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Analysis of Field-Effect Biosensors using Self-Consistent 3D Drift-Diffusion and Monte-Carlo Simulations

S. Baumgartner[a*], M. Vasicek[a], A. Bulyha[a], N. Tassotti[a], and C. Heitzinger[ab]*

[a]*Department of Mathematics, University of Vienna, Austria*
[b]*Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 0WA, UK*

Abstract

Field-effect biosensors based on nanowires enjoy considerable popularity due to their high sensitivity and direct electrical readout [1]. However, crucial issues such as the influence of the biomolecules on the charge-carrier transport or the binding of molecules to the surface have not been described satisfactorily yet in a quantitative manner. In order to analyze these effects, we present simulation results based on a 3D macroscopic transport model coupled with Monte-Carlo simulations for the bio-functionalized surface layer. Excellent agreement with measurement data has been found, while detailed study of the influence of the most prominent biomolecules, namely double-stranded DNA and single-stranded DNA, on the current through the semiconductor transducer has been carried out.

Keywords: field-effect biosensors, field-effect DNA sensors, silicon nanowire, sensor simulation;

1. Introduction

The detection principle of field-effect nanowire biosensors is based on the current change in the semiconductor transducer due to the binding of target molecules at a functionalized surface. Hence a large current response, i.e., a high sensitivity, is of great importance and is necessary to provide a reliable sensing result. Sensor designs can be improved by the model presented here due to a novel approach which includes all charge-carrier interactions.

* Corresponding author. Tel.: +43 1 4277 50715; fax: +43 1 4277 50650.
E-mail address: stefan.baumgartner@univie.ac.at, c.heitzinger@damtp.cam.ac.uk

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2. The Model

In order to quantify the screening of the partial charges of the biomolecules as realistically as possible and to gain a deeper quantitative understanding of the sensing mechanism, we have developed a macroscopic model coupled self-consistently with a Monte-Carlo algorithm for the functionalized surface at the electrolyte/semiconductor interface.

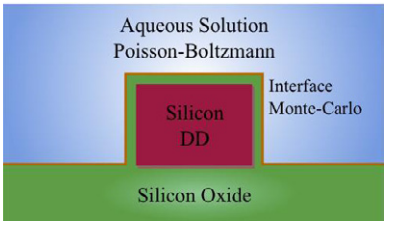
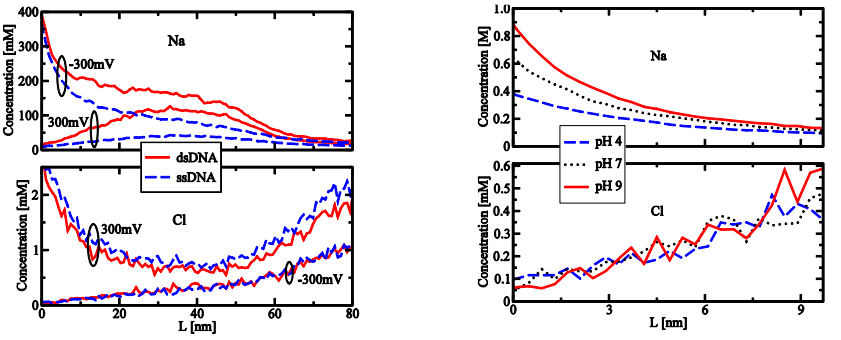


Fig. 1. Schematic cross section of the nanowire biosensor. The silicon nanowire is described by the drift-diffusion model, while the interface and the surface layer in the electrolyte are modeled by a Monte-Carlo approach.

The multiscale problem due to the biomolecules in the Angstrom range and the nanowire length in the micrometer range has been solved by a homogenization method [2]. The macroscopic part of the model is given by three material dependent systems of partial differential equations which include the electric potential in the whole domain and the charge carriers, i.e., the electrons and holes, in the semiconductor (see Figure 1). The charge transport in the nanowire is described by the drift-diffusion model and the aqueous solution is described by the Poisson-Boltzmann equation. The charge concentration in the bio-functionalized surface layer is calculated by Metropolis Monte-Carlo simulations in the constant-voltage ensemble [3] and is then transformed into interface conditions which are adequate to capture the impact of the surface layer in the transport model. In summary, it is possible to determine the concentration of the ions in the surface layer, which is crucial for the sensing mechanism, and the self-consistent PDE model allows us to calculate current-voltage characteristics.

3. Results

As mentioned before, the surface layer and the semiconductor are simulated in a self-consistent



(a) (b)

Fig. 2. (a) Na+ and Cl- concentration profiles with ssDNA and dsDNA immobilized on the surface at electrolyte voltages of -300mV and +300mV. (b) Ion concentration profile as functions of the distance from the surface at a surface voltage of -0.4V for different pH values.

manner. To that end, the sodium Na^+ and chloride Cl^- ion concentration profiles are calculated in each iteration of the self-consistent loop with respect to the electric potential at the surface. Such Monte-Carlo simulations for electrolyte potentials of 300mV and -300mV at a pH value of 7.5 for single-stranded DNA (ssDNA) and double-stranded DNA (dsDNA) in a simulation box of 80nm height are shown in Figure 2a.

The interplay between the Na^+ and Cl^- ion concentration is visible especially at 300mV, where the Na^+ concentration reaches a maximum at 40nm and the Cl^- concentration has a minimum. Furthermore, dsDNA bound at the surface – in comparison to ssDNA – increases the Na^+ concentration, while the Cl^- concentration remains nearly the same, especially in the -300mV case. Hence the sensitivity of this device is provided mainly from the sodium concentration. The same effect is achieved by varying the pH value in the electrolyte (see Figure 2b). Here the Na+ concentrations for different pH values are clearly distinguishable, while the Cl- concentrations show an unspecific behavior.

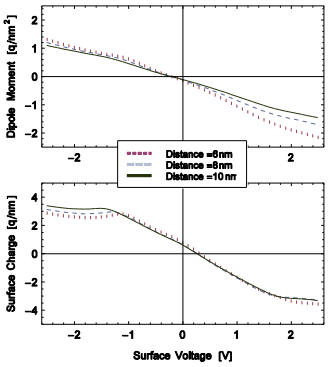
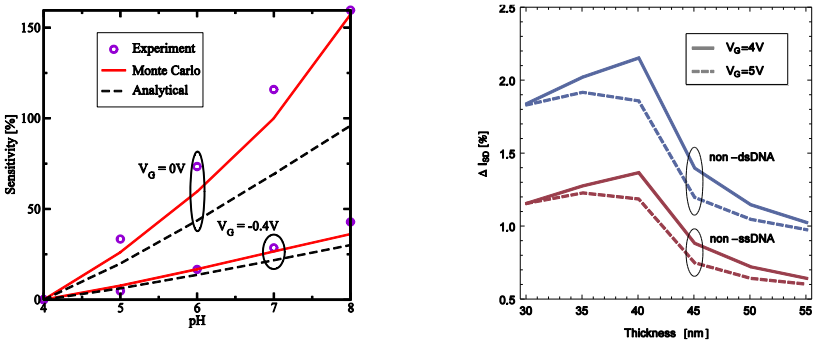


Fig. 3. Dipole-moment density and surface-charge density for different distances between dsDNA strands as a function of the surface voltage.

Based on these simulations, the macroscopic surface-charge density and the macroscopic dipole-moment density are calculated (see Figure 3). Parameters regarding the molecules such as the length of the linker, the angle of the DNA strands with respect to the surface, and the interspace between the DNA strands, as in Figure 3, are included.



(a) (b)

Fig. 4. (a) Comparison between experimental and simulated data. The sensitivity as a function of pH value of the electrolyte is calculated for gate voltages of 0V and -0.4V. The Monte-Carlo method outperforms the analytical model. (b) Current change, when molecules are detected, as a function of the nanowire thickness when ssDNA or dsDNA are present at the surface.

These values in turn change the electric potential in the semiconductor transducer, i.e., the charge carriers and the electric potential are the solutions of the drift-diffusion equations. Therefore the sensitivity of the sensor, expressed as the ratio of the conductivity change and the conductivity itself, can be investigated.

In Figure 4a, the sensitivity was calculated for different pH values. Our model clearly outperforms analytical models based on [4] and shows very good agreement with the experiments of [5]. Furthermore, geometrical and physical properties of the device can be investigated with respect to optimizing sensitivity. We note that due to the real-world boundary conditions and the spatial structure of the sensors, 3D simulations must be performed. The influence of the nanowire thickness on the current change for back-gate voltages of 4V and 5V for a 500nm long nanowire sensor is shown in Figure 4b. Here, non-dsDNA denotes the current change, in percent, from a non-functionalized surface to a surface with dsDNA, and similarly for the change from a non-functionalized surface to ssDNA. The maximum and hence the optimal sensitivity is reached at a thickness of 40nm for a back-gate voltage of 5V and it decreases very fast beyond 40nm. A change to a lower back-gate voltage shows a shift of the optimal point to a thinner nanowire. This example shows how certain device parameters can be varied to maximize sensitivity and that optimal designs exist. In future work, we will further investigate optimal designs and trade-offs between device parameters, also with respect to noise.

4. Conclusion

We have simulated field-effect biosensor characteristics using a drift-diffusion model self-consistently coupled with Monte-Carlo simulations. The Monte-Carlo simulations include all interactions between the free ions and the DNA strands and many parameters such as the angle of the DNA strands with respect to the surface and the length of the linker. The influence of different surface functionalizations and pH values on the Na^+ and Cl^- ion concentration profiles have been discussed as well as the dipole-moment density and the surface-charge density for different molecule interspaces. Emphases have also been given to sensitivity correlations with geometrical and physical parameters. In this way, optimal sensors can be designed and the underlying physics of the devices can be investigated by calculating potentials and concentrations that cannot be measured directly.

Acknowledgements

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