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Modeling of a Silicon Nanowire pH Sensor with Nanoscale Side Gate Voltage

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A silicon nanowire (Si-NW) sensor for pH detection is presented. The conductance of the device is analytically obtained, demonstrating that the conductance increases with decreasing oxide thickness. To calculate the electrical conductance of the sensor, the diffusion-drift model and nonlinear Poisson–Boltzmann equation are applied. To improve the conductance and sensitivity, a Si-NW sensor with nanoscale side gate voltage is offered and its characteristics are theoretically achieved. It is revealed that the conductance and sensor sensitivity can be enhanced by adding appropriate side gate voltages. This effect is compared to a similar fabricated structure in the literature, which has a wire with a rectangular cross section. Finally, the effect of NW length on sensor performance is investigated and an inverse relation between sensor sensitivity and NW length is achieved.

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Silicon nanowires (Si-NWs) have recently attracted considerable attention from many fields of healthcare and life sciences for the detection of biological and chemical species. Si-NW sensors have already been demonstrated for ultra-sensitive detection of pH levels,[1,2] proteins,[1,3] DNA,[4,5] and other biomolecules.[6,7] The detection ultra-sensitivity is associated with their small size which facilitates local charge transfers. The NWs act like field effect transistors (FETs) in a way that the sensing mechanism is indeed the result of a field effect parallel to applying a voltage.

In particular, ion-selective Si-NW sensors have shown high potential for the detection of ions in liquid solutions. The ability of such sensors was first demonstrated for pH detection.[5] A fundamental p-type Si-NW device was transformed to such a sensor by altering the Si oxide surface with 3-aminopropyltriethoxysilane (APTES), which results in amino (NH_2) groups as well as silanol (SiOH) groups at the NW surface. These groups are used as receptors for hydrogen ions which experience protonation/deprotonation reactions. The operation principle of such sensors is that when the surface charge on the Si-NW changes, the conductance changes as a consequence.

To enhance sensor performance, we can use a nanoscale side gate voltage close to the NW to give more control of the conductance. Adding different gate voltages makes the conduction channel be extended or squeezed and as a result, the sensor sensitivity can be increased by adding proper voltages.

Furthermore, this is understandable considering that the conductance and sensitivity of Si-NW sensors depend on device parameters such as doping density, device geometry and dimension especially NW length. These size dependent effects are fundamental to practical applications. However, despite advances in NW sensors, the principles for design and optimization of NW sensors have not been concentrated on much.

In this Letter, we provide an approach to obtain the conductance of Si-NW sensors and consequently the device sensitivity in pH detection. The approach is based on the solution of the reaction diffusion-drift model and the nonlinear Poisson–Boltzmann equation. To improve the conductance, a Si-NW pH sensor with nanoscale side gate voltage is presented and its conduction is achieved. The effect of side gate voltage on variations of conductance is investigated which shows improvement in conductance by increasing voltage. It is demonstrated there is an inverse relation between sensor sensitivity and NW length affecting sensor performance.

We propose a Si-NW pH sensor, the Si-NW of which is covered with a modified surface oxide layer (both amino (NH_2) and silanol (SiOH) groups). Figure 1 shows the schematic of such a Si-NW sensor.

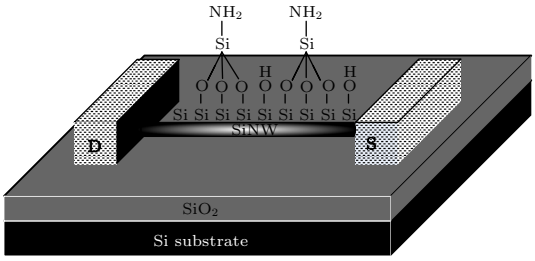

Fig. 1. Schematic of Si-NW sensor. The NW is covered by an oxide layer immersed in an electrolyte.

The channel structure contains three regions including coaxial Si NW, insulating oxide around the NW with thickness t_{OX}, and electrolyte. When the radius of the Si-NW is about 5 nm, a size quantization effect can exist. However, the quantum effect disappears at room temperature. At low temperature, we can observe quantized or at least nonlinear con-

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ductance in the NW. However, it was demonstrated that the current-voltage characteristics of the back-side gate Si-NW FETs are linear at room temperature in spite of the 5 nm radius of the NW and that the contact between the metal electrode and the Si-NW is ohmic. Therefore, we can use the diffusion-drift model for electronic transport inside the p-type Si-NW as

$$J_h(r) = q\mu_h n_h(r,z)\frac{V_{\rm DS}}{L_{\rm NW}} - qD_h\frac{\partial n_h(r,z)}{\partial z}, \quad (1)$$

where J_h is the hole current density, μ_h is the hole mobility, n_h is the hole density inside the Si-NW, D_h is the hole diffusivity, $V_{\rm DS}$ is the drain-source voltage, and $L_{\rm NW}$ is the NW length. Since the length of NW is much larger than the NW radius, the hole current density in the longitudinal path is about constant. Thus the longitudinal deviation of the hole density can be overlooked. The drain-source current through the Si NW can be obtained by

$$I_{\rm DS} = \int_0^{R_{\rm NW}} J_h(r)2\pi r dr, \quad (2)$$

where $R_{\rm NW}$ is the radius of NW. The electric displacement of p-type Si can be described by

$$\nabla \cdot \boldsymbol{D} = q(n_h - N_a), \quad (3)$$

where D is the electric displacement, and N_a is the concentration of p-type carriers. By using the divergence theorem, the following equation can be achieved

$$\int_0^{R_{\rm NW}} n_h(r)dr = R_{\rm NW}^2\Big(\frac{\sigma_{\rm NW}}{qR_{\rm NW}} + \frac{N_a}{2}\Big), \quad (4)$$

where $\sigma_{\rm NW} = D_r(R_{\rm NW})$ is the induced charge density. Thus the conductance in the coaxial Si-NW sensor is achieved,

$$G = \frac{I_{\rm DS}}{V_{\rm DS}} = q\pi\mu_h N_a\frac{R_{\rm NW}^2}{L_{\rm NW}} + 2\pi\mu_h\frac{R_{\rm NW}\sigma_{\rm NW}}{L_{\rm NW}}. \quad (5)$$

The first term on the right-hand side of Eq. (5), i.e. G_0, is the conductance of Si-NW without surface effects.

A comprehensive theory has been presented in Ref. [8] and it provides an analytic expression for the induced charge density. The theory is based on a self-consistent solution of analytic solutions of the Poisson–Boltzmann and reaction-diffusion equations. The induced charge density $\sigma_{\rm NW}$ can be expressed as[8]

$$\sigma_{\rm NW} = \frac{-\varepsilon_{\rm OX}\Psi_0}{R_{\rm NW}\big(1+\frac{t_{\rm OX}}{R_{\rm NW}}\big)\log\big(1+\frac{t_{\rm OX}}{R_{\rm NW}}\big)}, \quad (6)$$

where $\varepsilon_{\rm OX}$ is the oxide dielectric constant, $t_{\rm OX}$ is the oxide thickness, and Ψ_0 is the potential at the sensor surface. To achieve Ψ_0 the nonlinear Poisson–Boltzmann equation should be used as

$$-\nabla(\varepsilon_E\nabla\Psi(r)) + \kappa^2\sinh\Big(\frac{q}{k_BT}\Psi(r)\Big) = q\sum_n z_n\delta(r-r_n), \quad (7)$$

where ε_E is the dielectric constant of the electrolyte, Ψ is the electrostatic potential, κ^{-1} is the Debye–Huckel screening length, k_B is Boltzmann's constant, T is the temperature, and r is the spatial coordinate, $\kappa = q\sqrt{2I_0N_{\rm avo}(\varepsilon_E k_BT)^{-1}}$ with I_0 being the ion concentration in molar units and $N_{\rm avo}$ Avogadro's constant.

By applying Eq. (7) and the presented model in[8], Ψ_0 in the case of pH detection can be described as

$$\Psi_0 \cong \frac{2k_BT}{q}\Big(2.303a|pH - pK_a| - \frac{1}{2}\ln(I_0) + c\Big), \quad (8)$$

where $0 \le a \le 0.5$, $pK_a = -\log 10(K_a)$ (where K_a is the dissociation constant), and

$$c = \ln\left(qN_F\sqrt{\frac{1}{q^2k_BT\varepsilon_E N_{\rm avo}}}\right), \quad (9)$$

where N_F is the density of surface functionalization groups.

Figure 2 shows the conductance of sensor versus pH of solution for different ratios of $t_{\rm OX}$ to $R_{\rm NW}$. As is shown, the conductance varies linearly with variations of pH, which has been experimentally demonstrated before.[5] When the ratio of $t_{\rm OX}$ to $R_{\rm NW}$ becomes smaller, the conductance increases, implying that the thickness of the oxide layer affects the sensitivity. A thicker oxide layer reduces the sensitivity since the oxide layer screens the surface charges.

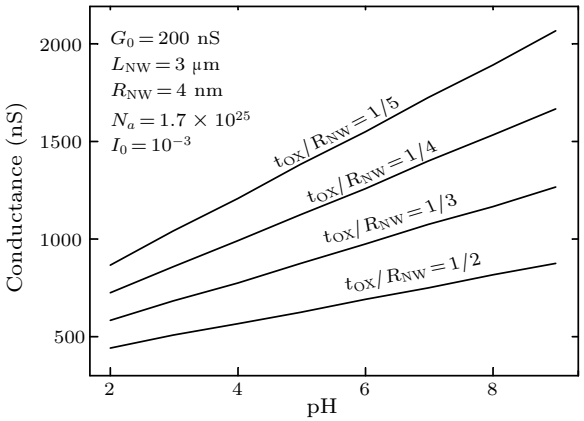

Fig. 2. Conductance of sensor versus pH of solution for different ratios of oxide thickness to NW radius.

Figure 3 shows a Si-NW sensor with nanoscale side gate voltage. This side gate electrode can be fabricated with complete control over its location and size. This side gate electrode provides the ability for controlled accumulation or depletion of surface charge carriers on the NW and so makes the conductance adjust in such a way to have better performance. To achieve the conductance of this sensor, G_v, we can use Eq. (5) and obtain the equation

$$G_v = G_0 + 2\pi\mu_h\frac{R_{\rm NW}}{L_{\rm NW}}\sigma_v. \quad (10)$$

When the NW length is larger than the length of the side gate (not much, for example, three times larger), the effect of side gate voltage can approximately be inserted with the following equation

$$\sigma_v \approx \sigma_{\rm NW} + \frac{\varepsilon_{\rm OX} V_{\rm GS}}{R_{\rm NW}\left(1+\frac{t_{\rm OX}}{R_{\rm NW}}\right)\log\left(1+\frac{t_{\rm OX}}{R_{\rm NW}}\right)}, \quad (11)$$

where $V_{\rm GS}$ is the side gate voltage.

Figure 4 shows the conductance versus pH for different side gate voltages. It is found that the conductance can be improved based on proper gate voltage. A positive gate voltage makes the charge carrier channel open analogous to the inversion layer in Si devices, while a negative gate voltage makes the charge carrier channel deplete or squeeze like the depletion layer. Therefore the conductance increases or decreases due to positive or negative gate voltage, respectively.

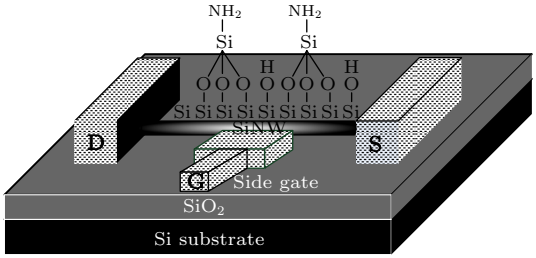

Fig. 3. Schematic view of Si-NW sensor with nanoscale side gate voltage next to the NW to enhance the sensor performance.

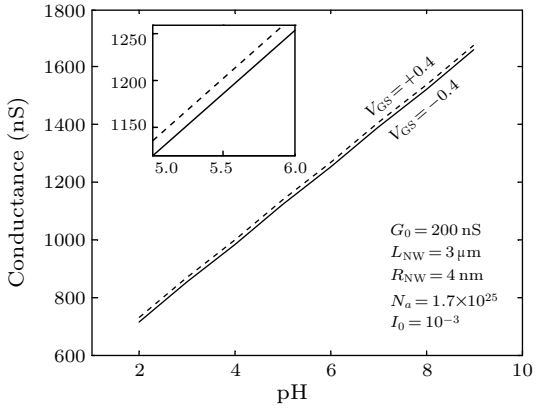

Fig. 4. Conduction versus pH for Fig. 3 with different values of side gate voltage. Inset shows these variations for pH between 5 and 6.

As was demonstrated in Ref. [9], the fabricated Si-NW with a rectangular cross section shows an almost linear relationship for variations of conductance versus the local gate voltage in the range from −0.4 V to 0.6 V. Hence for comparison between two structures only a specific range of gate voltages is considered.

Figure 5 exhibits the conductance versus the side gate voltage. The inset demonstrates the conductance versus local gate voltage for the reported rectangular-cross-section Si-NW sensor in Ref. [9]. As is shown, the two curves have a linear relationship between conductance and side gate voltage, which results in increasing conductance by the rising of the side gate voltage. The difference between the values of conductance is related to their geometrical and structural features. The wire in Ref. [9] has a rectangular cross section and it is 300 nm wide, 230 nm thick and 8 µm long, while the NW in this study has a circular cross section, a radius of 4 nm, and a length of 3 µm. This difference is understandable since NW with smaller dimensions in general provides a larger conductance and consequently a higher sensitivity.

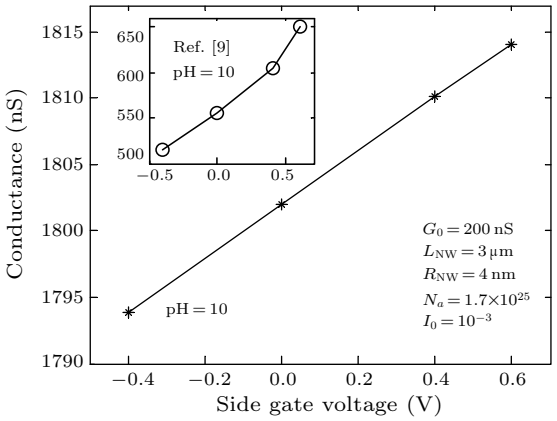

Fig. 5. Conduction versus side gate voltage. Inset shows these variations for the sensor presented in Ref. [9] with rectangular cross section.

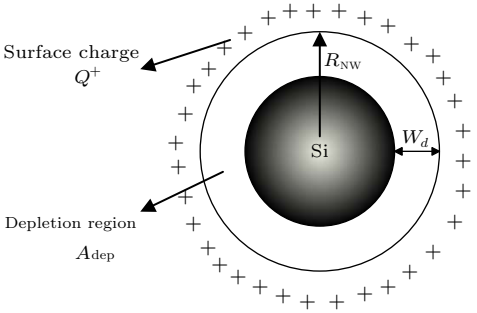

Fig. 6. Cross-sectional schematic of Si NW to show the depletion effect.

The sensitivity of a cylindrical Si-NW sensor with nanoscale side gate voltage S_v can be achieved,

$$S_v \equiv \frac{|G_v - G_0|}{G_0} = \frac{2\sigma_v}{qR_{\rm NW}N_a}. \quad (12)$$

To show the effect of length on sensitivity, we should consider another definition for sensor sensitivity, which is the relative change in resistance before and after exposure to a target as

$$S_v = \frac{|R_v - R_0|}{R_0}, \quad (13)$$

where R_v is the resistance with surface effects resulting from attaching the molecule on the NW surface, and R_0 is the initial resistance. Here the response of a p-type Si-NW sensor in a solution is considered based

on localized positive surface charge Q^+. The cross-sectional view of the p-type Si-NW sensor is depicted in Fig. 6.

In this case, sensitivity S_v can be achieved to read

$$S_v = \frac{Q^+\rho_{\rm Si}}{2\pi R_{\rm NW}L_{\rm NW}w_d} = \frac{Q^+\rho_{\rm Si}}{A_{\rm dep}L_{\rm NW}}, \qquad (14)$$

where Q^+ is the positive surface charge in the p-type NW, $\rho_{\rm Si}$ is the electrical conductivity of Si, w_d is the width of the depletion region and $A_{\rm dep}$ is the area of the depletion layer. As is shown, the sensor sensitivity varies inversely with change of the NW length. Thus it must be considered as a significant factor in the designing of the sensor. However, due to the technological difficulties related to the continued scaling of dimensions, the NW length cannot be reduced to any low value.

In summary, a Si-NW pH sensor with nanoscale side gate voltage is theoretically investigated. The dependence of conductance on pH of solution is demonstrated to show a linear relationship. The functionalized Si-NW can be controlled with local nanoscale side gate voltage to induce inversion or depletion layers. Therefore, the device sensitivity can be improved with adding proper side gate voltages. Moreover, the sensor sensitivity can be enhanced by reducing NW length in the possible range. These design considerations for the Si-NW pH sensor can be applied in practical aspects to give better sensor performance.

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