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Ion Concentration and Electromechanical Actuation Simulations of Ionic Polymer-Metal Composites

Tyler Stalbaum, Qi Shen, and Kwang J. Kim

Active Materials and Smart Living Laboratory
Department of Mechanical Engineering
University of Nevada, Las Vegas
Las Vegas, Nevada 89154-4027, USA

Email: tyler.stalbaum@unlv.edu
Web: https://sites.google.com/a/unlv.nevada.edu/tpstalbaum

Email: kwang.kim@unlv.edu
Web: www.kwangjinkim.org

UNLV Department of MECHANICAL ENGINEERING
University of Nevada, Las Vegas

Introduction

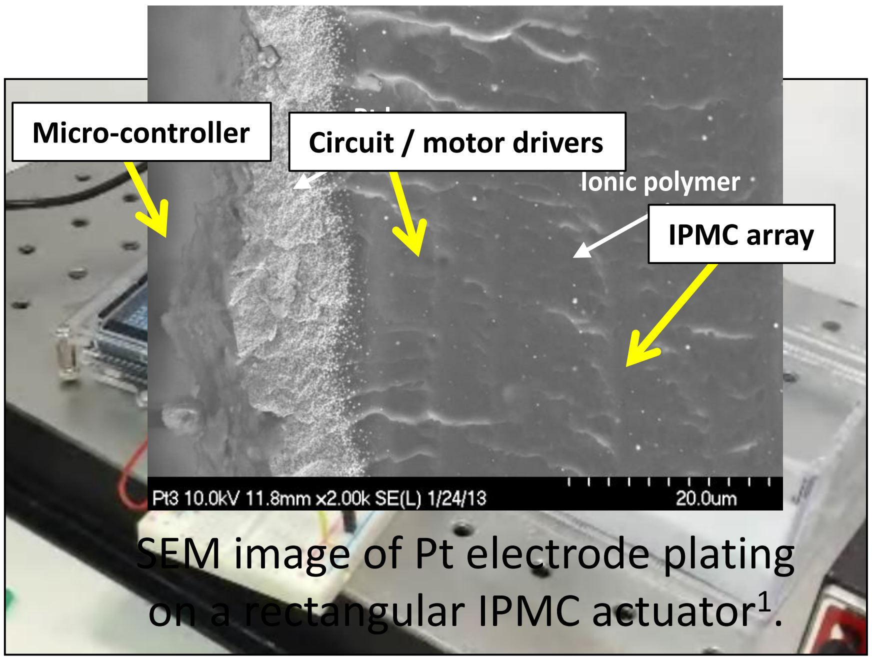
- An **electroactive polymer (EAP)** is a polymeric material which exhibits shape or size change in response to an external stimuli.
- These are of great interest for applications in soft-robotics and biomimicry as **actuators or sensors**.
- There are two primary types of EAP materials: **dielectric and ionic**.
- This study focuses on ionic type EAP materials, with specific focus on **Ionic Polymer-Metal Composite (IPMC)** actuators and sensors.
- The focus is to provide researchers with **simulation methods to assist in performance analysis, design, and development of ionic polymer-metal composites while simultaneously offering insight into the underlying physics**.

Methods

- **Ionic polymer-metal composite (IPMC)** materials have been studied for use as electroactive polymer actuator and sensor devices.
- This material type exhibits **large bending in response to an applied electric field**, due to **ion-migration within the membrane and a corresponding swelling/contraction near the metal electrodes**.
- In this way, IPMCs are an ideal candidate for **studies of ion-migration and deformation physics in electroactive polymer devices**.
- Therefore, IPMCs are selected as the primary material in physics-based modeling in this study.

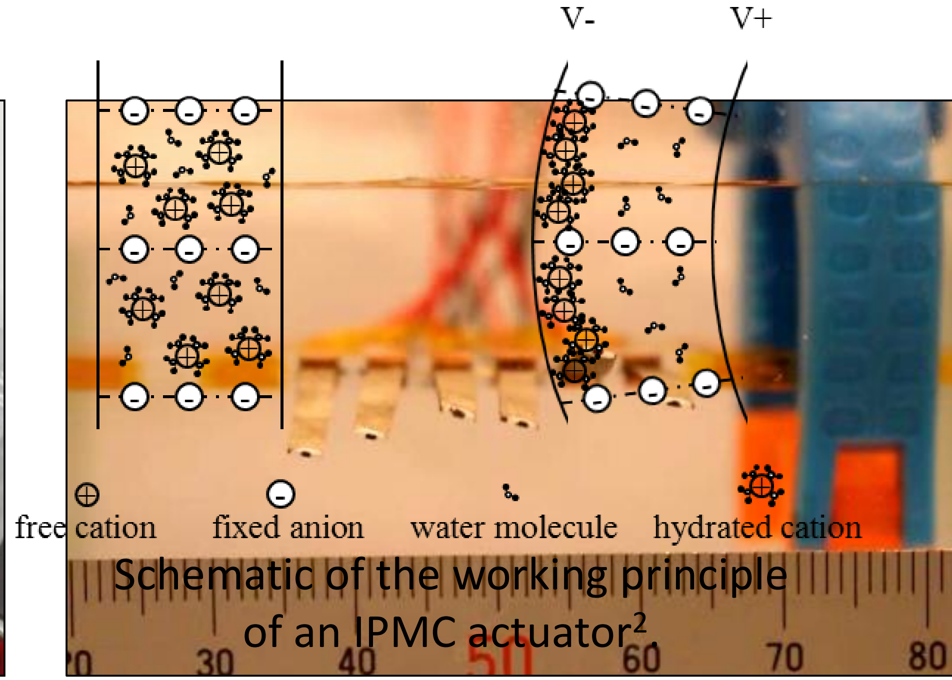
Background: IPMC materials

- IPMC materials are composed of a perfluorosulfonic acid membrane, typically **DuPont Nafion**, with separated noble metal electrodes plated to the surface.



SEM image of Pt electrode plating on a rectangular IPMC actuator[1].

Experimental setup for example IPMC application in actuation of a travelling wave



Schematic of the working principle of an IPMC actuator[2].

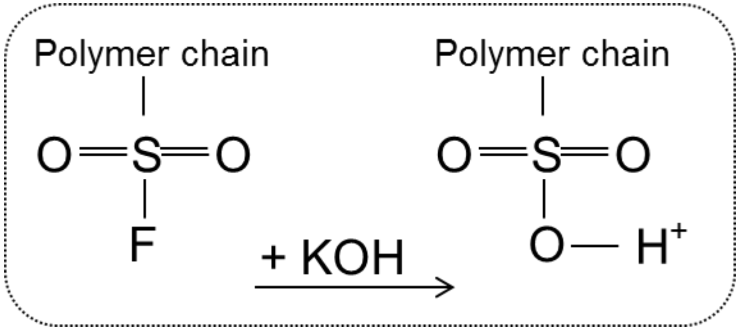
Example application of IPMCs as an array of actuators making a traveling wave motion

[1] Shen, Q., Palmre, V., Stalbaum, T., and Kim, K. J. "A comprehensive physics-based model encompassing variable surface resistance and underlying physics of ionic polymer-metal composite actuators." *Journal of Applied Physics,* 118 (2015): 124904

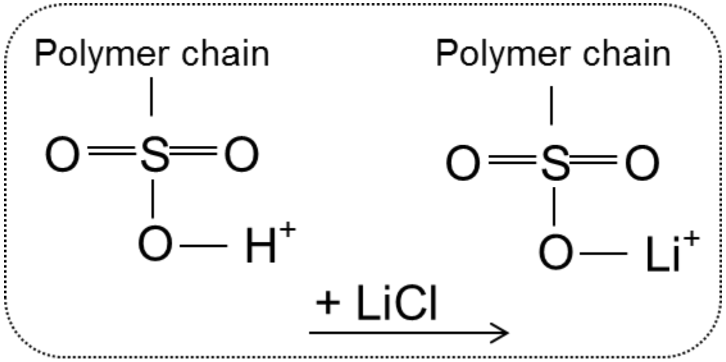
[2] Stalbaum, T., Pugal, D., Nelson, S. E., Palmre, V., and Kim, K. J. "Physics-based modeling of mechano-electric transduction of tube-shaped ionic polymer-metal composite." *Journal of Applied Physics,* 117 (2015): 114903

Materials fabrication

- IPMC fabrication consists of four primary steps.
- **Hydrolysis** of as-received Nafion 117

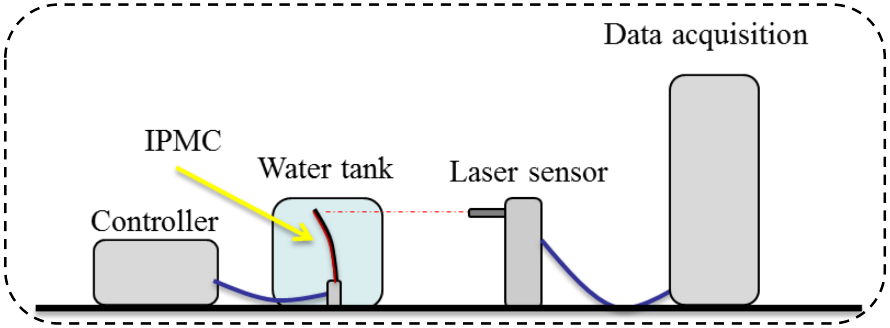


- Primary electrode plating by **impregnation reduction**
- Secondary electrode plating by **chemical deposition**
- **Ion exchange** for improved performance

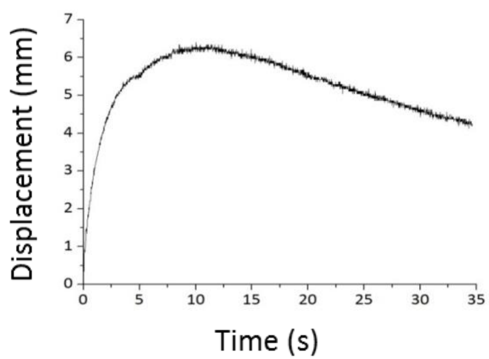


Experimental setups

- Electromechanical (actuation)

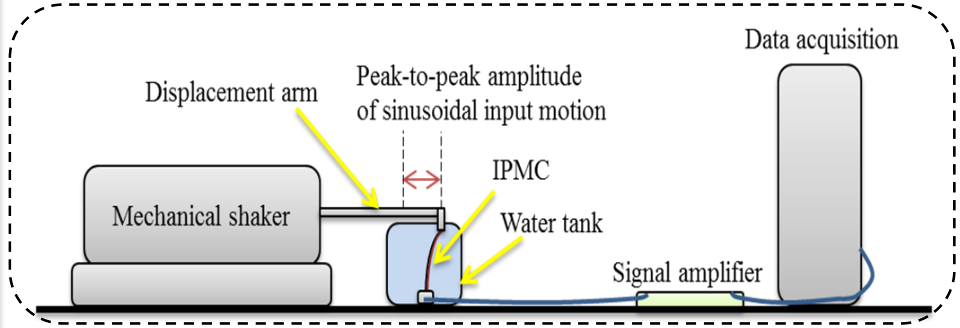


IPMC actuator experimental schematic.

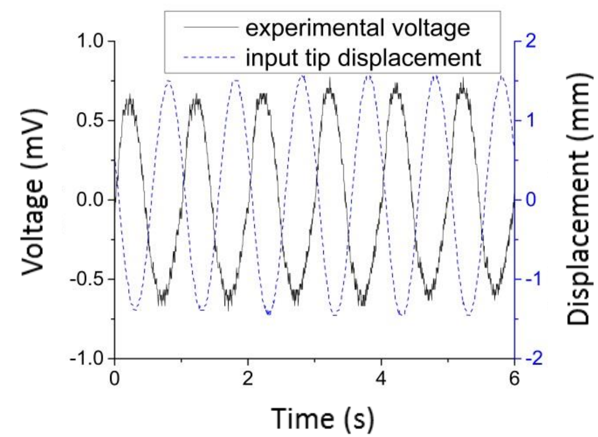


Example experimental trace for **electromechanical response of a rectangular IPMC** (dimensions ~10x51x0.5 mm) to a constant 3V DC input.

- Mechanoelectrical (sensing)



IPMC sensor experimental schematic.

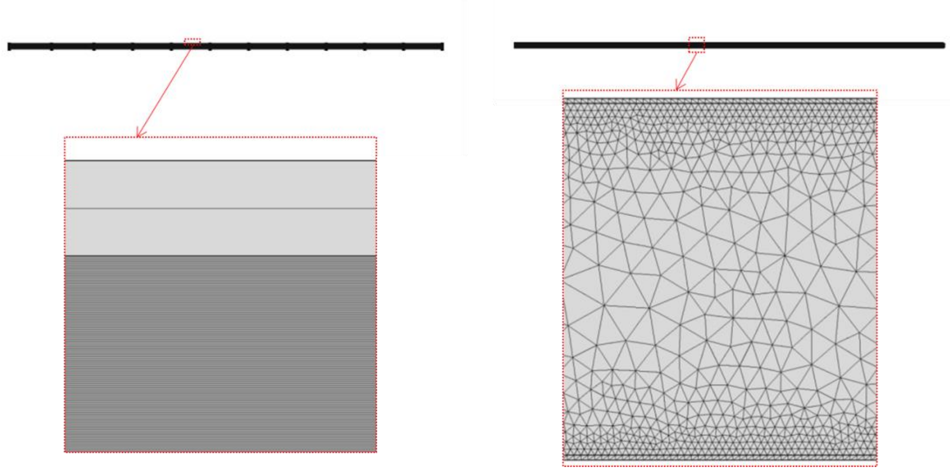


Example experimental data for **mechanoelectrical response of an IPMC** to an oscillating input of 1.5 mm tip-displacement at 1 Hz

Simulation tools

Due to the **multi-physics nature of the EAP transduction mechanisms**, COMSOL Multiphysics is an ideal software for use.

2D finite element simulations were performed using COMSOL Multiphysics software versions 4.3 – 5.2.



Meshes used in rectangular IPMC finite element simulations: (Left) Mesh sparsely mapped along length, (Right) triangulated mesh.

Physics modules utilized

- **Solid mechanics**
  - linear elastic material model
- **Transport of diluted species**
  - Cation/anion concentrations, electric potential, and charge density
    (Nernst-Planck equation)
- **General form PDE**
  - Utilized for Poisson's equation for electric potential gradient and charge density
- **Electric current**
  - For electric voltage potentials in the metal electrodes

Governing equations of IPMC transduction

The underlying cause of IPMC transduction is ion migration and resulting charge density in the vicinity of the electrodes.

Ionic current in the polymer for both cases can be described by the **Nernst-Planck equation**:

$$\frac{\partial C}{\partial t} + \nabla \cdot (\underbrace{-D\nabla C}_{\text{diffusive cation flux}} - \underbrace{z\mu F C \nabla \phi}_{\text{migration in elec. field}} - \underbrace{\mu C V_C \nabla P}_{\text{convective cation flux}}) = 0$$

Where:

C is cation concentration

μ is cation mobility

D is the diffusion coefficient

F is Faraday's constant

z is the charge number

V_C is the molar volume which quantifies the cation hydrophilicity

P is the solvent pressure

ϕ is the electric potential in the polymer

Governing equations: primary differences in actuation vs. sensing

An important difference between **IPMC electromechanical and mechanoelectrical transduction** is the magnitude, direction, and significance of individual terms in the Nernst-Planck equation.

In case of actuation, the electric potential gradient term is significantly more prevalent than the solvent pressure flux, that is:

$$zF\nabla\phi \gg V_C \nabla P$$

therefore the pressure flux term is often neglected in actuation model implementation.

However, **in case of sensing, these terms are of similar significance and neither should be neglected**.

Governing equations: charge density and electric potential

The electric potential gradient term can be described by **Poisson's equation**:

$$-\nabla^2\phi = \frac{\rho}{\varepsilon}$$

where ε is the absolute dielectric permittivity and ***ρ* is charge density defined as**:

$$\rho = F(C - C_a)$$

where C_a is local anion concentration, which is related to volumetric strain as:

$$C_a = C_0\left[1 - \left(\frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z}\right)\right]$$

Governing equations: solid mechanics

A **linear elastic material model** has been applied.

Hooke's Law in 3D for relating stress and strain in the polymer:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{13} \end{bmatrix} = \begin{bmatrix} 2\mu+\lambda & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & 2\mu+\lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & 2\mu+\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \end{bmatrix}$$

The constants μ and λ are Lame's constants, defined as:

$$\mu = \frac{E}{2(1+\nu)}, \qquad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$$

Newton's Second Law is used to describe time-dependent deformation:

$$\rho_p \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \nabla \cdot \sigma = \boldsymbol{F}$$

Governing equations: force-coupling in actuation

In case of rectangular IPMC actuator modeling, a linear proportionality is sufficient for **coupling the charge density in the polymer to the body force**, that is:

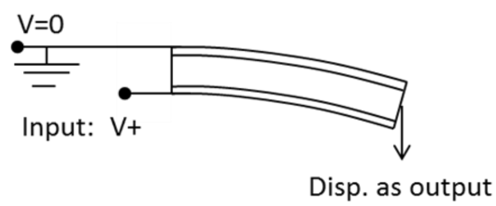
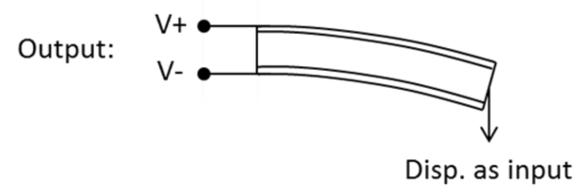
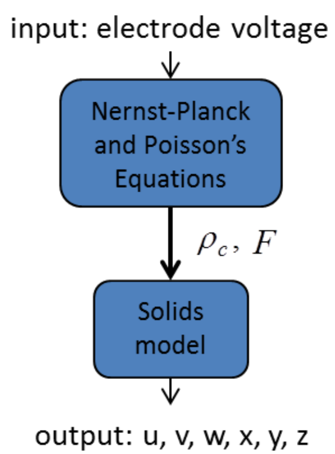
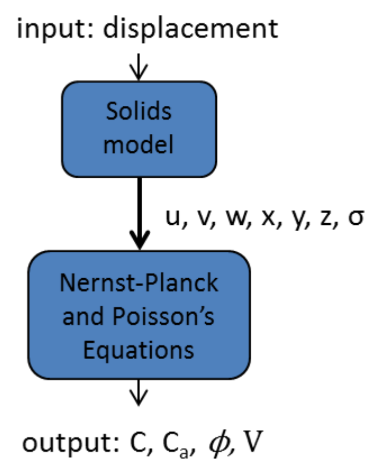
$$F_Z = \alpha\rho$$

However, in case of 3D models, a force-coupling of 2nd order which represents **the strong concentration at the electrodes** should be used, that is[3]:

$$F_z = \alpha \frac{sgn(\rho) + 1}{2}\rho^2 - \beta \frac{sgn(\rho) - 1}{2}\rho$$

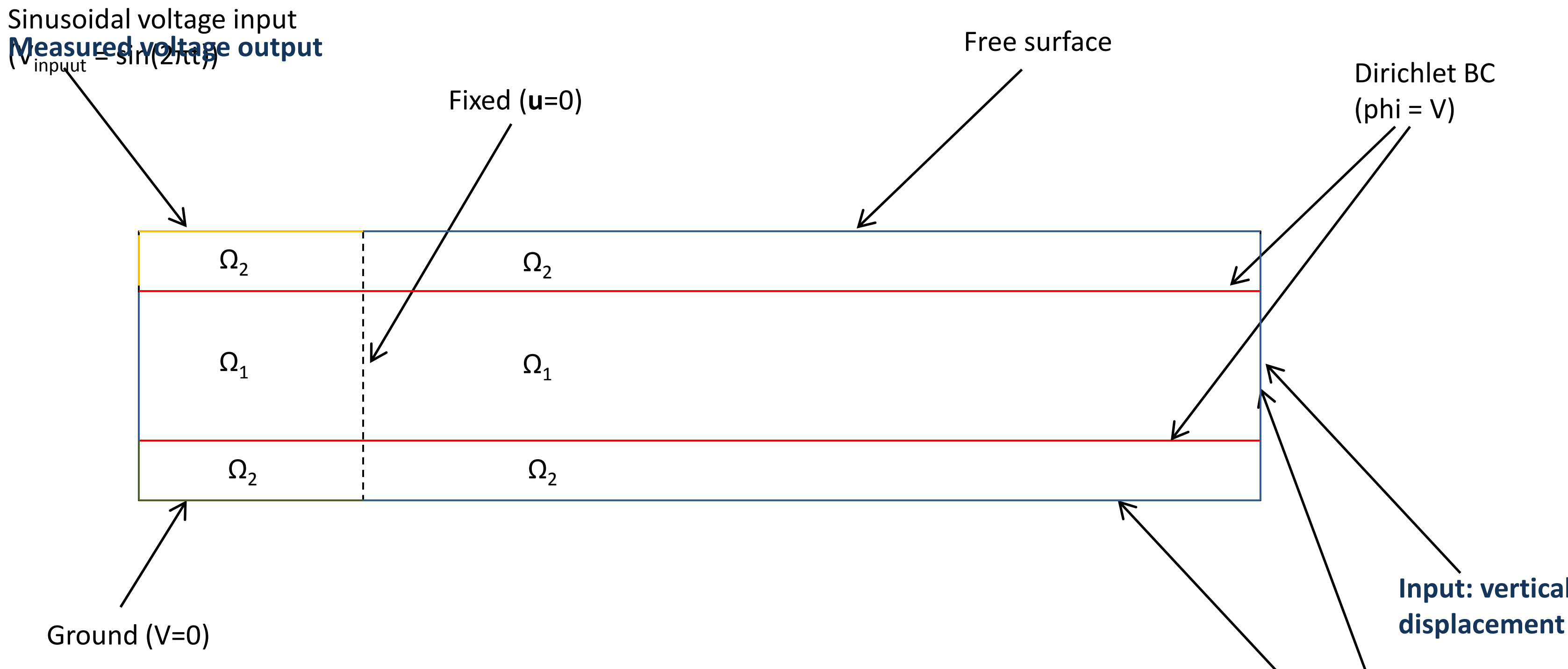
[3] D. Pugal., "Physics based model of ionic polymer-metal composite electromechanical and mechanoelectrical transduction," PhD dissertation, UNR, (2012)

Comparison of actuation to sensor model

Transduction mechanism	Electromechanical (Actuation)	Mechanoelectrical (Sensing)
Illustration of input / outputs		
Flow diagram of modeling approach		
Important differences	$C_a \approx C_0$ $zF\nabla\phi >> \Delta V \nabla P$	$C_a = C_0\left[1 - \left(\frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z}\right)\right]$ *Convective flux considered*

Domain physics and boundary conditions

IPMC actuator model / IPMC sensor model



Ω_1: P-N-P physics, solid mechanics

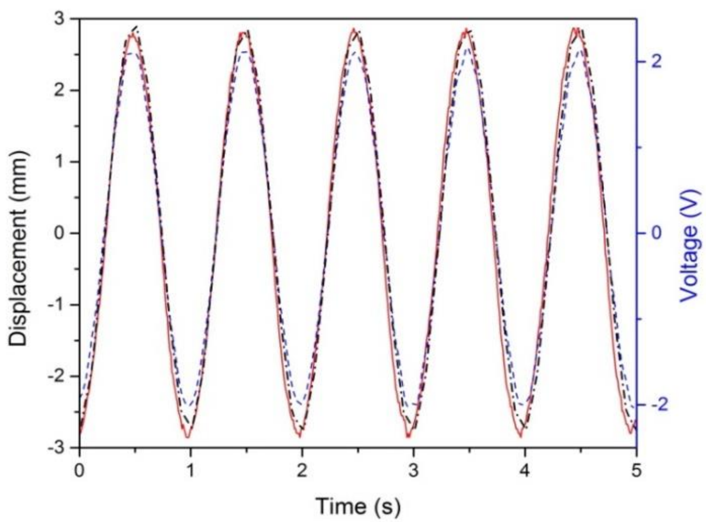
Ω_2: Ohm's law (ec), solid mechanics

Results: Response of rectangular IPMCs

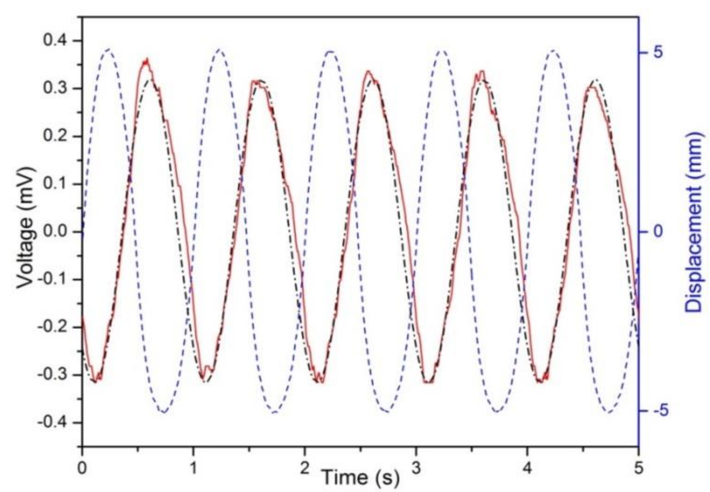
Example simulation results as compared to experimental for cases of AC actuation and sensing for rectangular IPMCs.

Rectangular IPMC of dimensions ~ 51 mm x 10 mm x 0.5 mm

IPMC as an actuator. Response to a sinusoidal input of 4V peak-to peak amplitude at 1Hz freq.



IPMC as a sensor. Response to sinusoidal free-end displacement of 10 mm peak-to-peak amplitude at 1 Hz.

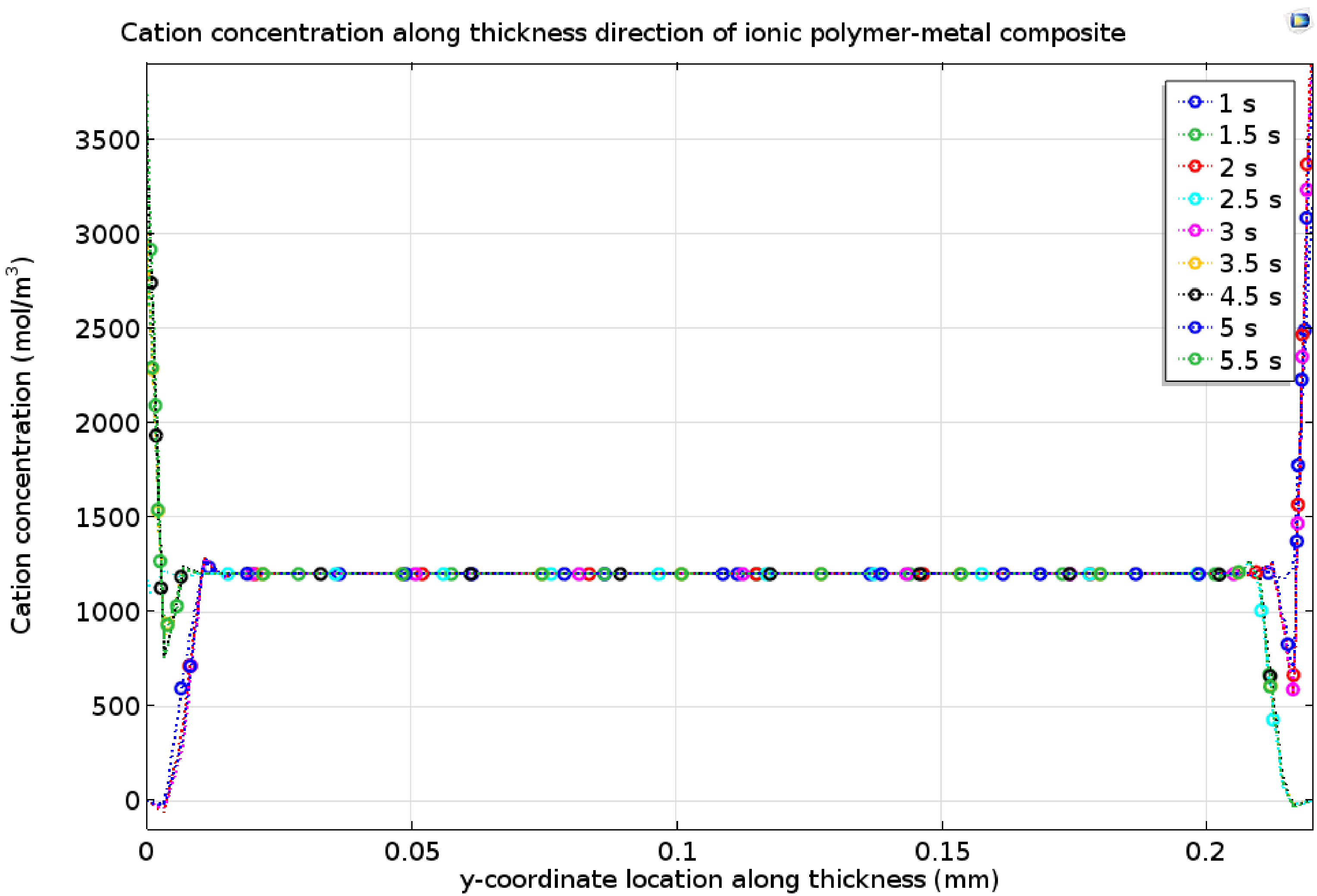


Red curve – experimental data

Black dotted curve – simulated results

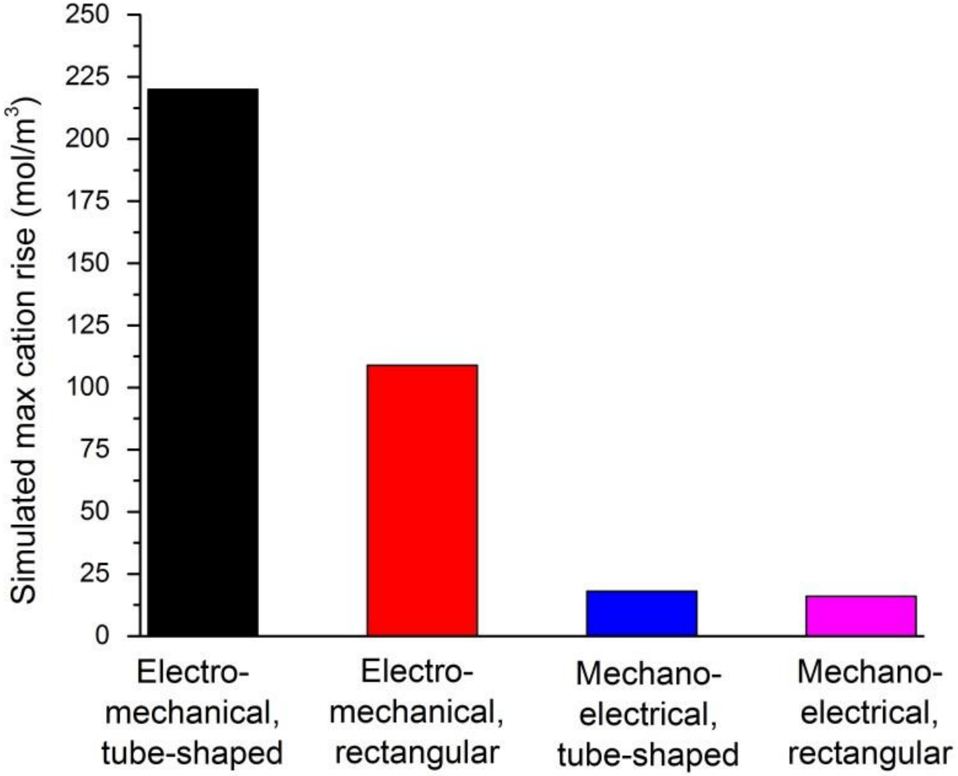
Blue dotted curve – input signal

Results: cation concentrations



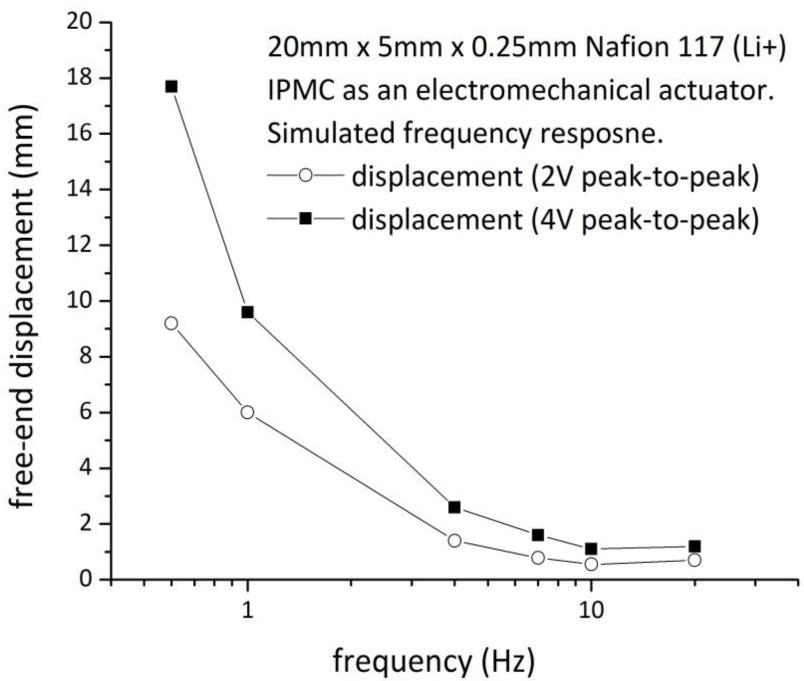
Simulation results: ionic concentrations

Simulated cation rise near the polymer-electrode interface for electromechanical and mechanoelectrical transduction of tube-shaped and rectangular IPMCs.

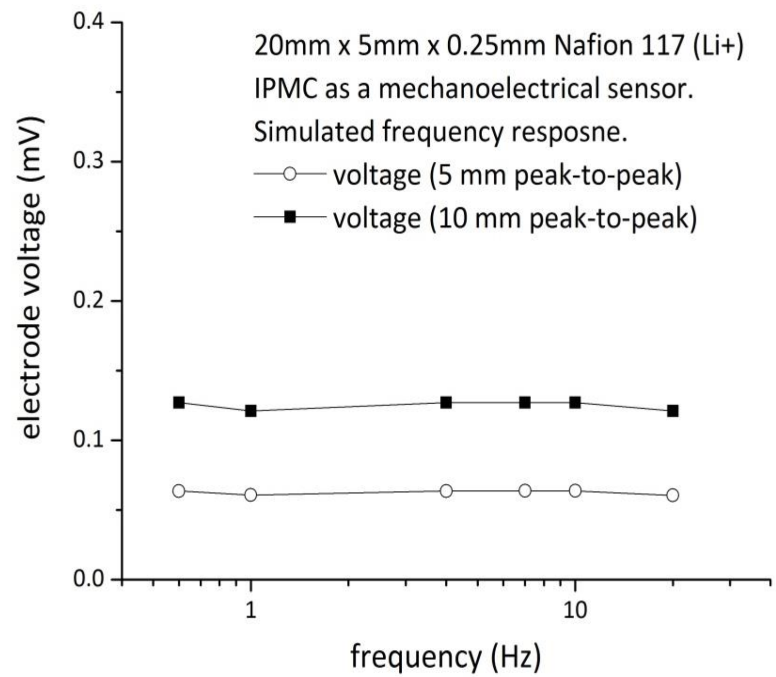


Simulation results: frequency response

IPMC as an actuator:
Frequency response to 2V and 4V peak-to-peak sinusoidal clamp voltage.



IPMC as a sensor:
Frequency response to 5mm and 10mm peak-to-peak sinusoidal free-end displacement.



$$\frac{\partial C}{\partial t} + \nabla \cdot \left(-D\nabla C - z\mu F C \nabla \phi - \underbrace{\mu C V_C \nabla P}_{\text{Dominant term, sensor model}}\right) = 0$$

Dominant term, sensor model

Conclusions and future work

CONCLUSIONS

- Simulations results using the modeling framework was presented with experimental verification for rectangular ionic polymer-metal composite devices.
- Cation concentration simulation results show large increase (order of 100-1000 mol/m^3) in a small subsurface region (<5µm) for actuation, whereas they show a small increase (~order of 10 mol/m^3) in the same small region for the case of sensing transduction.

  This is strong supporting evidence for the proposed theories of actuation and sensing mechanisms in IPMCs.

FUTURE WORK

- Experimental visualization of cation migration in the IPMC to compare with simulations.
- Propose design improvements of IPMC devices for soft-robotics applications based-on simulation results.

Acknowledgements

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