10-22-2006

Investigation of Device Parameters for Field-Effect DNA-Sensors by Three-Dimensional Simulation

Eddie Howell
Norfolk Sate University

Clemens Heitzinger
Purdue University, Main Campus

Gerhard Klimeck
Purdue University, Main Campus, gekco@purdue.edu

MEO3

Investigation of Device Parameters for Field-Effect DNA-Sensors by Three-Dimensional Simulation

Eddie Howell*, Clemens Heitzinger†, and Gerhard Klimeck†
*School of Science and Technology, Norfolk State University, Norfolk, VA, USA
Email: e.l.howell@nsu.edu
†School of Electrical Engineering, Purdue University, West Lafayette, IN, USA
Email: ClemensH@Purdue.edu

I. Introduction

The development of a DNA field-effect transistor (DNAFET) simulator is described and implications on device structure and future experiments are discussed. In DNAFETs the gate structure is replaced by a layer of immobilized single-stranded DNA molecules which act as surface probe molecules [1, 2]. When complementary DNA strands bind to the receptors, the charge distribution near the surface of the device changes, modulating current transport through the device and enabling detection (cf. Fig. 1 and 5). Arrays of DNAFETs can be used for detecting single-nucleotide polymorphisms and for DNA sequencing. The advantage of DNAFETs over optical methods of detection is that DNAFETs allow direct, label-free operation.

II. Simulation method

Conventional and silicon-nanowire DNAFETs are investigated using a rigorous and comprehensive approach [3, 4].The simulator constructs the specified DNA oligomers and calculates the electrostatic potential due to the partial charges of the DNA molecules by solving the three-dimensional Poisson-Boltzmann equation. For modeling silicon-nanowire DNAFETs we use a modified three-dimensional self-consistent mode-space non-equilibrium Green function (NEGF) simulator [5], and conventional SOI structures are simulated by MiniMOS [6]. The silicon-nanowire simulation uses small-signal AC analysis with a bias of 50 mV and a frequency of 79 Hz.

III. Simulation results and discussion

Figure 2 shows that by decreasing the length of the sensor area that is exposed to the analyte, the effects of DNA hybridization on conductance are greater. The physical dimensions of the sensor area play an important role in the capabilities of the device. Previous research has shown that the hybridization efficiency of the target strands to the probes depends on the packing density of the probe molecules [7]. Higher packing densities lead to lower hybridization efficiencies due to electrostatic effects. It has been shown that at a probe spacing length of 3 nm the hybridization efficiency is ≈ 10%, while at 7 nm the hybridization efficiency is ≈ 90% [7]. Figure 3 shows the correlation between the packing density and hybridization which implies there is a trade-off between the two. Figure 3 shows that a device with a probe spacing of 7 nm is more sensitive to DNA hybridization than a device with 3 nm spacing. Figure 4 shows that increasing the salt concentration in the analyte solution decreases the sensitivity of the device, due to increased shielding. However, a minimum salt concentration is necessary for DNA hybridization.

In the silicon-nanowire simulations there is only one probe molecule in the middle of the device (cf. Fig. 5). This device shows the possibility of being a single-molecule sensor. Figure 6 shows that the sensitivity of the device is a function of its diameter. As expected, the larger the diameter of the device, the less sensitive it is due to the decreased surface area-to-volume ratio. Fig. 2 & 3 show the great influence of binding efficiency, therefore rigorous modeling of surface chemistry is necessary to understand and predict device performance.

Acknowledgment

This material is based upon work supported by the National Science Foundation under Grant No. EEC-0228390, the Indiana 21st Century fund, and the Semiconductor Research Corporation. We thank Siegfried Selberherr for providing the source code of MiniMOS 6.1. Interested readers can run simulations online at http://www.nanohub.org.

References

[1] M. J. Schöning and A. Poghossian, "Recent advances in biologically sensitive field-effect transistors," The Analyst, vol. 127, pp. 1137-1151, 2002.

[2] J. Hahm and C. M. Lieber, "Direct Ultrasensitive Electrical Detection of DNA and DNA Sequence Variations Using Nanowire Nanosensors," Nano Letters, vol. 4, no. 1, pp. 51-54, 2004.

[3] C. Heitzinger and G. Klimeck, "Computational Aspects of the Three-Dimensional Feature-Scale Simulation of Silicon-Nanowire Field-Effect Sensors for DNA Detection," in *Proc. 11th Int. Workshop Comput. Electron. (IWCE 11)*, Vienna, Austria, May 2006.

[4] C. Heitzinger and G. Klimeck, "Computational Aspects of the Three-Dimensional Feature-Scale Simulation of Silicon-Nanowire Field-Effect Sensors for DNA Detection," J. Comp. El., 2006. Submitted for publication.

[5] J. Wang, E. Polizzi, and M. Lundstrom, "A three-dimensional quantum simulation of silicon nanowire transistors with the effective-mass approximation," J. Appl. Phys., vol. 96, no. 4, pp. 2192-2203, 2004.

[6] S. Selberherr et al., *MiniMOS 6.1 User's Guide*, Institute for Microelectronics, Technical University, 1999.

[7] A. W. Peterson, R. J. Heaton, and R. M. Georgiadis, "The effect of surface probe density on DNA hybridization," Nucleic Acids Research, vol. 29, no. 24, pp. 5163-5168, 2001.

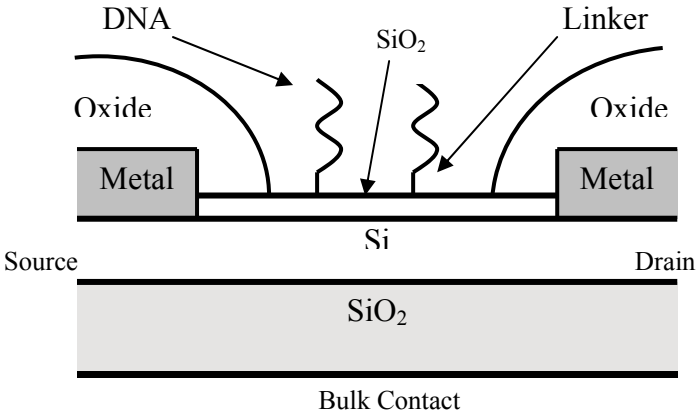

Figure 1. This is a schematic diagram of the conventional SOI DNAFET structure. The DNA molecules are bound to the SiO_2 surface layer by an uncharged linker molecule.

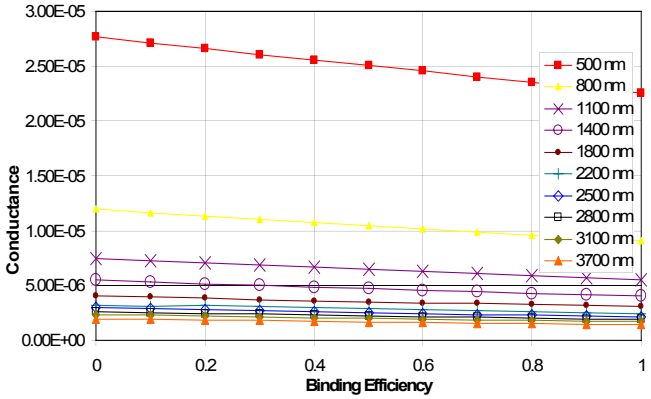

Figure 2. Conventional structure simulation with a probe spacing length of 10 nm and a surface oxide thickness of 4 nm. The absolute values of the conductance were calculated, and for smaller devices the relative change in conductance was greater than that for larger-sized devices.

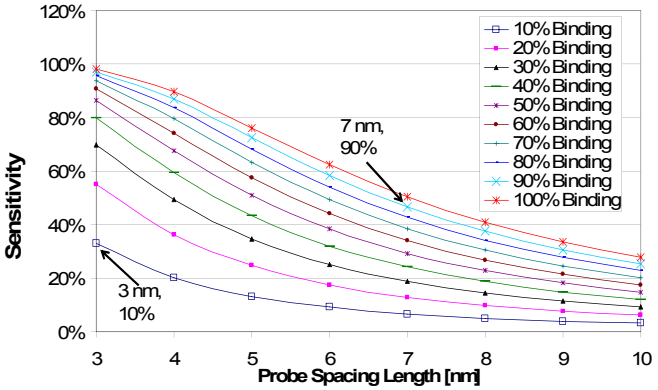

Figure 3. Conventional structure simulation with a sensor length of 3 and a surface oxide thickness of 4 nm. 0% binding is calculated with only probe molecules attached to the surface. The baseline is the 0% binding level. Sensitivity is defined as the difference between the conductance with two strands and the conductance with one strand divided by the conductance with one strand.

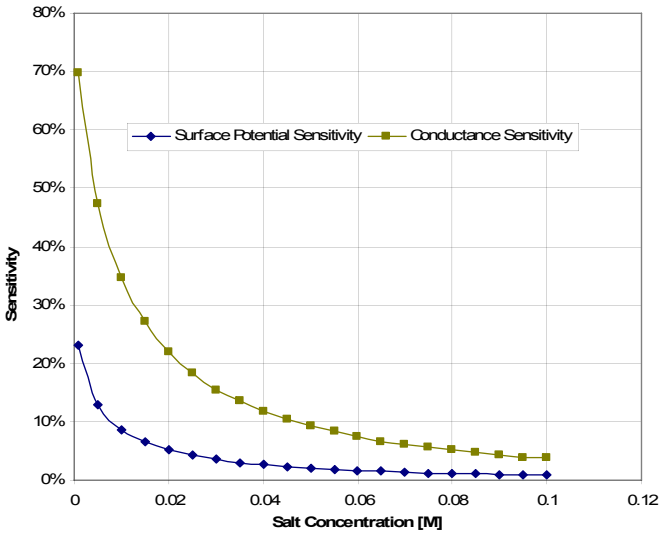

Figure 4. Conventional structure simulation with a probe spacing length of 10 nm and a surface oxide thickness of 4 nm. The conductance and surface potential were calculated in two states; initially with only the probe molecules attached to the surface and then with the probe molecules bonded with the target molecules. Sensitivity is defined as the difference between the values with two strands and the potential with one strand divided by the value with one strand.

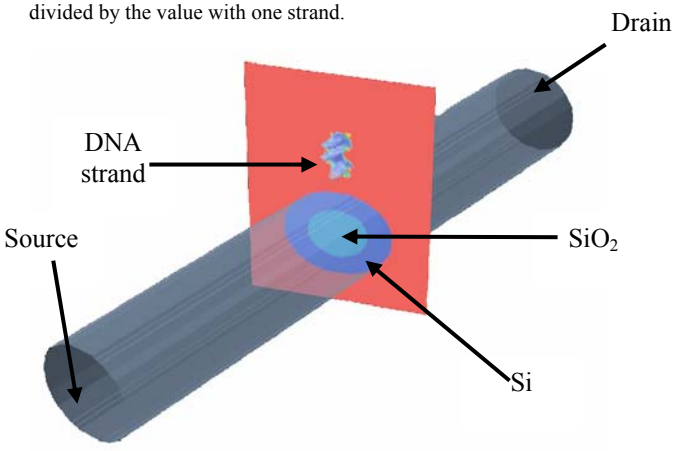

Figure 5. Silicon nanowire DNAFET diagram.

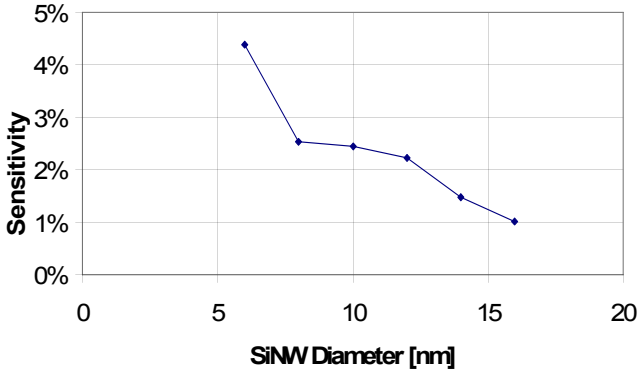

Figure 6. Silicon nanowire structure simulation with a channel length of 20 nm and a surface oxide layer thickness of 2 nm.