Simulation of ionic current through the nanopore in a double layered semiconductor membrane.

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Abstract
Starting with a description of an electrostatic model of a double-layered semiconductor membrane immersed in an electrolyte solution, we provide a comparison of the electric potential and ionic concentrations in a nanopore for different nanopore geometries (double-conical, single-conical, cylindrical) and for various voltages applied to the membrane. Voltage-current characteristics for ionic currents, as well as their rectification ratios are calculated using a simple ion transport model. The rectification ratio is found to be a linear function of potential variation in the pore. Based on our calculations, we find that the double layered semiconductor membrane with a single-conical nanopore with a narrow opening in the n-Si layer exhibits the largest range of available potential variations in the pore, and thus, may be better suited for transport selectivity through the nanopore.

Model of the solid-state membrane
Concentrations of electrons and holes in silicon are

\[ n = N_i^{eff} \frac{q}{kT} \exp \left( \frac{-\phi}{kT} \right) \]

\[ p = N_i^{eff} \frac{q}{kT} \exp \left( \frac{-\phi}{kT} \right) \]

where

- \( N_i^{eff} \) is the equivalent volumetric concentration of the oxide surface charge (\( n_{ox} \)) on the boundary with [KCl].
- \( \phi \) is the electric potential.
- \( q \) is the electronic charge.
- \( k \) is the Boltzmann constant.
- \( T \) is the temperature.

The considered system demonstrates significant ionic current rectification, with a strong dependence on the gate voltage \( V_g \). There is a current saturation region for \( V_g < 0 \), and \( K^+ \) ions are the major charge carriers. We also show that such a system performs the comparable membrane with a thicker n-Si layer in terms of the gate voltage effectiveness.

Simulation results

- \( V_{DS} = -0.4 \) V, \( V_{GS} = 0 \) V:

- \( V_{DS} = 0.4 \) V, \( V_{GS} = 0 \) V:

Numerical Method
The system of equations is solved self-consistently using finite difference method. In order to do it, potential \( \phi \) and concentrations \( n, p, [C^+] \), and \([K^+] \) were replaced with their discrete representations on a grid with variable grid-point size from 0.2 nm to 0.8 nm. Gummel’s method is implemented for Poisson’s equation to speed up its convergence. Finally, all systems of linear equations are solved using Gauss-Seidel method.

Different systems
If the n-Si layer is large, so that the thickness of the oxide layer is equal to 0.8 nm everywhere, we obtain the following I-V curves:

References
[1] Simulation of ionic current through the nanopore in a double-layered semiconductor membrane. A. Nikolaev and M. Gracheva (Accepted for publication in Nanotechnology, 2011).