Elucidating the Mechanisms of Charge and Temperature Modulated Ionic Transport in Nanochannels

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Abstract

The transport of fluid through nanochannels is of importance in a variety of technological applications, including biological sensing, energy storage and conversion, chemical separation and many others. Synthetic nanofluidic architectures that mimic the gating functions of biological ion channels have attracted broad interest in both fundamental research and applications because of the outstanding performance on the modulation of molecule and ion transport. Several parameters influence the transport process in nanoscale channels, including the geometry of the channel, the applied voltage, the electrolyte ionic strength, etc. In this work we propose two types of nanodevices that make use of surface charge density and temperature, respectively, to modulate and control the ion/molecule transport process.

Experiments:
Porous anodic alumina (PAA) nanochannels were fabricated by two-step anodic oxidation. In the charge-based device, the top surface of PAA membranes was covered with a graphene oxide (GO) sheet and both the PAA membrane and GO sheet were dipped in polydopamine solution to coat the surfaces. The device displays an ionic current rectification (ICR) behavior when immersed in 1mM KCl solution with different pH values under a voltage that periodically varies between -1 and 1 V at a rate of 0.1 V/s. The ICR ratio was found to be dependent on the pH value of the solution. In the temperature-based device, the surface of the PAA membrane was modified with gold nanorods (AuNRs). The AuNRs exhibit localized surface plasmon resonance (LSPR) in the presence of electromagnetic excitation, which leads to significant optical absorption in the visible or near infrared range and, therefore, enhances the energy conversion of light to heat. The response of dynamic transport process to laser excitation was investigated by monitoring the concentration of Ru(bpy)3Cl2 in the permeating cell via the fluorospectro photometer. The experimental measurement shows that the diffusion flux is enhanced with increasing temperature in the nanochannel, which can be controlled by adjusting the power of illuminating laser.

Modeling:
The mechanisms of both devices were elucidated based upon principles of physics and thermodynamics via finite element simulation in COMSOL Multiphysics® simulation software. The 3D geometry of nanochannel was simplified in equivalence with a 2D axis-symmetric geometry. The underlying mechanisms are governed by three interacting physical phenomena: creep flow, electrostatics, and transport of ionic species. The CFD

module, AC/DC module, and Chemical Species Transport module were integratively utilized to solve the fluid flow, electric field distribution and transport of ions in the nanochannel. In addition, RF module and Heat Transfer module were used to simulate the electrothermal effect of localized surface plasmon resonance (LSPR) of gold nanorods. The modeling results show satisfactory agreement with experimental observations. With obtained in-depth knowledge of how interacting physics induce these intriguing phenomena, we believe that these simple devices that can modulate transport process would be applicable in areas such as biosensing and ion transport in confined environments.