKB) approximation. In a ballistic regime, the transmission probabilities give IV curves for Mol–FETs. Further possibility to control the Fermi level in the channel will allow one to obtain an optimal switch which ON/OFF ratio for a single scatterer may approach 40%.

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