A Multi-physics Study of the Ion Transport in Wireless Bipolar Nanopore Electrodes

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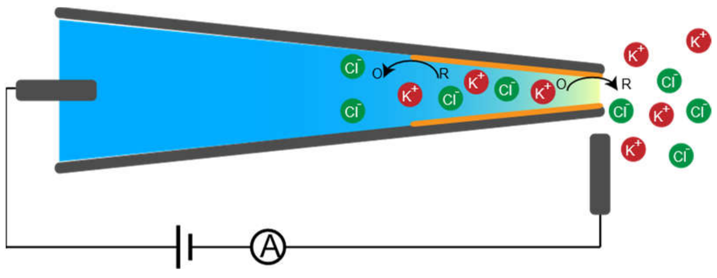
Introduction

Wireless Bipolar Nanopore Electrode (WNE) as a new type of nanoelectrode offers a novel and generally accessible tool for analyzing single molecules/ions, discriminating single particles and probing single cells. The WNE fabricates by a metal coated quartz nanopore, which owns a gold nanostructure at the tip. As exposed to an external electric field in a solution, the conductive nanotip of WNE exhibits a certain polarization potential difference at its two terminals due to the bipolar electrochemistry. The ionic current as the most basic principle for the detection of translocated analytes can be easily influenced by the interactions between the electrolyte and the surface charge on nanopore walls, particularly for the metal-coated nanopores. Despite the behavior of ion transport in nanopores have been modeled widely, description of the polarization metal is still a challenge for WNEs. In this study, the COMSOL MultiphysicsR software is used to study the ion transport in WNEs. Poisson-Nernst−Planck (PNP) and Navier−Stokes (NS) equations have been used to simulate steady-state solutions for ionic current and potential distribution at room temperature of 298 K in a 2D axial symmetric geometry model. For solving the ununiform distribution of charge in the nanopore wall, we have used optimum junction location in the polarization metal and the ununiform charge distribution could be successfully described. The simulation results have successfully explained the ionic current blockade, ion current rectification, ununiform peotential distribution and the fluid motion in the tip of the nanopore electrodes.

Wireless nanopore electrode



Wireless nanopore electrode(WNE)

A **Nernst-planck equation**

$$\boldsymbol{J}_i = -D_i \nabla c_i - \frac{z_i F}{RT} D_i c_i \nabla \boldsymbol{\Phi} + c_i \boldsymbol{u}$$

Possion equation

$$\nabla^2 \boldsymbol{\Phi} = -\frac{F}{\epsilon} \sum_i z_i c_i$$

Navier-stockes equation

$$\boldsymbol{u} \nabla \boldsymbol{u} = \frac{1}{\rho} \left(-\nabla p + \eta \nabla^2 \boldsymbol{u} - F\left(\sum_i \sigma_i c_i\right) \nabla \boldsymbol{\Phi}\right)$$

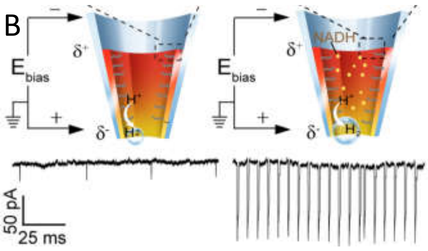


Figure 1 │ The scheme of the wireless nanopore electrode(WNE). Metal layers are fabricated in the inner surface of the glass nanopore. Redox reaction is occur on the each side of the metal layer. A. Poisson-Nernst−Planck (PNP) and Navier−Stokes (NS) equations have been used to simulate steady-state solutions for ionic current and potential distribution at room temperature of 298 K B. Detection of the nanobubble generated in the tip of the nanopore by the WNE.

2D axisymmetric geometry of WNE

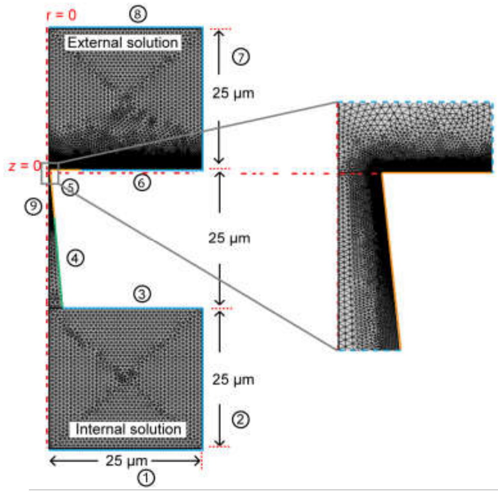
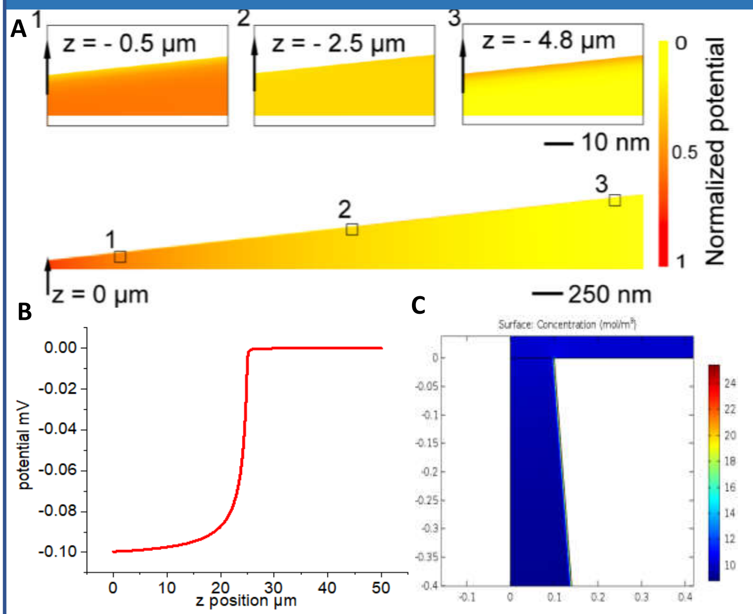


Figure 2 │ The 2D axisymmetric geometry, the mesh for the finite-element simulation, and the boundary settings of the nanopore for the simulation of the potential distribution. Blue lines (1, 2, 3, 6, 7, 8) are the internal bulk solution and external bulk solution. Green line of 4 is the surface of glass. Yellow line of 5 is the metal layer of the WNE and the length of the yellow line is about 15 μm.

SURFACE	NERNST-PLANCK	POSSION	NAVIER-STOKES
8	c_K+=10 mM c_{Cl}-=10 mM	V=0	P=0
2,3,4,6,7	No flux	No charge	No slip
5	No flux	$\sigma=\sigma_0 \frac{2}{(1+\exp[-k(z-z0)]} - 1)$	No slip
1	c_K+=10 mM c_{Cl}-=10 mM	V=Vbias	P=0
9	Axial symmetry	Axial symmetry	Axial symmetry

Results



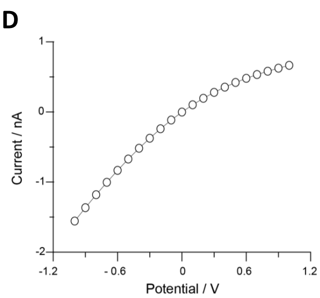


Figure 3 │ **Distribution of the potential in the WNE. A.** Normalized potential drop at the Au layer/solution interface at an applied potential of −0.6 V. Images 1−3 from left to right represent three parts of the nanopore at z-lengths of 0, − 2.5, and −4.8 μm, respectively. **B.** Potential drop in the WNE along with the nanopore at -100 mV. **C.** Distribution of K+ concentration and the diffuse double layer in the wall of the WNE. **D.** The simulated I-V response of the ANE with 2D axisymmetric geometry.

Conclusion

- Using PNP-NS equation and the diffuse double layer in the surface of the electrode could be built.
- Using optimum junction location in the polarization metal and the ununiform charge distribution could be successfully described.
- The potential of the WNE has rapidly drop in the tip of the wireless nanopore electrode.

References

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