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Screening model for nanowire surface-charge sensors in liquid

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The conductance change of nanowire field-effect transistors is considered a highly sensitive probe for surface charge. However, Debye screening of relevant physiological liquid environments challenge device performance due to competing screening from the ionic liquid and nanowire charge carriers. The authors discuss this effect within Thomas-Fermi and Debye-Hückel theory and derive analytical results for cylindrical wires which can be used to estimate the sensitivity of nanowire surface-charge sensors. They study the interplay between the nanowire radius, the Thomas-Fermi and Debye screening lengths, and the length of the functionalization molecules. The analytical results are compared to finite-element calculations on a realistic geometry. © 2007 American Institute of Physics. [DOI: 10.1063/1.2779930]

Imagine a sensor so small and compact that it can fit almost everywhere and detect all kinds of chemical substances in real time. Such a sensor could, in principle, monitor and detect unwanted bacteria and viruses instantaneously in, e.g., your blood or drinking water. Sensors based on semiconductor nanowires have already been fabricated7 and shown to work, for example, as a pH sensor, where the concentration of hydrogen ions H+ in a surrounding liquid is detected.5 Moreover, application in label-free detection and biological sensing addressing, e.g., DNA in low concentration is now being explored.5–6 In general, the conductance G of a nanowire is in the literature considered a promising can-

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with Γ being a dimensionless function, between zero and unity, quantifying the actual sensitivity in the presence of Debye screening in the electrolyte and a finite Thomas-Fermi screening in the nanowire. We show that Γ scales with the electron density n0 as n0−2/3 in the dilute limit, thus leading to a prediction of a n0−2/3 dependence, contrasting the intuitively expected n0−1 dependence. However, high sensitivity is, of course, still associated with low densities.

Above, P is the perimeter of the nanowire cross section (the fraction supporting the surface charge), A is the cross-sectional area, and e is the electron charge. For a cylindrical wire of radius R, we have P/A = 2/R, thus clearly illustrating the benefit of scaling the wires to the nanoregime. Obviously, screening in the liquid will suppress the sensitivity below the bound given by Eq. (1), and a n0−1 dependence (the limit Γ = 1) can only be expected when the Thomas-Fermi screening in the nanowire is much stronger than the Debye screening in the electrolyte surrounding the nanowire so that changes in the density of the electron gas fully compensates the additional surface charge. In our screening model, we consider the induced electrical potential due to a surface-charge density σS on the outside of an oxide-covered nanowire (see Fig. 1). For the nanowire we employ the Thomas-Fermi model (see, e.g., Ref. 11), while for the dilute electrolyte we consider a Debye-Hückel approximation (see, e.g., Ref. 12).

These approximations we arrive at the following linear differential equation for the induced electrical potential φ:

\[
\nabla^2 \phi = \begin{cases} 
\lambda_{TF}^{-2} \phi, & \mathbf{r} \in \Omega_1 \\
0, & \mathbf{r} \in \Omega_2 \\
\lambda_D^{-2} \phi, & \mathbf{r} \in \Omega_3 \cup \Omega_4,
\end{cases}
\]

where λTF is the Thomas-Fermi screening length in the nanowire domain Ω1 and λD is the Debye screening length in the

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The induced charge-density, $\nu$, and the corresponding surface-charge density $\sigma_0$, are determined at the surface $\Omega_1$ of the oxide layer domain by the Poisson equation.

In the following, we consider the case of a surface-charge density $\nu$ in the analyte solution equals the isoelectric point of the surface. In general, the oxide layer will be charged unless the functionalization molecules supporting the charge which for $\delta<\delta_S$ residing directly on the outside of the oxide layer of the nanowire. In the static limit, water is highly polarizable and $\epsilon_1\sim78\epsilon_0$ while for silicon $\epsilon_1\sim12\epsilon_0$. Thus, for a fixed $n_0$ the ultimate sensitivity, Eq. (1) with $\Gamma=1$, requires a very short Thomas-Fermi screening length, but at the same time one would like to benefit from the $n_0^{-1/3}$ scaling in Eq. (5).

The oxide layer has a thickness $\delta_S$, thus calling for nanowires with densities supporting screening at the true nanometer scale. A simple estimate of $\lambda_{TF}=\sqrt{\hbar^2/\mu e^2n_0^{1/3}}$ also yields $\lambda_{TF}\sim1$ nm for a carrier concentration of $10^{19}$ cm$^{-3}$. Taylor expanding Eq. (5) in the dilute carrier limit, $\lambda_{TF}\gg R$, we get

$$\Gamma \approx \frac{1}{2} \left[ \frac{\epsilon_1}{\epsilon_3} \frac{\lambda_{TF}K_0(R/\lambda_{TF})}{\lambda_{TF}R} \right]^2 \approx n_0^{1/3}$$

Figure 2(a) illustrates the dependence of the sensitivity on the Debye screening in the electrolyte. The lower trace is for a nanowire of circular cross section with $\lambda_{TF}/R=0.02$. The dashed line shows Eq. (5) valid for a negligible oxide-layer thickness, i.e., $\delta<\delta_S$, while the data points are the result of finite-element simulations (Comsol MultiPhysics) taking into account a finite oxide layer of width $\delta/R=0.005$ and with $\epsilon_1\approx4$. As seen, Eq. (5) accounts well for the numerical exact results. The upper trace shows finite-element results for a nanowire with a trapezoidal cross section with aspect ratio $w/r=2$ and etching defined angle $\theta\sim54.7^\circ$ corresponding to the fabricated structure in Ref. 5 [see Fig. 2(b)]. The oxide layer has a thickness $\delta/\ell_{TF}=0.02$, and for the Thomas-Fermi screening, we have $\lambda_{TF}=\ell_{TF}=0.02$, which is somewhat stronger than for the circular case shown in the lower trace. Note how the two curves have the same overall shape and dependence on the Debye screening length, though the stronger Thomas-Fermi screening for the upper case makes $\Gamma$ approach unity for more moderate Debye screening lengths than in the lower case. Figure 2(b) illustrates a typical distribution of the induced charge-carrier density in the nanowire and the superimposed contours show the equipotential lines. As expected,
the excess carrier density is induced near the surface of the wire supporting the surface-charge density $\sigma_S$.

Finally, let us discuss the prospects for sensing of point-like charges located at a distance $\ell$ further away from the conductor. Obviously, the additional Debye screening in the layer of thickness $\ell$ (see Fig. 1) will further reduce the induced carrier density in the nanowire, and in a simple picture (neglecting curvature) we would qualitatively expect a reduction proportional to $\exp(-\ell/\lambda_D)$. In the following, we let $N$ denote the average number of molecules absorbed on the wire of length $L$ and we imagine that the chainlike functionalization molecule supports a charged group, with charge $Q$, situated at a distance $\ell$ from the surface. Smearing out these charges results in an equivalent surface-charge density

$$\sigma_S = N Q / [2 \pi (R + \ell) L]$$

at $r = R + \ell$. Solving the problem in Eqs. (2a) and (2b) for a finite $\ell$, we get $\Gamma \rightarrow \Gamma^\ell \times \Gamma$ with

$$\Gamma^\ell = 2 \frac{R}{R + \ell} \left[ 1 + \sqrt{\frac{R}{R + \ell}} \exp \left( \frac{\ell}{\lambda_D} \right) \right]^{-1}.$$

Here, we have used the large-argument exponential asymptotes for the Bessel functions. The extra factor $0 \leq \Gamma^\ell \leq 1$ illustrates the additional, close to exponential, suppression by Debye screening when the charge is supported by a functionalization molecule of length $\ell$. We note that, in principle, the $\lambda_D$ entering the expression for $\Gamma^\ell$ could differ from the Debye screening length of the electrolyte, e.g., due to the surface functionalization.

In conclusion, we have used Thomas-Fermi and Debye-Hückel theory to formulate a simple screening model for surface-charge sensing with conducting nanowires. The two screening mechanisms act in concert and our model illustrates the nontrivial interplay between the nanowire radius $R$, the Thomas-Fermi screening length $\lambda_{TF}$, the Debye screening length $\lambda_D$, and the length $\ell$ of the functionalization molecules.

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