Investigations of the Potential Jump at the Surface of BioFETs Using a Multi-scale Model

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A BioFET (biologically active field-effect transistor) is a biosensor whose transducer consists of a semiconductor, usually silicon. The device structure of a BioFET is similar to a MOSFET whose gate structure has been replaced by a functionalized oxide surface and an aqueous solution (see Fig. 1). BioFETs can be viewed as generalizations of ISFETs (ion-selective FETs) [1]. In the last decade experiments have shown that as the analyte binds to the functionalized surface, the change in the charge distribution near the oxide surface affects the conductance of the semiconductor and this conductance change enables detection [2, 3]. The detection of ssDNA, a highly charged biomolecule, is a prime example with many health-care applications.

To arrive at predictive simulations of BioFETs, the electrostatic potential must be calculated on a straight line perpendicular to the sensor surface containing the aqueous solution, the oxide layer, and the semiconductor (i.e., parallel to the x-axis in Fig. 1). This modeling effort is complicated by the multi-scale nature of the device: the lengths of the exposed sensor areas in experiments are at least a few micrometer, whereas the DNA diameter is about 2nm and the packing density of the probe molecules is between 3nm and about 10nm. In previous work we presented results from a first-order approximation to the solution of this problem [4, 5]. Here we present a model based on a rigorous solution of the mathematical multi-scale problem by homogenization of the boundary conditions at the oxide/solution interface.

Our model is based on the Poisson–Boltzmann equation including both the mobile ions in the solution and the carriers in the semiconductor (the mobile charges follow a Boltzmann distribution). The original problem whose solution varies rapidly on the nanometer scale is replaced, after homogenization of the boundary conditions at the oxide/solution interface, by a homogeneous equation in the solution, a homogenized potential, and matching interface conditions. The two interface conditions are interpreted as a jump in the homogenized potential that arises from the dipole moment of partial charges of the molecules (a linear term) and from the dipole moment of the mobile Boltzmann charges (a nonlinear term); and as a jump in the field that arises from the partial charges plus a nonlinear term. The Poisson–Boltzmann PDE together with the interface conditions and the boundary conditions for the reference electrode and bulk contact is a well-posed problem.

Fig. 2 shows the homogenized potential on a straight line normal to the sensor surface of a DNAFET. In summary, the model can be applied comprehensively to all classes of BioFETs.

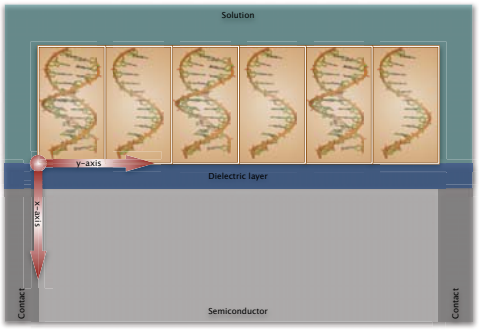

Figure 1: Schematic diagram of a BioFET. Here the oxide surface has been functionalized with single-stranded DNA (or PNA) to create a DNAFET. In the multi-scale BioFET model the surface area is covered by boxes and each box is occupied by a probe molecule and potentially a target molecule.

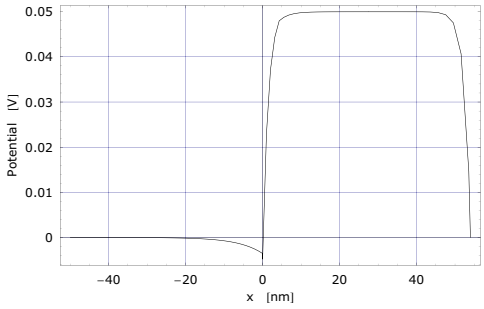

Figure 2: This example shows the homogenized electrostatic potential perpendicular to the sensor surface (parallel to the x-axis of Fig. 1) of a DNAFET SOI structure (consisting of 50nm of 1:1 electrolyte on the negative x-axis, a 4nm oxide layer, a 20nm silicon layer, and 30nm bulk oxide). The jump in the homogenized potential and field is seen at $x = 0$nm. The binding efficiency of target strands to probes is 100% target strands. The difference in the surface potential on the semiconductor side between 0% and 100% binding efficiency is ≈ 4.2mV.

REFERENCES

[1] P. Bergveld, "Development of an ion-sensitive solid-state device for neurophysiological measurements," *IEEE Trans. Biomed. Eng.*, vol. BME-17, pp. 70–71, 1970.

[2] E. Souteyrand, J. Cloarec, J. Martin, C. Wilson, I. Lawrence, S. Mikkelsen, and M. Lawrence, "Direct detection of the hybridization of synthetic homo-oligomer DNA sequences by field effect," *J. Phys. Chem. B*, vol. 101, pp. 2980–2985, 1997.

[3] M. Schöning and A. Poghossian, "Recent advances in biologically sensitive field-effect transistors (BioFETs)," *Analyst*, vol. 127, pp. 1137–1151, 2002.

[4] C. Heitzinger and G. Klimeck, "Computational aspects of the three-dimensional feature-scale simulation of silicon-nanowire field-effect sensors for DNA detection," *Journal of Computational Electronics*, 2006. *(In print).*

[5] C. Heitzinger and G. Klimeck, "Investigation of conventional DNAFETs for genome-wide detection of polymorphisms," in *Proc. Eurosensors XX 2006*, (Göteborg, Sweden), Sept. 2006.