Modelling Nanofluidic Diodes

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Background

The control of ionic flows at the nanoscale is a key ingredient in the design and functionality of nanofluidic devices. Similar to solid-state electronic circuits, integrated nanofluidic circuits would contain diodes and transistors but with properties that mainly derive from the interaction between electrolytic solutions and the domain boundaries of nanoscopic pores through which these fluids flow. In recent years, various nanofluidic diodes and transistors have been produced but advanced device modelling has not evolved at the same pace.

Project Summary - Methodology

This theoretical research project focuses on physical models for deformable nanofluidic diodes which would extend the functionality of conventional devices to nature-inspired soft media. Soft materials are expected to exhibit richer dynamics, owing to the interaction of the fluid flow and the surrounding, fluid-containing structure.

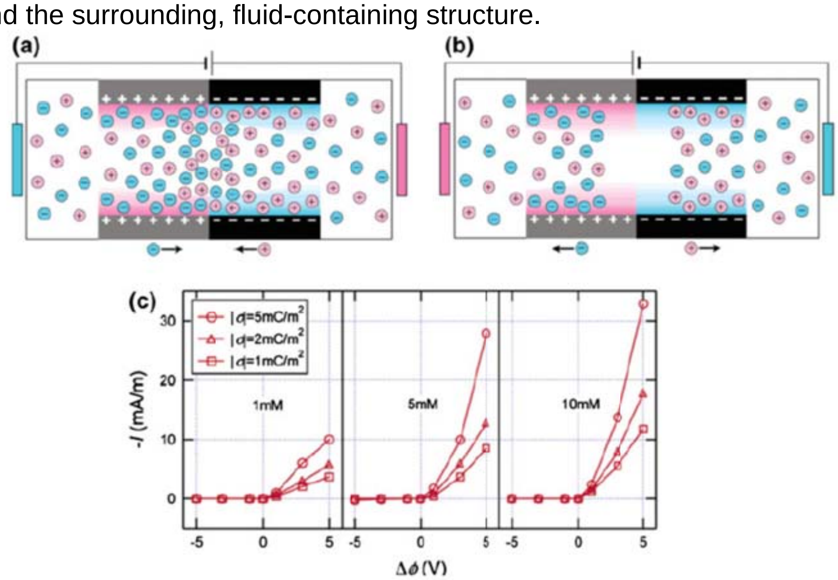

Fig. 5 Working principle of a nanofluidic diode utilizing a nanochannel with half positively charged wall and half negatively charged wall. In case (**a**), the voltage is applied from the negatively charged wall to the positively charged wall (positive voltage), cations and anions are both concentrated to the middle of the nanochannel, leading to enhanced ionic conductance and large electric current. While in case (**b**), the voltage is applied from the positively charged wall to the negatively charged wall (negative voltage), cations and anions are both depleted from the nanochannel, leading to reduced ionic conductance and negligible electric current. The corresponding current–potential relationship is presented in (**c**) which clearly shows the behavior of ionic rectification (Daiguji et al. 2005)

(source: reference [10])

The **main goal** of this project is to derive a simplified one-dimensional model for a deformable nanopore with non-uniform wall charges, representing a dynamic, nanofluidic diode. While any type of electrolyte is generally of interest, we will begin to study this problem for nanopores in polymer electrolyte membranes (PEM) which only contain mobile water, mobile protons and fixed, negative wall charges. These ionomer membranes serve as a solid electrolyte in PEM fuel cells and PEM electrolysers.

The pore geometry will be determined by the fluid-wall force balance and may impact the functionality of the pore. This effort is based on previous work of our group [1-3,6,7] and serves to illustrate that deformable pores may have richer dynamics than conventional ones.

Mathematically speaking, this problem boils down to the derivation and numerical solution of nonlinear ordinary differential equations. This can be done in Matlab, C, C++, Python or any other language that the student may prefer.

This work includes a collaboration with the Weierstrass Institute for Applied Analysis and Stochastics (WIAS) in Berlin, Germany. Further details can be discussed with the project supervisor, Peter Berg, at any time.

References

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