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

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Motivation

- Field-effect biosensors provide **high sensitivity** and a **direct electrical readout** [1]
- **Influence of biomolecules** on the charge transport or **binding of molecules** to the inferface are **not satisfactorily described** yet
- **Mathematical modeling** of the charge transport with partial differential equations leads to **predictive and realistic simulations**

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 developed the following model [2].

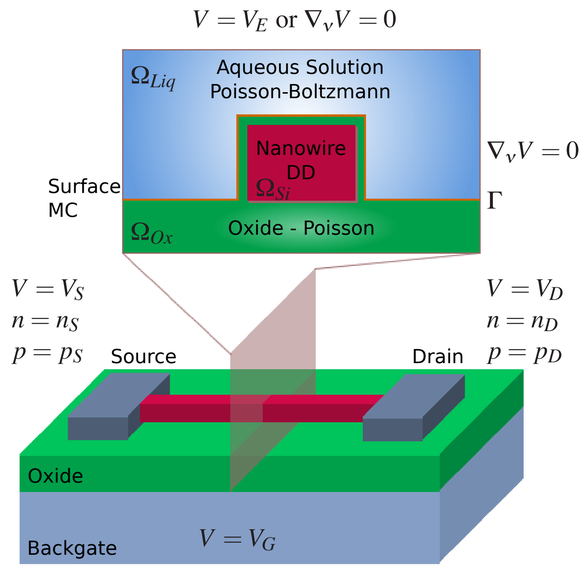
- Three material dependent systems of partial differential equations describe the electric potential and the charge carriers (see Fig. 1):
  - **Drift-diffusion equations** for the charge transport in the nanowire

$$-\nabla\cdot(\varepsilon_{Si}\nabla V) = q(p-n+C_{dop})$$
$$\nabla\cdot(D_n\nabla n-\mu_n n\nabla V) = R$$
$$\nabla\cdot(-D_p\nabla p-\mu_p p\nabla V) = -R$$

  - A **Poisson-Boltzmann** model for the aqueous solution

$$-\nabla\cdot(\varepsilon_{Liq}\nabla V) = \sum_{\sigma\in\{-1,1\}}\eta\sigma e^{-\sigma\beta V},$$

  - The **Poisson equation** for the dielectric layer
- **Metropolis Monte-Carlo simulations** in the constant-voltage ensemble are computed to obtain the charge concentration in the biofunctionalized surface layer [3].



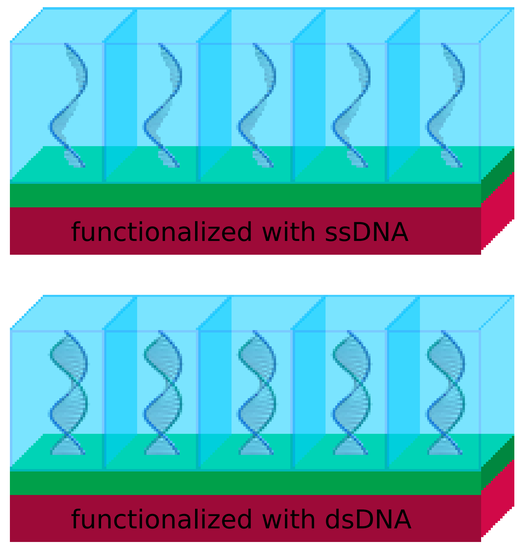


Fig. 1. Left: schematic cross section of the nanowire biosensor. The silicon nanowire is described by the drift-diffusion model, while the interface and the surface layer in the electrolyte are modeled by a Monte-Carlo approach. Boundary conditions are also indicated. Right: a nanowire functionalized with ssDNA as probes without any target molecules (top) and a nanowire functionalized with ssDNA with a target ssDNA strand (dsDNA, bottom).

- A **homogenization method** solves the multiscale problem of the biomolecules in the Angstrom range and the nanowire length in micrometer range [4]. Therefore, the continuity equations at the interface are replaced by jump conditions including the surface-charge density α and the dipole-moment density γ:

$$V(0+,y,z) - V(0-,y,z) = \frac{\gamma}{\varepsilon_{Liq}}$$
$$\varepsilon_{Liq}\nabla_x V(0+,y,z) - \varepsilon_{Ox}\nabla_x V(0-,y,z) = -\alpha(y,z)$$

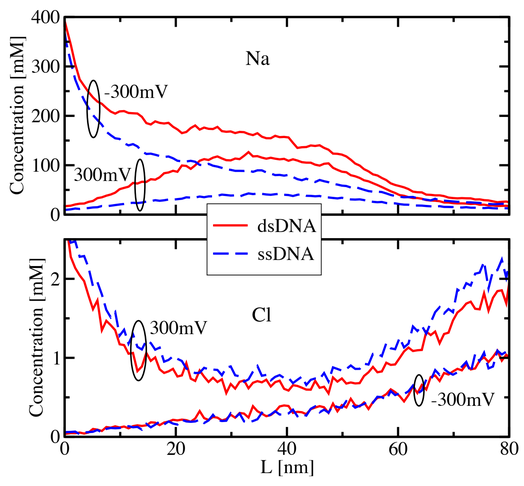


Fig. 2: NaCl concentration profile.

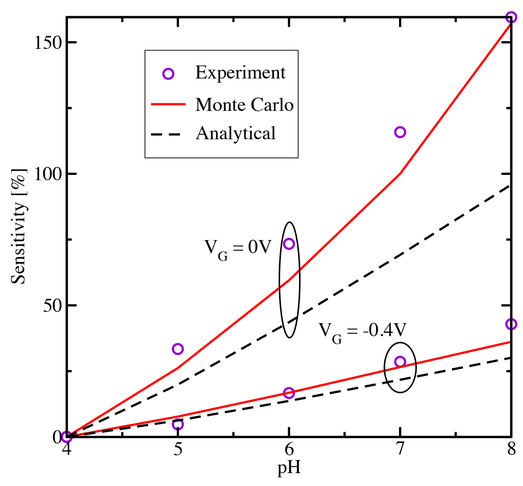


Fig. 3: Comparison between experimental and simulated data .

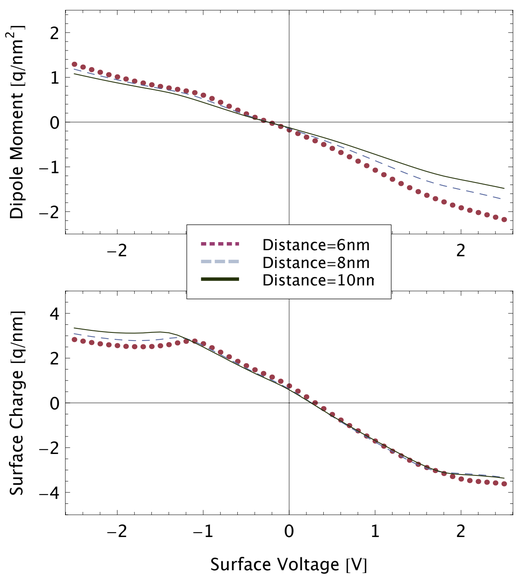


Fig. 4: Dipole moment density and surface charge density.

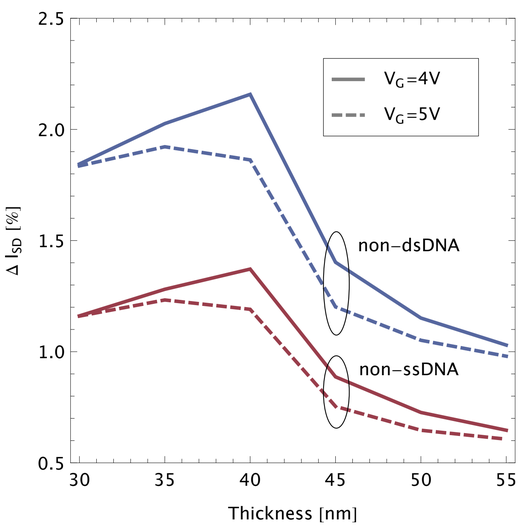


Fig. 5: Current change as a function of the nanowire thickness.

Numerical Methods

- The **Scharfetter Gummel iteration scheme** in connection with the finite volume method for the drift-diffusion equations
- The **finite volume method** for the Poisson-Boltzmann equation
- A **FETI (finite element tearing and interconnecting) method** for the parallelization of the simulator
- A **Metropolis Monte-Carlo algorithm** in the constant voltage ensemble for the computation of the surface charges

Results

- **Sodium Na^+** and **chloride Cl^-** ion concentration profiles are calculated with a Metropolis Monte-Carlo algorithm in the constant voltage ensemble with respect to the electric potential at the surface (see Fig. 2).
- Many parameters can be adjusted in order to obtain reliable and realistic results. Some of them are
  - the electrolyte potentials,
  - the pH value,
  - the angle of the DNA strands to the surface,
  - and the interspace between the DNA strands.
- The interface conditions, the **dipole-moment density** and the **surface-charge density**, are computed from the ion concentration profiles and are then implemented in the self-consistent loop of the Scharfetter Gummel iteration scheme (see Fig. 4).
- The electric potential and the charge carriers are obtained in a self-consistent loop. Current, current-voltage characteristics and the sensitivity of the sensor can be computed.
- Sensitivity simulations for different pH values show **very good agreement with experiments** of [5] and our model clearly outperforms analytical models based on [6] (see Fig. 3).
- The simulations of the electric potential and the charge carriers are in 3d and hence physical as well as geometrical properties can be tested on their contribution to sensitivity [7]. We show in Fig. 5 that nanowire thickness for a 500nm long nanowire has an **optimal point of sensitivity** at 40nm. The molecules at the surface are dsDNA and ssDNA and the computed current of them is compared with a non-functionalized nanowire.

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