Investigation of Silicon Nanowire Biosensors Using the 2D Drift-diffusion Model

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ABSTRACT

Experiments for silicon biosensors with gate lengths in the range of 200nm to 500nm have not been extensively carried out. In this paper, simulations were performed for gate lengths proportionally smaller and greater than regular experimental gate lengths. The sensitivity of the biosensors was simulated using a 2D drift-diffusion model in cylindrical coordinates using the Prophet simulator. In this study simulated conductance results and the respective experimental values [2] are compared. The good agreement between simulation and experiment enables us to predict and optimize the sensitivity of the DNA sensors.

The sensitivity was studied in terms of conductance by varying the gate length, probe spacing, binding efficiency and angle of probe from normal.

Keywords: BioFET, DNA-FET, biosensor, silicon nanowire.

1 INTRODUCTION

DNA-FETs are DNA sensors consisting of a semiconductor transducer and a functionalized surface. Their device structure is similar to a MOSFET, but the gate has been replaced by the functionalized surface. The charge distribution near the surface of DNA-FET changes due to binding of complementary DNA strands to the receptors on the oxide layer of the transducer. Thus current transport through the device is modulated, enabling detection. Since DNA-FETs allow direct label-free operation, they offer several advantages compared to optical detection methods, e.g. real-time and continuous operation. Furthermore, it is possible to integrate the read-out circuitry into the device in a straight-forward manner.

Experiments have been performed for biosensors with active sensor areas in the range of 1.5μm to approx. 5μm. For such large structures, a 2D drift-diffusion model is suitable. The Prophet simulation framework was used with definitions of the 2D drift-diffusion equations in cylindrical coordinates in this work. Previously a simulator was developed at our group to obtain the potential at the surface of the oxide layer of the DNA-FET due to different parameter specifications [1,3]. These parameters include the probe spacing, the binding efficiency of the probe molecules to the oxide layer surface and the angle deviation of the probe from the normal. The simulator is available online at nanoHUB.org, an NCN project.

2 PARAMETER DESCRIPTIONS

Among all the parameters characterizing the system, those which were observed to have the most sensitive relationship with the conductance were dealt with in more detail in the simulations. Two of these parameters, deviation of probe angle from normal and probe spacing are shown in Figure 1. Conventionally a uniform probe spacing and deviation angle is used throughout the structure and the values which provide us with the greater conductance are used. Binding efficiency is refers to the extent to which the probe molecules bind to the surface of the oxide layer. In the simulations binding efficiencies varying from 0% to 100% efficiency were considered. In experiments efficiencies of up to 90% can be achieved. Simulations for 0% to 100% efficiency in steps of 10% were carried out to help characterize the behavior of the system. While dealing with the device structure, the source-drain length was changed to values higher and lower than those used in experiments [2]. The oxide layer thickness used for the simulations was 1 nm and the wire thickness was in the range of 0.5μm.

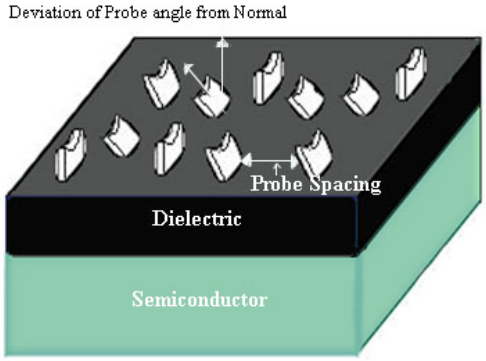

Figure 1: Schematic diagram of conventional Si BioFET structure.

3 BIOSENSOR BEHAVIOUR

It is observed from Figure 2 that the surface potential change of the oxide layer due to the partial charges of the DNA molecules is higher for smaller probe spacing. This directly implies that smaller probe spacing increases the capacity of the oxide layer to feel changes due to the partial charges. This gives us a definite direction on what the probe spacing should be for better sensitivity since the surface potential change determines the sensitivity of the sensor.

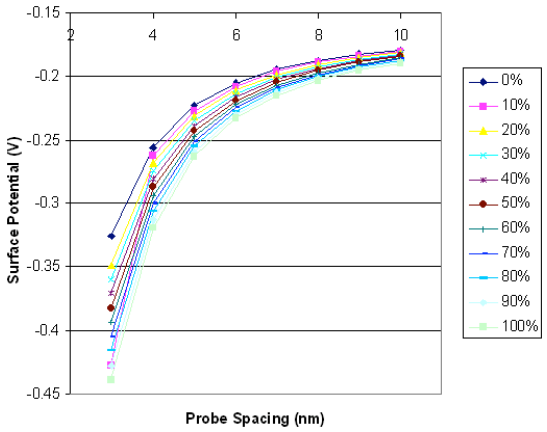

Figure 2: Surface potential on oxide layer as a function of probe spacing and binding efficiency.

Figure 3 indicates that as the deviation of the probe angle from the normal is increased a greater potential change is observed on the oxide layer. This suggests that greater probe angles *increases* the sensitivity. It is also observed that for higher binding efficiencies there is a greater surface potential change with respect to the oxide layer. This indicates that a higher binding efficiency of the probe to the surface also *increases* the sensitivity.

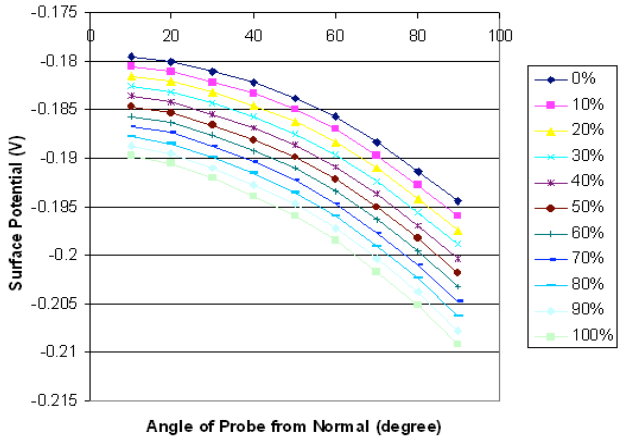

Figure 3: Surface potential as a function of angle of probe from normal and binding efficiencies.

Figure 4 shows that a smaller probe spacing has a significant impact on the conductance of the nanowire. This is in accordance with the findings of Figure 2 in providing a more definite relation of the probe spacing to the conductance of the device. This figure also confirms the increased conductivity with increased binding efficiency. It is also clear from the graph that probe spacing has a greater impact on the final conductance as compared to the binding efficiencies. Comparisons with experimental measurements [2] show that the conductance values obtained from these simulations are below the experimental conductance measurements. This is likely due to the usage of the more sensitive PNA receptors in the experiments as compared to the DNA receptors in the simulations.

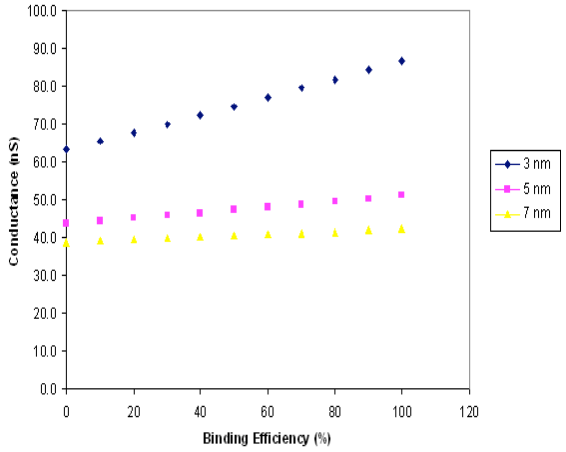

Figure 4: p-Si nanowire simulation of conductance vs. binding efficiency with 1micron gate length and 1nm oxide layer thickness at a drain voltage of 1V.

Figure 5 shows a significant increase in the conductance with decreasing sensor area exposure to the analyte. It is especially observed that an exposure of 200nm gives us an exceptionally large conductance value. We note here that the simulations are based on a classical drift-diffusion approach, which does not limit conduction to discrete conductance quanta at very small nanowire diameters.

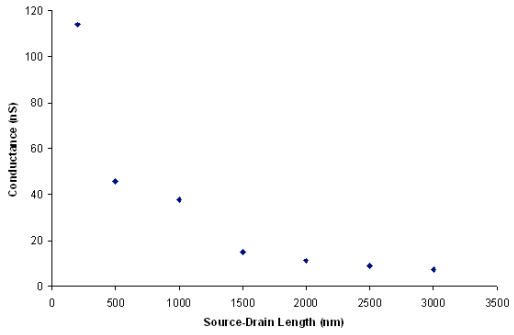

Figure 5: Conductance vs. source drain length at constant drain source voltage of 1V and 1nm oxide layer thickness.

Sensitivity has the same dependence as conductance on probe spacing and binding efficiency.

$$S = (G_i - G_0)/G_0 \quad (1)$$

S is the sensitivity, Gi is the conductance with that particular binding efficiency and G_0 is the conductance of 0% efficiency.

So Figure 6 shows the direct effect of probe spacing and binding efficiency on sensitivity. Also in the figure has been added the corresponding sensitivity [2] for 100 fM, 30 fM and 10 fM DNA sample for comparison purposes. These experimental results have a close correlation with the simulations obtained.

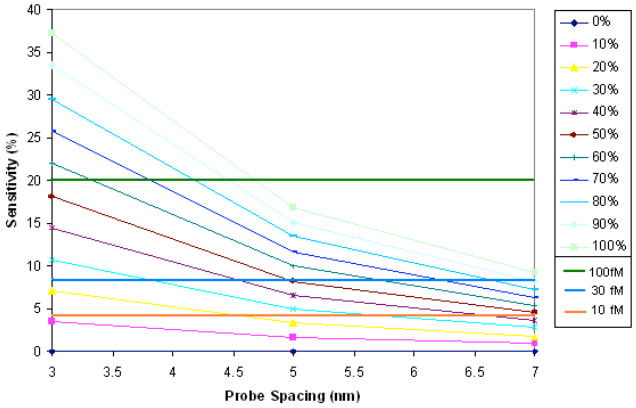

Figure 6: Sensitivity vs. probe spacing for different binding efficiencies at a constant drain voltage of 1V and oxide layer thickness of 1nm. Corresponding experimental sensitivity [1] has been added for 100 fM, 30 fM and 10 fM DNA sample for comparison.

4 RESULTS AND DISCUSSION

It has been found out that a trade-off between probe spacing and binding efficiency based on the simulations is necessary to make realistic biosensors [1]. Coupling those results with the source-drain length simulations provides us with a realistic model of the device itself. Since both the effect of molecular attachment to the oxide surface and their consequent effect on the conductance have been simulated correspondingly, the results present a very accurate model of biosensors of those specifications. In addition the conductance values obtained for the biosensors in the range of 200nm to 1000nm source-drain length were reasonably high. These values indicate immense capacity in making sensitive silicon biosensors with the mentioned specifications.

5 CONCLUSION

From the simulations for different gate lengths, silicon biosensors respective sensitivity has been studied for binding efficiency, probe spacing and angle of probe from normal. The simulations obtained provide us with insight into the characteristics of silicon biosensors which would yield the most sensitivity. It thus provides a definite direction for the development of accurate biosensors using silicon.

6 ACKNOWLEDGMENTS

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[6] See http://www.nanohub.org/tools/prophet/ for more information on Prophet.