Sensitivity Analysis of Nanowire FET Biosensor

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Abstract. A nanowire junctionless FET biosensor has been modelled with COMSOL Multiphysics. The high sensitivity of the device in depletion regime was observed. The sensitivity dependence on variations of species concentration in analyte surrounding the nanowire has been studied. It has been demonstrated that the thinner is the nanowire, the higher is the sensitivity and even a single molecule affects the drain current. The model is useful for sensor optimization.

Keywords: biosensor, nanowire, COMSOL Multiphysics

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1. Introduction

Nanowire based bio-chemical sensors are of great interest due to their high sensitivity and simple fabrication process. For sensing applications, the surface of semiconductor nanowire (NW) is usually functionalized with receptors to be sensitive to specific chemical or biological molecules. The surface functionalization allows to immobilize biomolecules on NW surface and enables a direct detection of disease-related molecules [1, 2].

The modelling of physical and chemical processes in biosensors is important for the device optimization and for further improvement in sensing selectivity. Here we introduce computational model of NW junctionless (JL) field effect biosensor using COMSOL Multiphysics.

2. Methodology: COMSOL model

An n-type Si NW surrounded with an analyte solution in cylindrical volume is assumed. The metallic cylinder is considered as third electrode (in our model we use Ag) for applying the gating voltage or the reference potential. Source and drain contacts are built at the bottom and at the top of the NW, respectively (see Fig. 1). The NW is covered with an array of y-shaped nanopillars designed for biomolecules binding to its surface. The internal surface of nanopillars (marked as “2” in Fig. 1) is coated with a biologically active material that adsorbs biomolecules in the sample solution. The density of nanopillars on NW surface is controllable, and in the model 16 nanopillars along 0.5μm NW length are implemented. The injected species concentration ($c_{\_oo}$) is defined at outer interface of analyte (marked with “3”, in Fig 1).

2.1 COMSOL model structure

The COMSOL model applies the Semiconductor Module to the NW domain, the AC electrostatic and Chemical Reaction Engineering Modules to the analyte domain. Ordinary Differential Equations (ODE) model is applied to the interface between NW and analyte (interface marked as “1” in Fig. 1) for adjusting the potential from both sides. Transport of Diluted Species module is applied to solve mass transfer equation in analyte assuming species transfer in porous media.

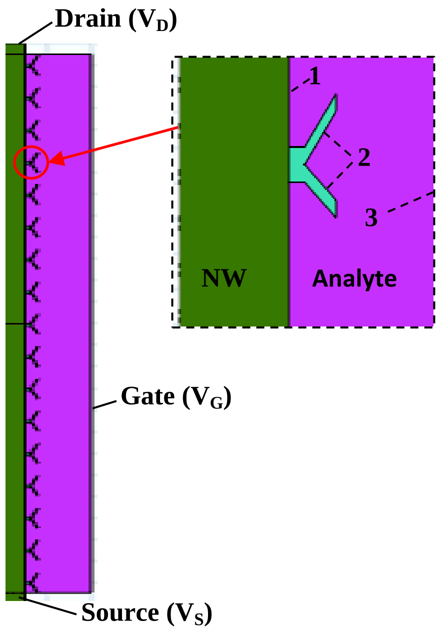

Fig. 1. The cross section of modeled structure.

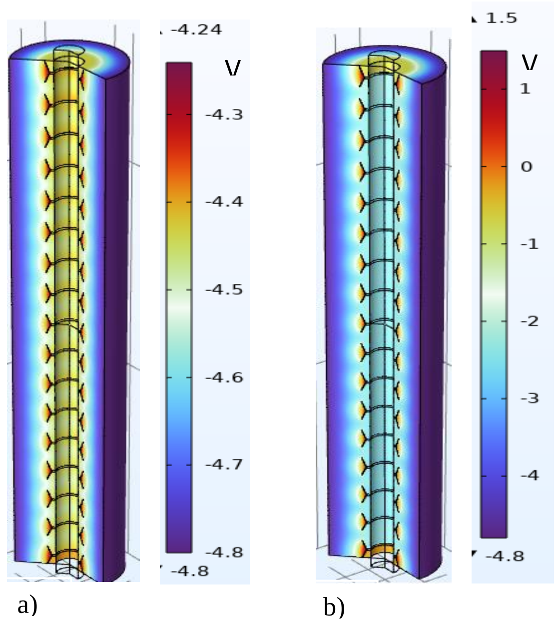

Fig. 2. Volume potential in analyte at t=0 s (a), and t=1,5 s (b).

The model allows to study the concentration distribution in the analyte and the surface coverage of adsorbed species. The Surface Reactions interface from Chemical Reaction Engineering Module in COMSOL Multiphysics is used to model the chemical reactions on pillar's surface.

2.2 Surface reactions

The adsorption-reaction-desorption are the main steps of surface reactions in biosensors. Analyte molecules (P) can adsorb and desorb from surface sites (S) on the nanopillar surfaces according to $P + S \leftrightarrow PS$.

The adsorbed analyte (PS) can transform into a quenched state (QS) that does not contribute to the sensor signal, and the quenching reaction is reversible: $PS \leftrightarrow QS$.

The rate of adsorption is proportional to the concentration of species in solution ($c_{\_oo}$), whereas the desorption rate is proportional to the surface concentration (c_{o_s}), of absorbed species. The reversible quenching mechanism is also considered. To model surface reactions on pillars surfaces we follow to Biosensor module demonstrated in [3].

3. Results and discussion

It is worth to note that the surface reactions are time dependent and consequently the surface concentration of species is time dependent.

A Si NW with doping density $N_D=5\cdot10^{18}$ (cm^{-3}), and a pure water as an analyte are considered. Fig. 2 illustrates potential distribution in analyte volume at the initial moment of injected species and later at t=1.5 (s), when surface reactions are already stabilized. In these calculations the following parameters are used: $c_{\_oo}=5$ (mol/m^3), the zero-gate voltage and drain voltage: $V_d=0.5$(V). In COMSOL simulations by default the reference level for potential distribution is vacuum level.

To validate the NW behaviour as a FET, the drain current dependence on the gate voltage at different species concentration is illustrated in Fig. 3. It is seen that the species concentration variation causes the drain current variation. This is explained by the influence of nanopillars surface charges on NW conductivity. The sensor operation is studied in depletion regime (below flat band condition), as it is the most sensitive regime for NW JL FET sensor [4-6].

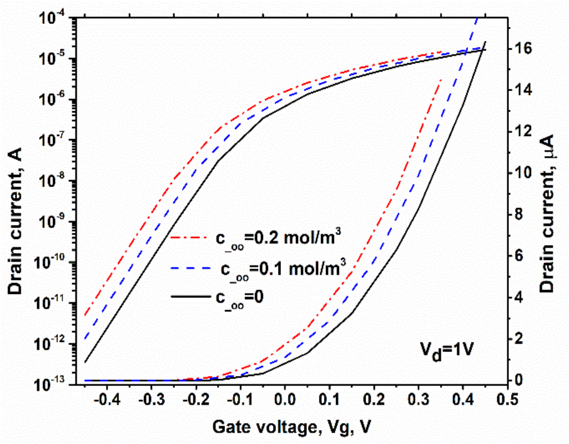

Fig. 3. The drain current versus gate voltage at different species concentration.

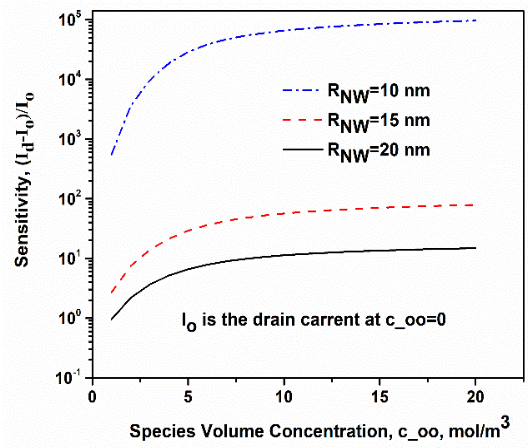

Fig. 4. The NW sensor sensitivity versus species volume concentration at different NW radii.

The influence of geometrical parameters on sensor sensitivity is studied in Fig. 4. As it was expected, as smaller is the NW radius, the higher is the NW sensitivity. Due to higher surface to volume ratio of thinner NWs the gating effect is higher for NWs with smaller radius, and consequently the sensitivity is also higher. In this plot the sensitivity is calculated, as the relative drain current difference, $(I_d- I_o)/ I_o$, where I_o is the drain current at the absence of species in analyte. For this and the following simulations the gate voltage is set to zero.

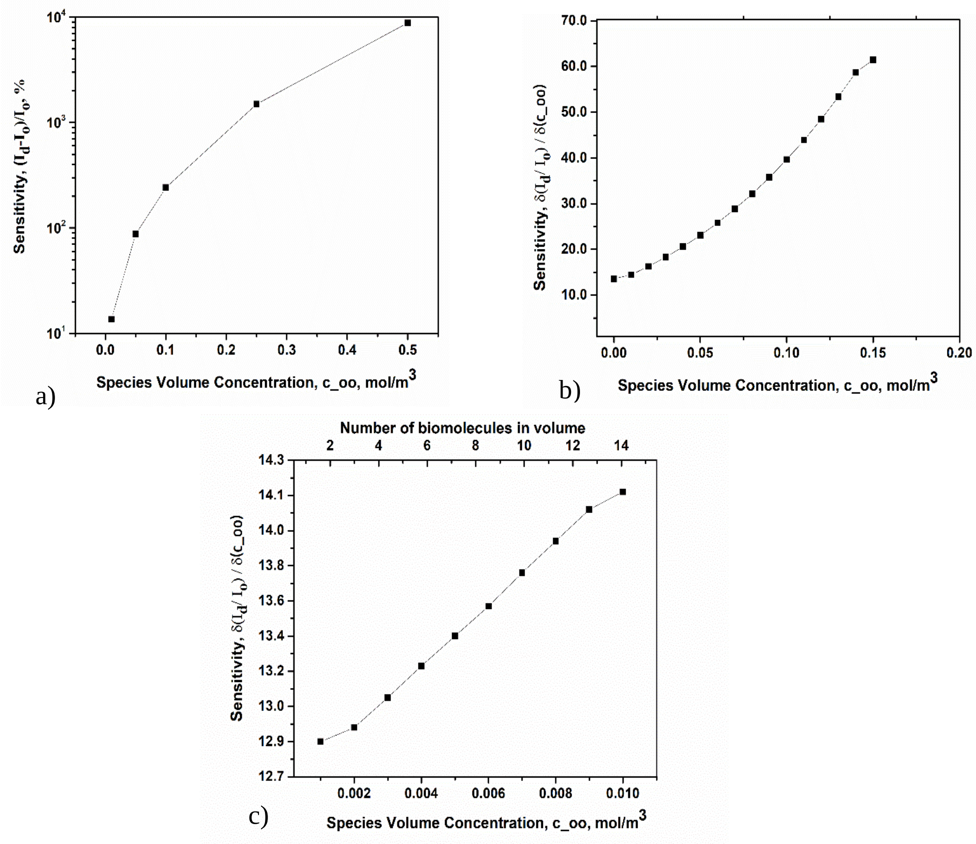

Fig. 5. The NW sensor sensitivity versus species volume concentration.

It is seen that at very high concentration the device sensitivity approaches to the saturation. This makes evident that NW sensors are more attractive for detecting the variations of small concentrations. The sensitivity calculations for a NW with radius R=10 (nm) is illustrated in Fig. 5. The NW sensor sensitivity versus injected species volume concentration calculated as the relative current difference, and is depicted in Fig 5(a). The sensitivity is plotted in logarithmic scale to make visible the large alternation of the sensitivity with the variation of species concentration from 0 to 0.5 (mol/m^3). The sensitivity values calculated for the given concentrations are depicted with the connected points.

To accurately calculate the sensor sensitivity at very small concentration variations the derivative of the relative current in respect to concentration is calculated and illustrated in Fig. 5(b) and (c). The numbers of biomolecules corresponding to concentrations given in (mol/m^3) and depicted on the bottom axis are available on the top axis, in Fig. 5(c). The performed simulations make evident that NW JL FET biosensor detects even a single molecule, as it was previously mentioned in experimental works [1, 2].

4. Conclusion

The developed Multiphysics model can serve as a basic model for further investigations of NW junctionless field effect sensor in different mediums and at the presence of different species. The model allows to accurately predict the device performance at wide range of species concentration and the system geometrical parameters. By our knowledge, this is the first COMSOL model developed for NW junctionless field effect biosensor.

Acknowledgements

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