

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

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 $\varphi|_{x=-L_x}=V_S+V_0^{KCl},$ 

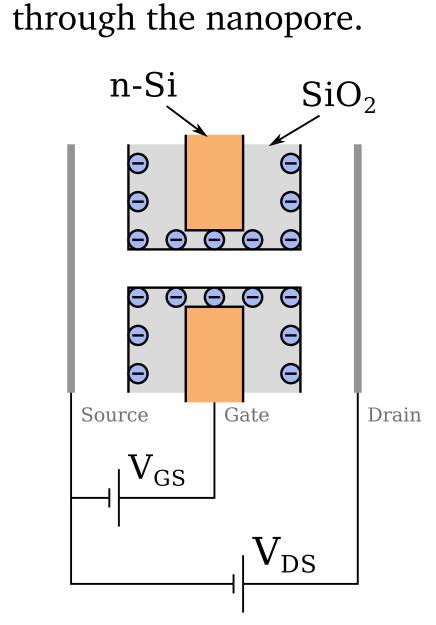
 $\varphi|_{x=L_x} = V_D + V_0^{KCl},$ 

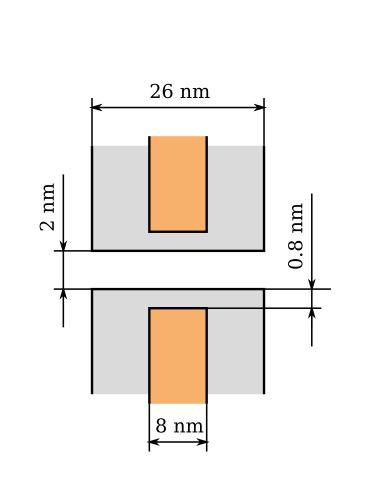
 $\frac{\varphi}{dy}\Big|_{y=\pm L_y} = \frac{\varphi}{dz}\Big|_{z=\pm L_z} = 0.$ 

**I-V Curves** 

#### **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 control of polymer translocation





#### Parameters of the system

$$N_A^-, N_D^+ = 2.0 \cdot 10^{20} \ cm^{-3}$$
 $\sigma_{
m surf} = -0.25 \ e/nm^2$ 
 $arepsilon_{Si} = 11.70$ 
 $arepsilon_{SiO_2} = 3.9$ 
 $arepsilon_{KCl} = 80.0$ 
 $[KCl] = 0.1 \ M$ 
 $D_{Cl}^-, D_{K^+} = 2.0 \cdot 10^{-5} \ cm^2/s$ 

#### Validation of Continuum Approach in the Nanopore.

Continuum approaches are widely used to model electrostatic and ion transport phenomena in confined spaces such as nanopores and nanochannels. The validity of the continuum PNP approach which we use to calculate the ionic current in the nanopore, has been confirmed for pore radii larger than the Debye length [3]. In [3], the ionic current and conductance were calculated via the PNP model and systematically compared with the results of BD simulations of the ionic solution in nanopores with radii varying from 4 Å to 16 Å. A convergence between two theories occurred in pores with radius of  $\sim$ 2 Debye lengths. Thus, the continuum approach can be used for our nanopore geometry as long as the ionic strength of the solution is large enough to result in Debye lengths that are smaller than the nanopore radius.

#### Model of the solid-state membrane

Concentrations of electrons and holes in silicon are

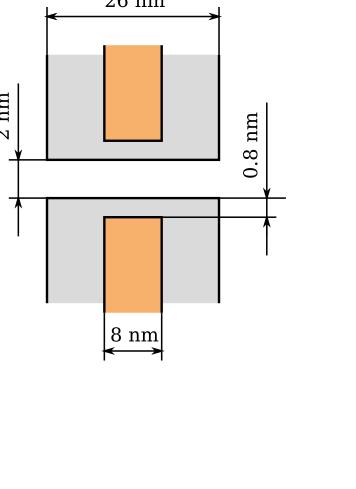
$$n=N_C^{eff}~\mathscr{F}_{1/2}igg(rac{q(arphi-V_G)-rac{E_g}{2}}{kT}igg),$$
  $p=N_V^{eff}~\mathscr{F}_{1/2}igg(rac{-q(arphi-V_G)-rac{E_g}{2}}{kT}igg),$  where

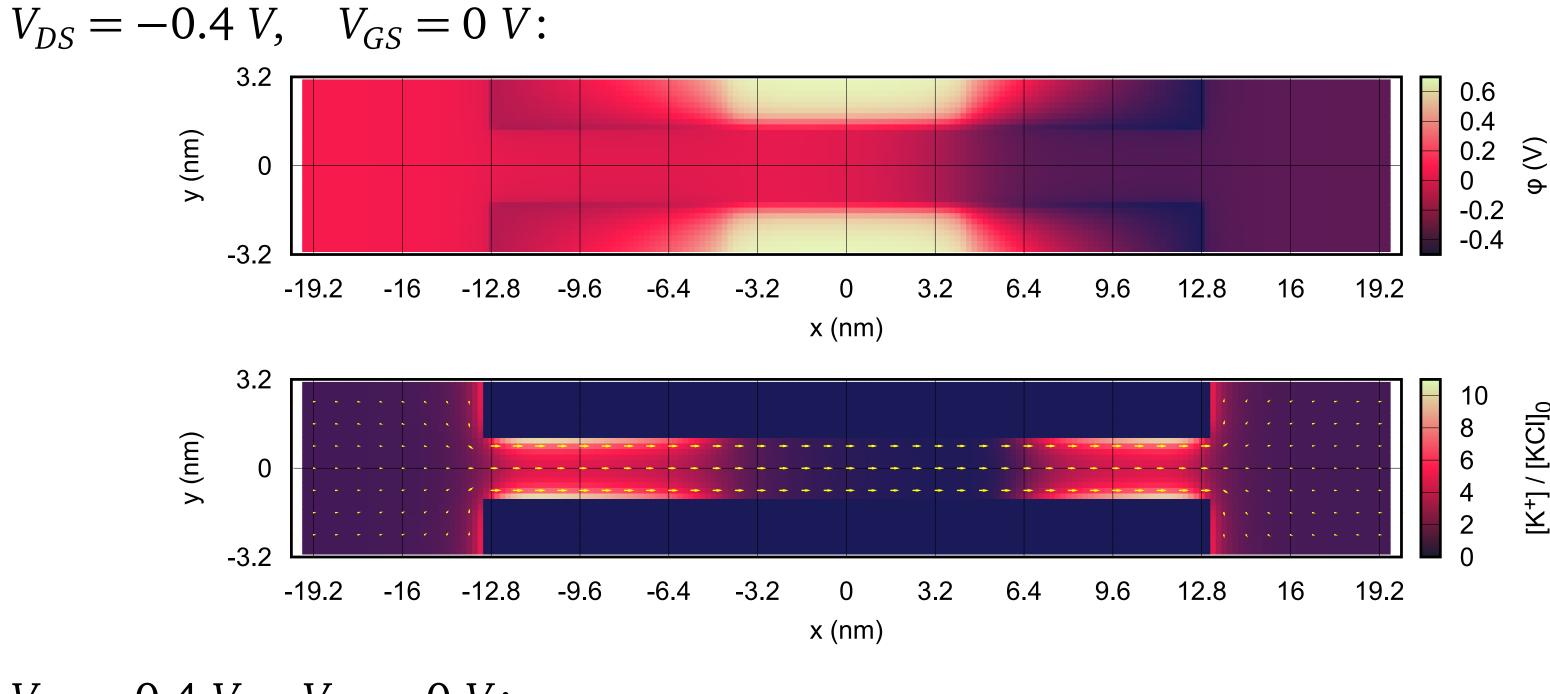
$$N_C^{eff} = 2\left(\frac{2\pi \, m_n^* \, k_B T}{h^2}\right)^{3/2}, \quad N_V^{eff} = 2\left(\frac{2\pi \, m_p^* \, k_B T}{h^2}\right)^{3/2}.$$

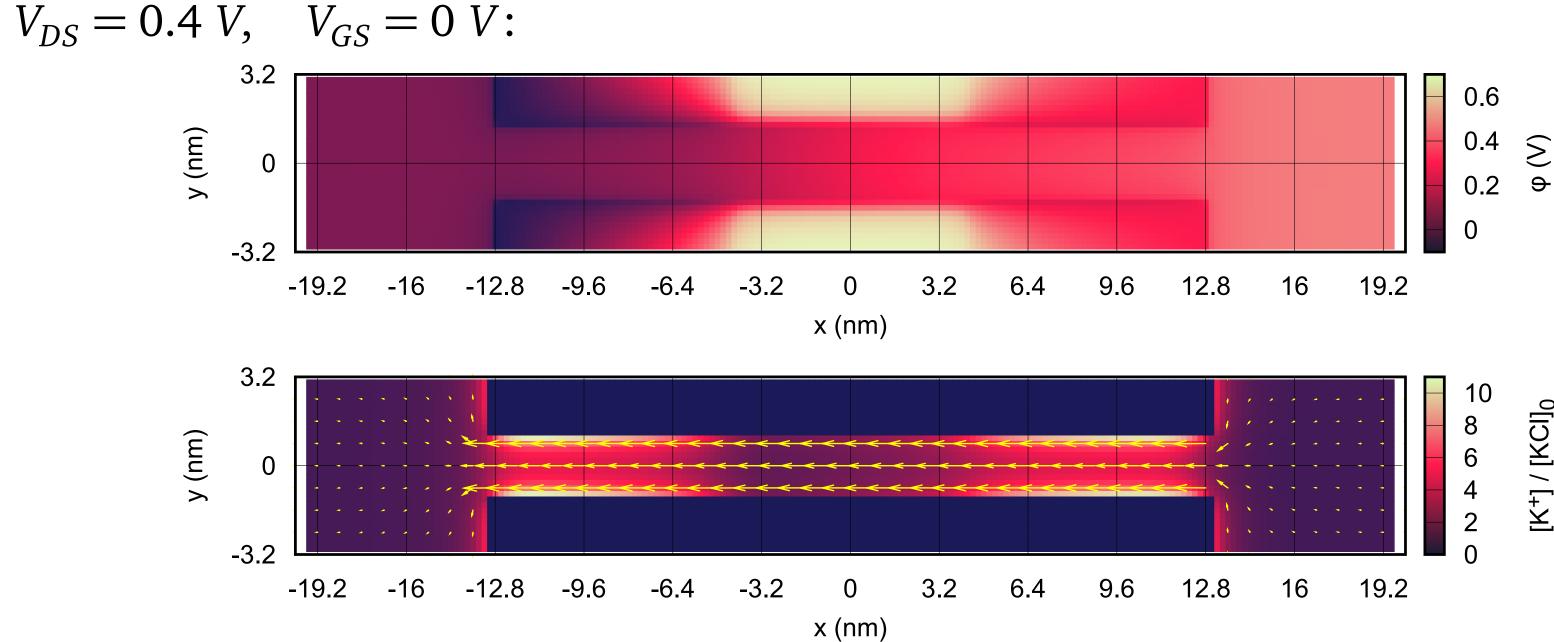
 $m_n^*$  and  $m_n^*$  are effective masses of electrons and holes.

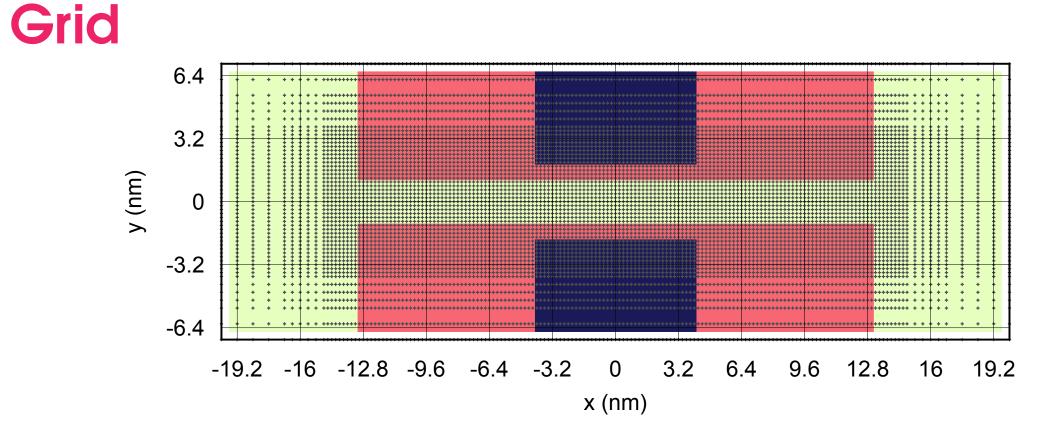
 $N_{\Delta}^{-}$ ,  $N_{D}^{+}$  are concentrations of dopant atoms.  $E_{\sigma}$  is the band gap in Si. See [1] and [2] for details.

### Simulation results









Simulations are performed on a grid with a variable grid-point size that is equal to 0.2 nm in the center, and 0.8 nm on the periphery.

### Boundary Conditions For potential For ion Poisson's equation

$$\nabla(\varepsilon\nabla\varphi) = -\frac{\rho}{\varepsilon_0}, \text{ where}$$

$$\rho = q(-n+p-N_A^- + N_D^+ + N_{\text{surf}} - [Cl^-] + [K^+]).$$

 $\varepsilon$  is the relative permittivity,

 $N_{\text{surf}}$  is the equivalent volumetric concentration of the oxide surface charge ( $\sigma_{\rm surf}$ ) on the boundary with [KCl].

## Nernst-Planck equations for ions

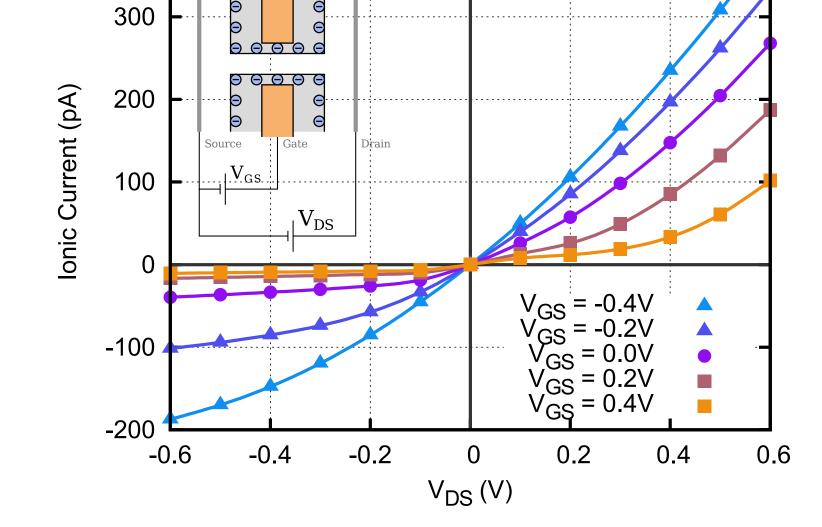
Current densities are

$$\vec{J}_{Cl} = -q\mu[Cl^{-}]\nabla\varphi + qD\nabla[Cl^{-}],$$
 
$$\vec{J}_{K} = -q\mu[K^{+}]\nabla\varphi - qD\nabla[K^{+}].$$

The Nernst-Planck equation  $\nabla \vec{J} = 0$ :

$$\nabla(-\mu[Cl^{-}]\nabla\varphi + D\nabla[Cl^{-}]) = 0,$$

$$\nabla(-\mu[K^+]\nabla\varphi - D\nabla[K^+]) = 0.$$

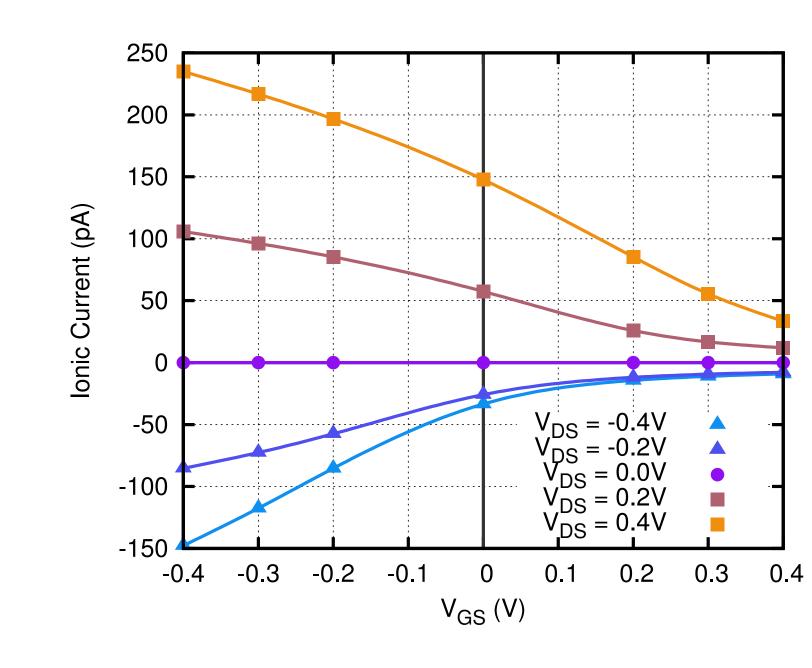


For ionic concentrations

 $\rho|_{x=\pm L_x}=[KCl],$ 

 $(\vec{J} \cdot \hat{j})|_{y=\pm L_y} = 0,$ 

 $(\vec{J}\cdot\hat{k})|_{z=\pm L_z}=0.$ 



#### Conclusion

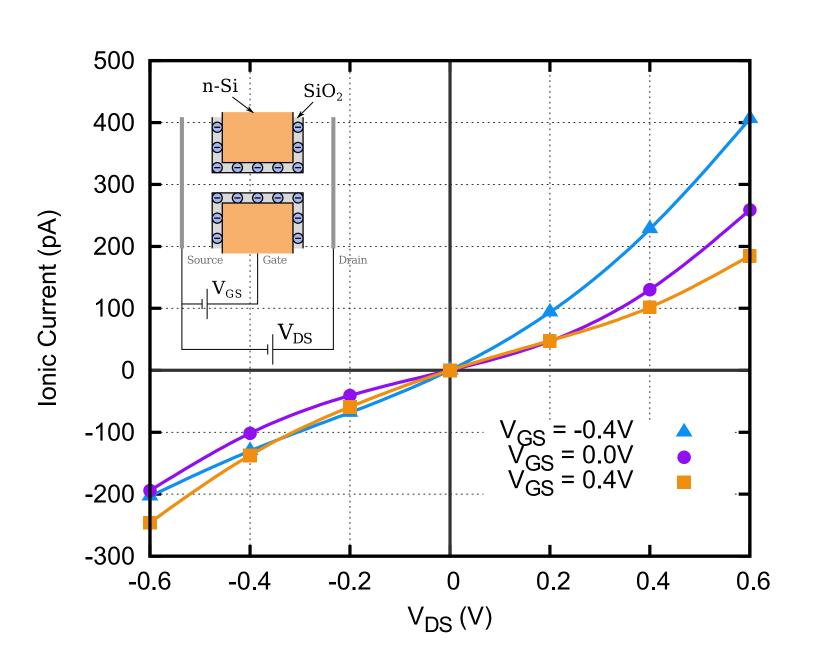
The considered system demonstrates significant ionic current rectification, with a strong dependence on the gate voltage  $V_G$ . There is a current saturation region for  $V_{DS} < 0$ , and K<sup>+</sup> ions are the major charge carriers. We also show that such a system outperforms the comparable membrane with a thicker n-Si layer in terms of the gate voltage effectiveness.

## **Numerical Method**

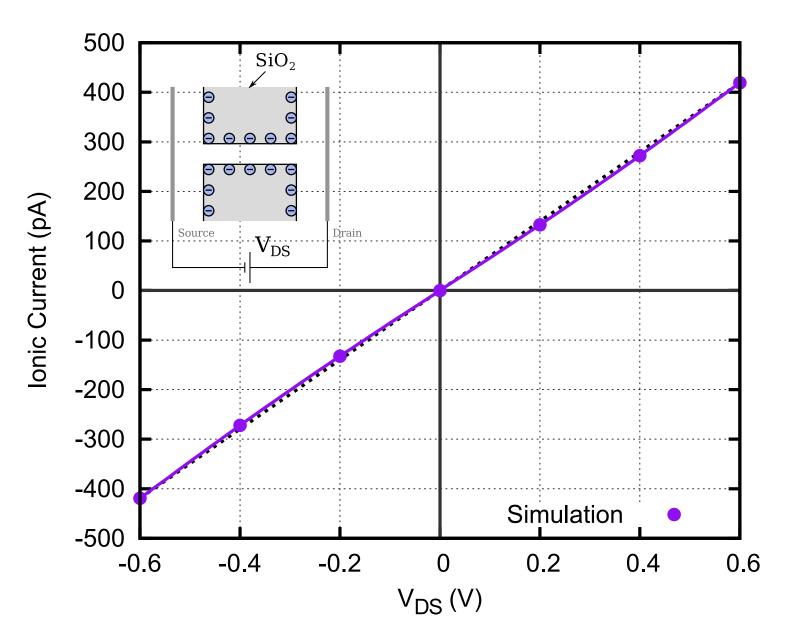
The system of equations is solved self-consistently using finite difference method. In order to do it, potential  $\varphi$  and concentrations n, p,  $[Cl^-]$ , and  $[K^+]$ were replaced with their discrete representations on a grid with variable grid-point size from 0.2 *nm* to 0.8 *nm*. Gummel's 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:



Currents through the membrane that consists of only  $SiO_2$  (with the same surface charge,  $-0.25 e/nm^2$ ) are shown below. The curve is almost linear, and the dotted black line is added as a reference.



#### 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).
- [2] p-n Semiconductor Membrane for Electrically Tunable Ion Current Rectification and Filtering. M. E. Gracheva, J. Vidal and J.-P. Leburton 2007 *Nano Lett.* **7** (6) pp. 1717–22.
- [3] Tests of continuum theories as models of ion channels. II. Poisson-Nernst-Planck theory versus brownian dynamics. B. Corry, S. Kuyucak, and S. H. Chung 2000 *Biophys J.* **78** (5) pp. 2364–2381.