Theoretical model for the detection of charged proteins with a silicon-on-insulator sensor

Stefan Birner[1], Peter Vogl

For a bio-sensor device based on a silicon-on-insulator structure, we calculated the sensitivity to specific charge distributions in the electrolyte solution that arise from protein binding to the semiconductor surface [1]. This surface is bio-functionalized with a lipid layer so that proteins can specifically bind to the headgroups of the lipids on the surface. We consider charged, artificial proteins that consist of a variable number of aspartic acids. We calculate self-consistently the spatial charge and electrostatic potential distributions for different ion concentrations in the electrolyte. We determine the potential change at the binding sites as a function of protein charge and ionic strength. Screening effects in the electrolyte are taken into account using the Poisson-Boltzmann equation which is superior compared to the simplified Debye-Hückel approximation. The quantum mechanical charge densities in the semiconductor are calculated self-consistently by solving the Schrö-dinger equation in the silicon channel. The Schrödinger and Poisson equations are coupled via the electrostatic potential and the charge densities. Fig. 1(b) shows the calculated conduction band edge and the electron density in the silicon channel for a backgate voltage of U_{BG} = 25 V. Indicated is also the position of the Fermi level E_F and the electrostatic potential. Specifying a value for the potential U_G of the reference electrode in the electrolyte is equivalent to a Dirichlet boundary condition for the electrostatic potential of the Poisson-Boltzmann equation. An increase of U_G leads to higher electron densities in the right channel. Therefore, the variation of U_G and the backgate voltage U_{BG} allows one to increase the sensitivity of the sensor by adjusting the ratio of the densities of the two channels. Our calculations

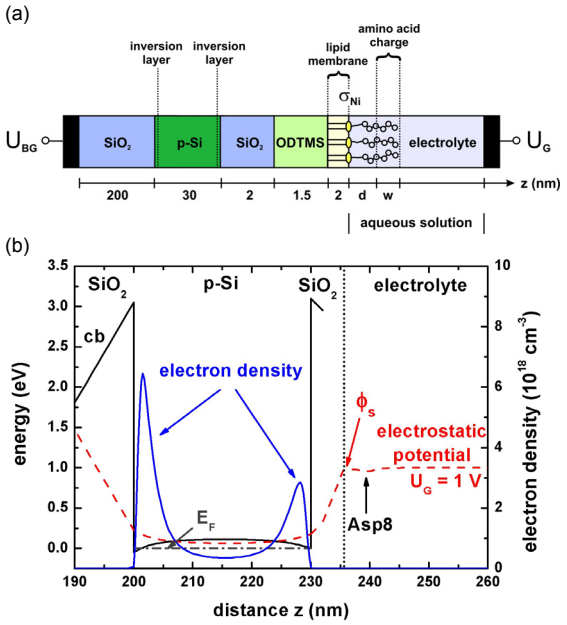

***Fig. 1**: (a) Schematic layout of the SOI structure. There is a negative interface charge density σ_{Ni} at the lipid/electrolyte interface. The amino acid charge is assumed to be distributed homogeneously over a width w. The electrolyte region includes the histidine-tagged amino acids as well as the neutral part of the tag of length d. (b) Calculated conduction band edge (black solid line) and electrostatic potential (dashed line) at a salt concentration of 50 mM KCl. The electron charge density (blue solid line) of the two inversion layers is shown. Upon binding to the lipid membrane, the charge of the aspartic acid (Asp8) modifies the surface potential ϕ_s. The interface between the lipid membrane and the electrolyte is indicated by the vertical dotted line.*

[1]phone: +49-89-289-12752, fax: +49-89-289-12737, email: stefan.birner@nextnano.de

yield channel densities of the order of a few 10^{12} cm^{-2}. They are modulated slightly by the actual configuration of the system in terms of ion concentrations and protein charges. Since a lower surface potential ϕ_s yields a lower electron density in the inverted silicon channel, the source-drain current is expected to decrease if negatively charged proteins bind to the functionalized sensor surface.

The artificial proteins that we consider consist of several aspartic acids. Figure 2(a) shows the calculated potential distributions for a varying number of aspartic acids, i.e. various protein charge distributions, at 50 mM KCl concentration in the electrolyte solution. The magnitude of the negative protein charge density increases with the number of aspartic acids. This results in a lower electrostatic potential in the protein region. Also, the surface potential ϕ_s decreases with increasing protein charge. Fig. 2(b) shows the calculated change of surface potential $\Delta\phi_s$ at the bio-functionalized semiconductor surface for a varying number of aspartic acids at salt concentrations of 50 and 140 mM KCl. Comparison with experiment is very good. One can clearly see that the sensitivity of the structure is enhanced at low ion concentrations. We demonstrated that our numerical approach - the self-consistent solution of the Schrödinger and Poisson-Boltzmann equation [3] - is well suited to model semiconductor based bio-sensors in a systematic manner, which is a requirement in order to both understand and optimize their sensitivity.

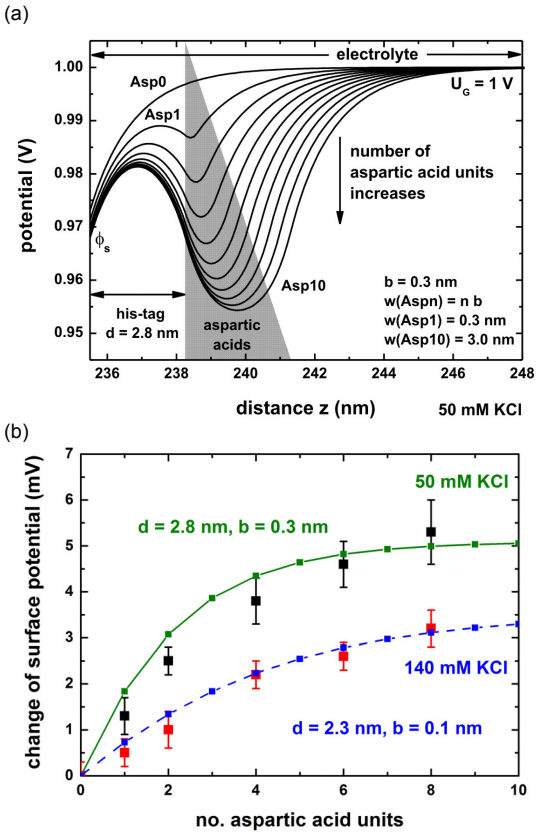

***Fig. 2**: (a) Calculated electrostatic potential distributions for varying protein charge at 50 mM KCl. The number of aspartic acids is n = 0,1,2,...,10 and increases from top to bottom. The width w=nb of the negative protein charge distribution is assumed to increase linearly with the number of acids (indicated schematically by the shaded triangle). (b) Calculated surface potential change $\Delta\phi_s$ at the lipid membrane as a function of the number of aspartic acids in the artificial protein for different salt concentrations (solid line: 50 mM KCl, dashed line: 140 mM KCl). The experimental data points are from Ref. [2].*

[1] S. Birner, C. Uhl, M. Bayer, P. Vogl, J. Phys.: Conf. Ser. **107**, 012002 (2008)
[2] S.Q. Lud, M.G. Nikolaides, I. Haase I, M. Fischer, A.R. Bausch, ChemPhysChem **7**, 379 (2006)
[3] This algorithm has been implemented into the software package next**nano**^{3} which can be obtained from www.nextnano.de.