Original talk title:

# The influence of sample’s shape on Poisson's ratio

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Changed talk title:
# Modeling IPMC cantilever actuator

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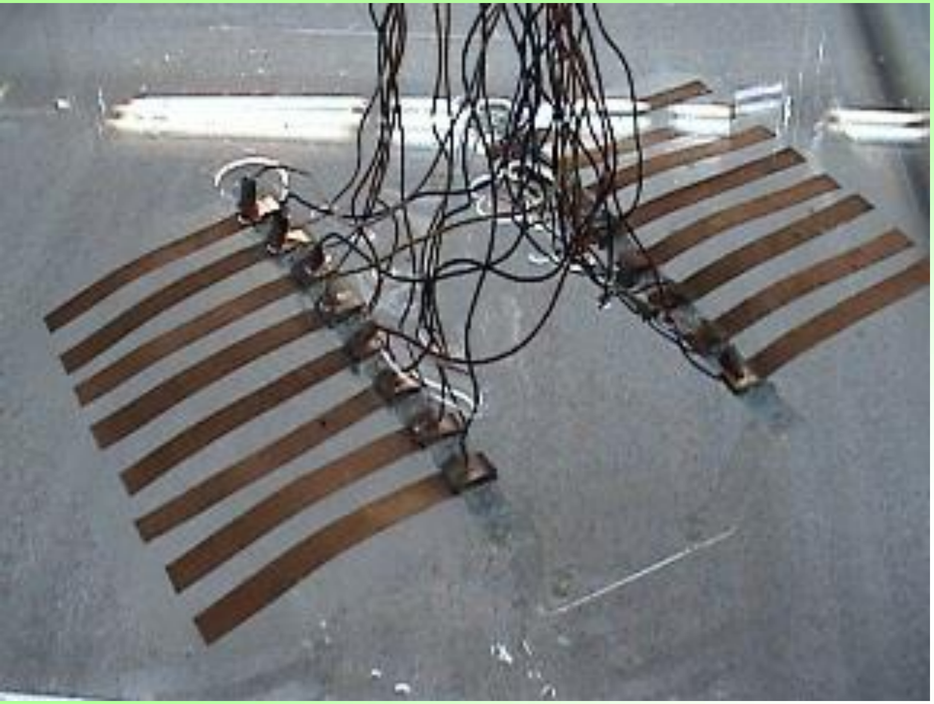
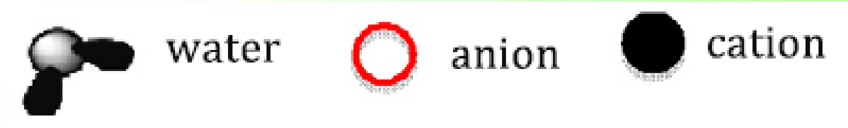
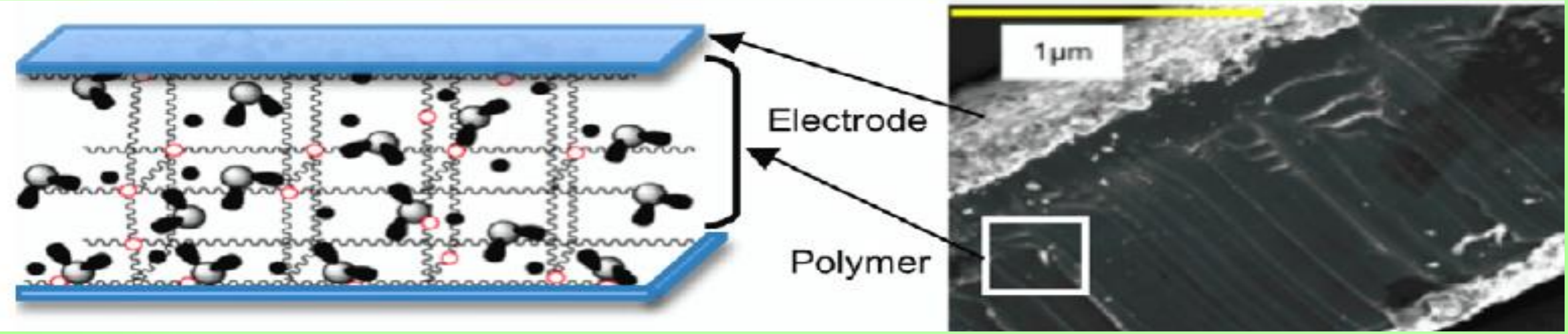
# IPMC: Electro-active polymers controlled using low voltage



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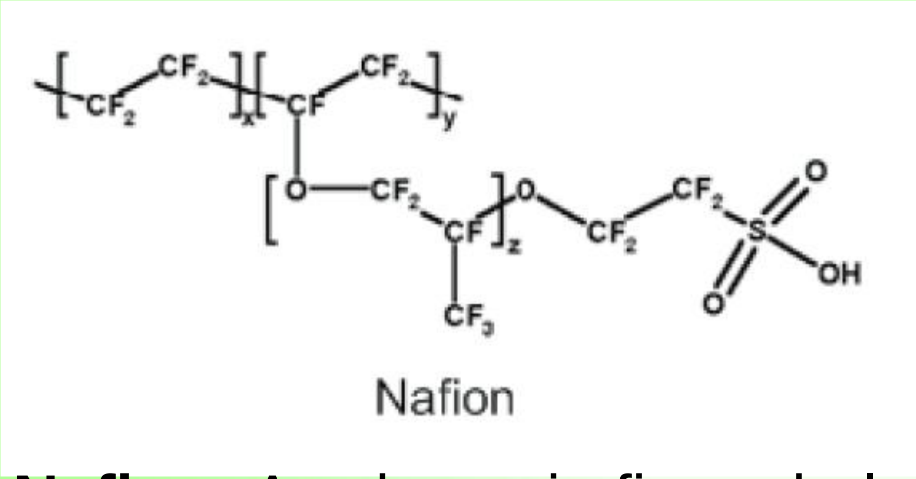
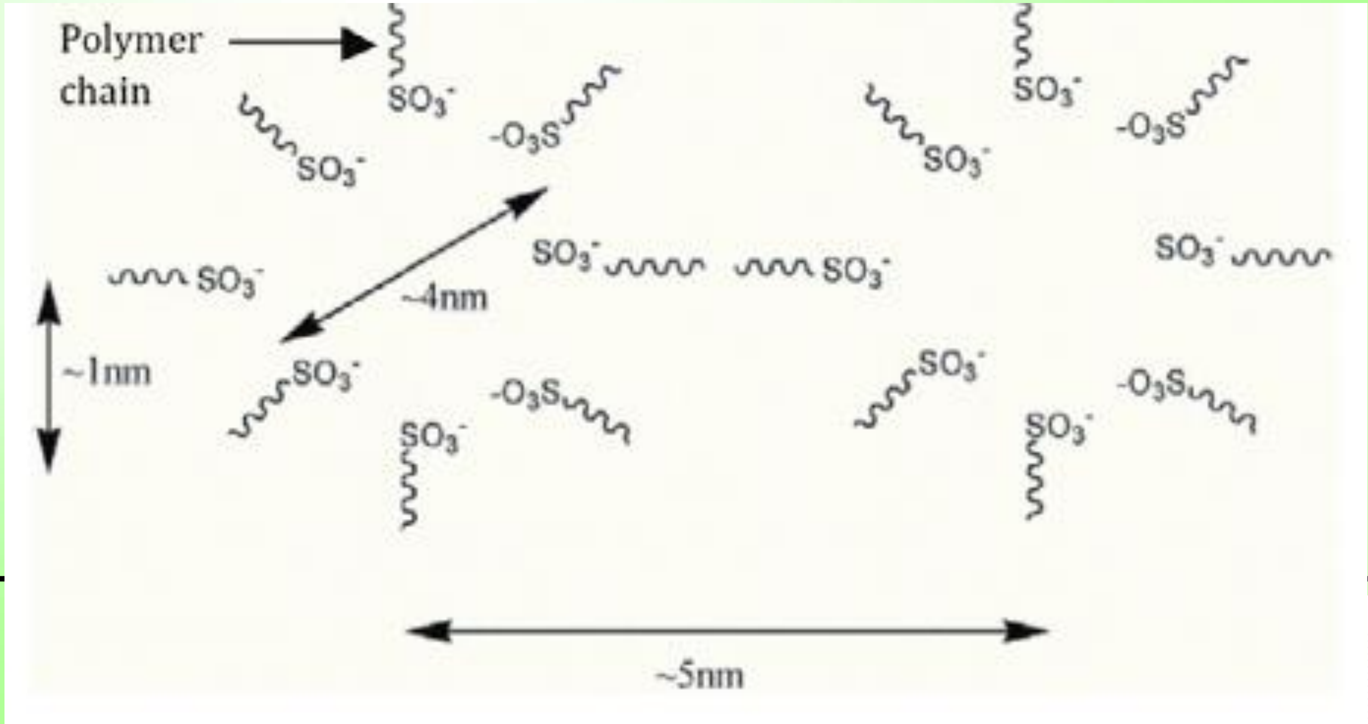



**Nafion:** As shown in figure below, **clusters of diameter 4 nm** are formed **due to** the **reorientation of a hydrophilic side chain and hydrophobic backbone**.

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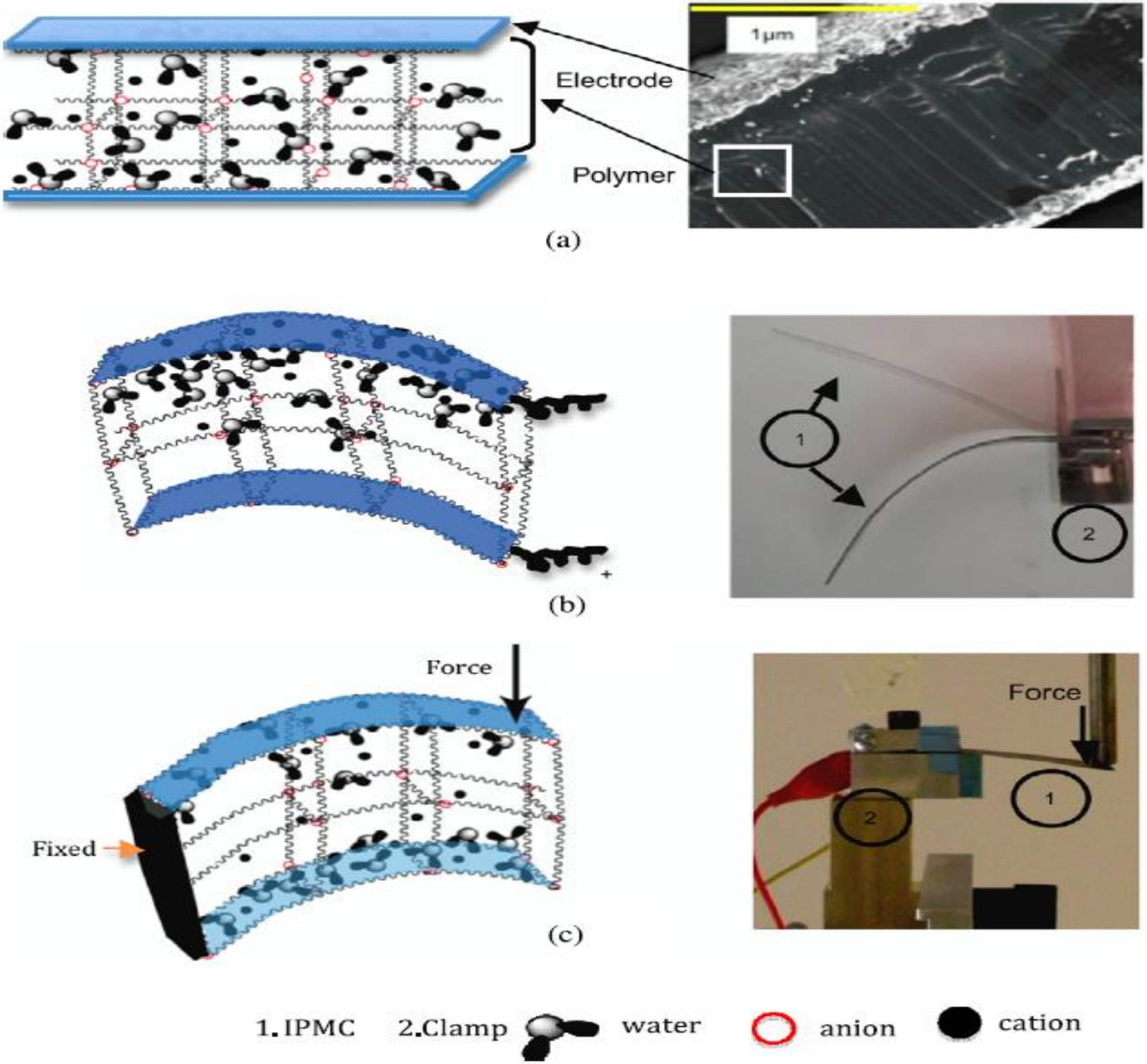
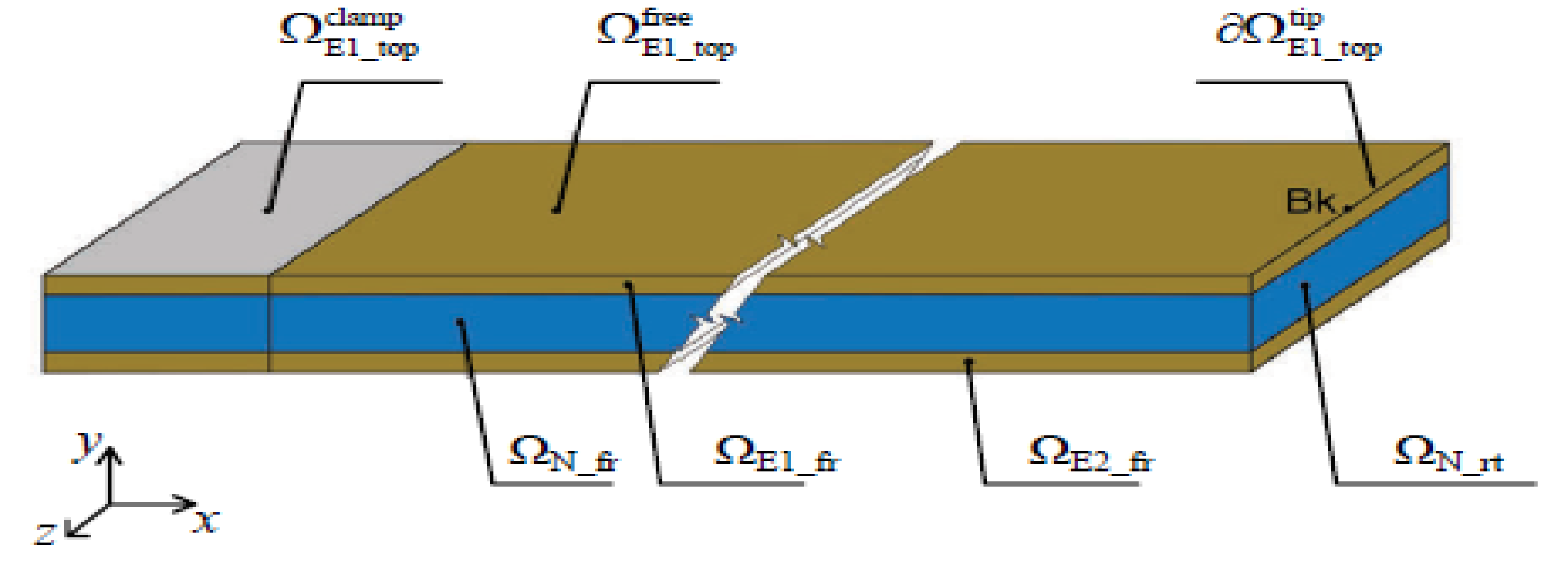


1μm
Electrode
Polymer
(a)
1
2
+
(b)
Force
Fixed
Force
1
2
(c)
1. IPMC
2. Clamp
water
anion
cation

**Source**: D. Vokoun, Q. He, L. Heller, M. Yu, Z. Dai. Modeling of IPMC cantilever’s displacements and blocking forces. Journal of Bionic Engineering 12 (2015) 142-151.

The model can work with Nafion with **various thicknesses** and **Young’s moduli**.

The **purpose** of the model is simulation of **IPMC’s tip movement** and simulation of **blocking force**.

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# Poisson-Nernst-Planck (PNP) equation system

The **PNP system** is strongly non-linear. The key variables of the PNP system are **concentration of the mobile ions**, *c*, and **electric potential**, φ.

Then, **diffusion** and **electromigration** of mobile ions in the Nafion domain is described by flux ***J***

$$\boldsymbol{J} = -D\nabla c - \mu F c \nabla \phi,$$

where *D, μ, F* are the **diffusivity**, the **mobility of free ions**, and the **Faraday constant**, respectively.

Then, the **Nernst Plank equation** has the following form:

$$\frac{\partial c}{\partial t}+\nabla \boldsymbol{J}=\frac{\partial c}{\partial t}-\nabla\left(D\nabla c\right)-\nabla\left(\mu F c\nabla\phi\right)=0.$$

The **Poisson equation** has a form

$$-\nabla^2\phi=\frac{F\rho}{\varepsilon}=\frac{F}{\varepsilon}\left(c-c_0\right),$$

where ρ, ε and c0 are the **charge density**, the Nafion's **electric permittivity** and the **constant concentration of Nafion's $SO_3^-$ anions**, respectively.

in the **domains of metal electrodes** the Poisson's equation transforms to $\nabla^2\varphi = 0$

## Boundary conditions of the 3D PNP system

we require the **Neumann boundary condition** $d\varphi/d\boldsymbol{n} = 0$ (n is the normal vector to the boundary)

Furthermore, we require the **Dirichlet boundary conditions** $\varphi = V$ and $\varphi = 0$ on the respective outer surfaces of the electrodes.

In our work, potential V is periodic, varying in time as:

$$V = 3 \cdot \sin(0.2\pi \cdot t).$$

As for **concentration of free cations, c**, we need to fulfil the **Neumann boundary** condition $dc/d\mathbf{n} = \mathbf{0}$ on all the boundaries of the **Nafion domain**. The **initial condition** for concentration c is $c = c0$ at time t=0.

## Concentration-stress coupling

How stress relates to concentration and why?

As **cations in the Nafion** in **an electric field** are moving, they take **molecules of water** with them.

Changes of pressure inside →change of strain → bending

We can decompose the total stress tensor into deviatoric and isotropic parts

$$\sigma_{ij}^{tot} = (\sigma_{ij}^{tot} - \frac{1}{3}\delta_{ij}\sigma_{kk}^{tot}) + \frac{1}{3}\delta_{ij}\sigma_{kk}^{tot}.$$

The **hydrostatic pressure** of the solvent due to the **concentration change** contributes to the **isotropic part of the total stress tensor**

$$\frac{1}{3}\sigma_{kk}^{tot} = \frac{1}{3}\sigma_{kk} - p_c,$$

where $p_c$ is the hydrostatic pressure

$$\frac{1}{3}\sigma_{kk} = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) \text{ is the isotropic part}$$

Pressure $p_c = 0$ in **the electrode domains**. For the **Nafion domain**, we assume a **linear relationship** between the **pressure** $p_c$ and **concentration** of free cations, $c$

$$p_c = \beta_N \cdot (c - c_0)$$

$\beta_N$ is a constant coefficient

## Structural mechanics

Connecting the **Newton's law of motion** and the **force balance**, the structural mechanics of cantilever is described as:

$$\nabla \boldsymbol{\sigma}^{tot} + \boldsymbol{F}^V = \rho_i \frac{\partial^2 \boldsymbol{u}}{\partial t^2}$$

where $\boldsymbol{\sigma}^{tot}$, is the **total stress tensor**,

$\boldsymbol{F}^V$, is the **force vector per volume area**,

$\rho_i$ is the **mass density** of respective material ($i=\{N,E1,E2\}$)

and $\boldsymbol{u} = (u,v,w)$ is the **displacement vector**, Because of the **slow actuation** in our experimental setup, we neglect the **dynamic term** of the right side of Eq.+neglecting volume force

So $\nabla \boldsymbol{\sigma}^{tot} = 0$ .

We assume that Nafion and the electrodes are **elastic isotropic** materials either one characterized by two elastic constants, **Young's modulus** and **Poisson's ratio** denoted as $E_N$, $\nu_N$, $E_E$, $\nu_E$, respectively. According to the **Hooke's law**, we have:

$$\sigma_{ij}^{tot} = 2G_i \varepsilon_{ij} + [(3K_l - 2G_l)(\frac{1}{3}\varepsilon_{kk}) - p_c]\delta_{ij},$$

# Boundary conditions for the equations of structural mechanics

We have to distinguish two cases: **(i)** the **boundary conditions** for a **free movement of the IPMC's tip**.
**(ii)** the **boundary conditions** for the **constrained IPMC's tip**. In this case we simulate the blocking forces.

**Free tip case:** we require u=v=w=0 at clamped part of IPMC cantilever (Dirichlet boundary conditions).
Otherwise, we require $n_1\sigma_{i1} + n_2\sigma_{i2} + n_3\sigma_{i3} = 0$ for i=1, 2, 3 (the Neumann boundary conditions) at the other IPMC boundaries where **n**=($n_1$, $n_2$, $n_3$) is the **normal vector** to the boundary.

**blocking force measurements:** We apply the conditions of the free IPMC's tip, except the boundary condition at the **place where the force sensor is placed** (the cantilever's tip). In the area of force measurement **we require** *v=0* (the Dirichlet condition).

# Model parameters and input data

| Variable/constant | Value and unit |
|---|---|
| Diffusivity, $D$ | $1\times10^{-10}$ m$^2$·s$^{-1}$ |
| Mobility at room temperature, $\mu$ | $2.9 \times 10^{-15}$ mol·s·kg$^{-1}$ |
| Faraday constant, $F$ | 96485.337 C·mol$^{-1}$ |
| Dielectric permittivity of Nafion, $\varepsilon$ | $2.8 \times 10^{-3}$ F·m$^{-1}$ |
| concentration of $SO_3$- anions, $c_0$ | 1000 mol·m$^{-3}$ |

There are various values of $E_N$ (Young's modulus of Nafion) and $t_N$ (thickness of Nafion layer) **in Table** corresponding to the **five manufactured IPMC samples**.

**The Pt Young's modulus not determined now**

| Variable/constant | Value and unit |
|---|---|
| Young's modulus of Nafion, $E_N$ | 0.22 GPa, 0.63 GPa, 0.76 GPa, 0.82 GPa, 0.83 GPa |
| Poisson ratio of Nafion, $\nu_N$ | 0.49 |
| Young's modulus of Pt electrodes, $E_E$ | various values in the range 1 GPa – 5 GPa |
| Poisson ratio of Pt electrodes, $\nu_E$ | 0.38 |
| Length of the free part of the IPMC cantilever, $L$ | 2.5 cm |
| Length of the fixed part of the IPMC cantilever, $L_{fix}$ | 5 mm |
| Thickness of the Nafion layer in the IPMC cantilever, $t_N$ | 0.22 mm, 0.32 mm, 0.42 mm, 0.64 mm, 0.80 mm |
| Thickness of the Pt layer in the IPMC cantilever, $t_E$ | 10 μm |
| Depth of the IPMC cantilever, $wd$ | 5 mm |

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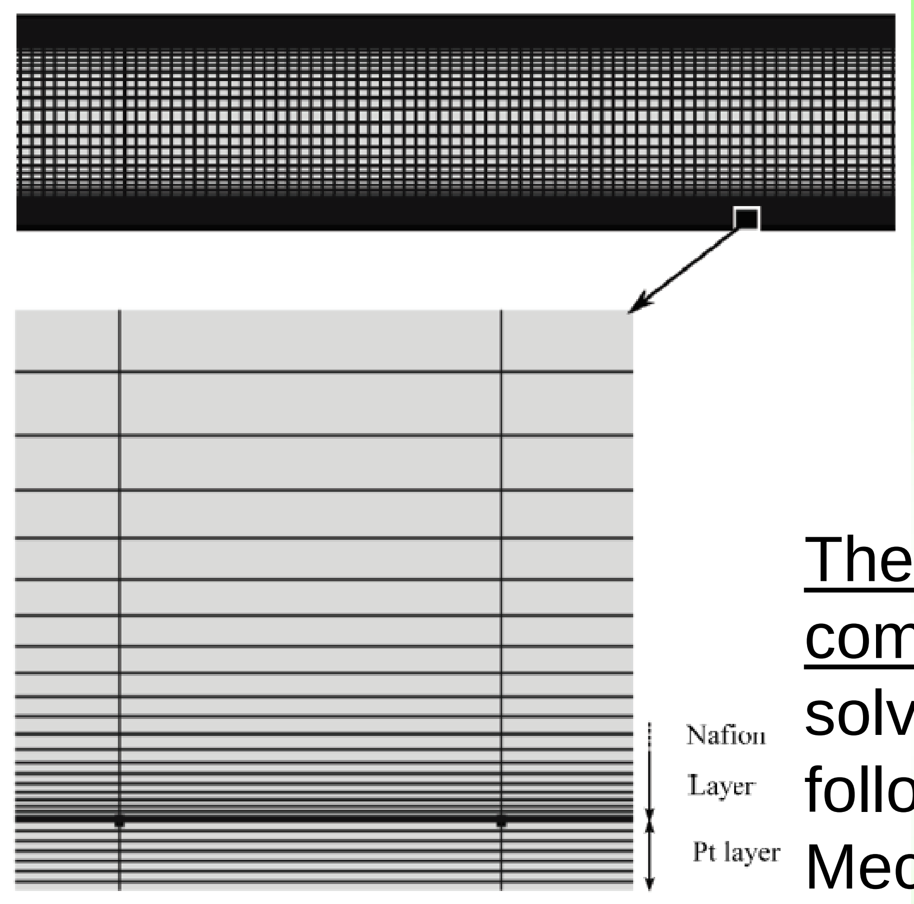
## About realization of the simulation:

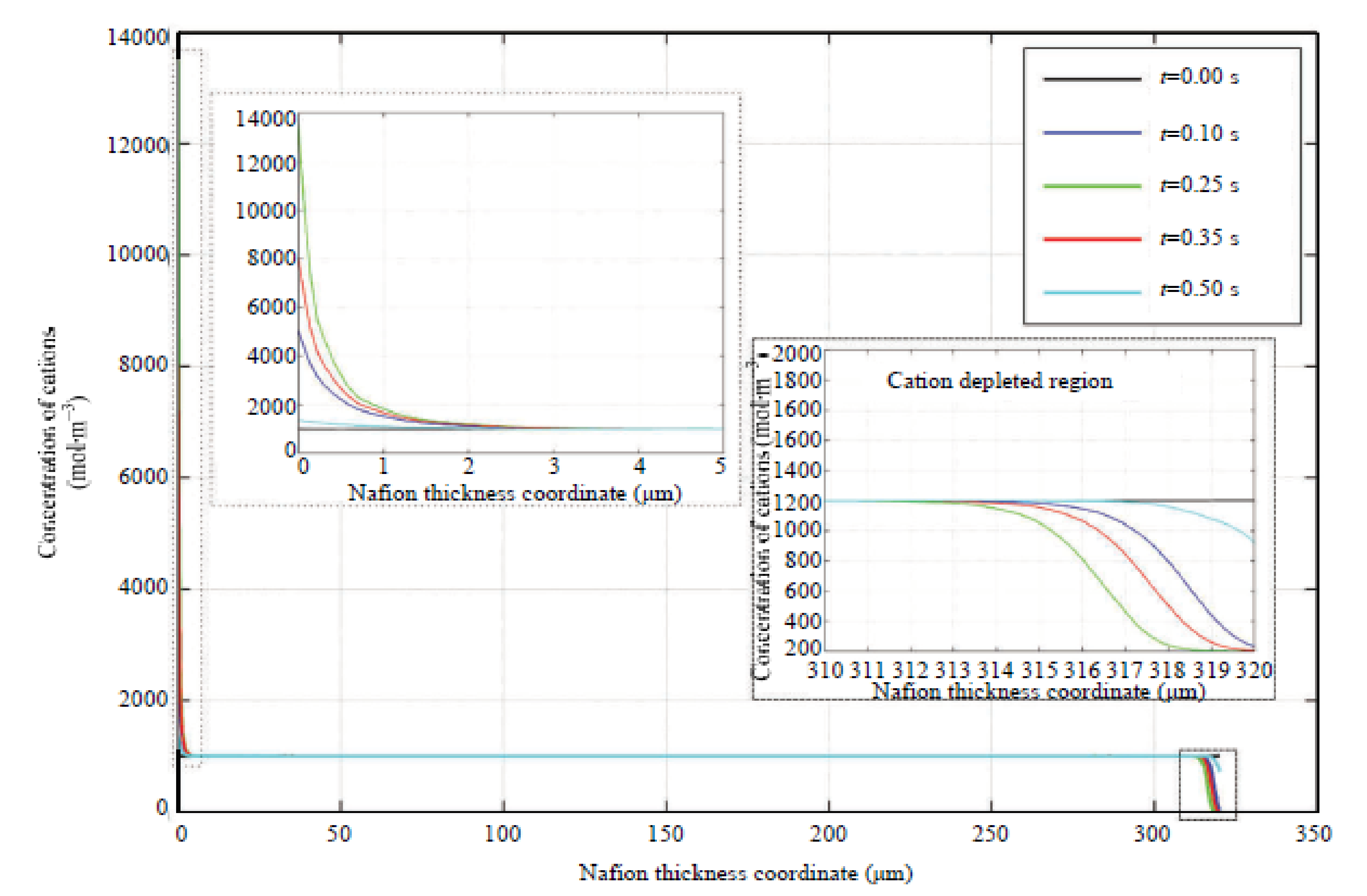
We use FEM implemented in **Comsol software** and work with the **general form PDE modules** of **Comsol software.**

A special care has to be taken when choosing and **distributing a mesh for finite elements**. The **finest mesh network** has to be formed in the places with the highest change of concentration c.



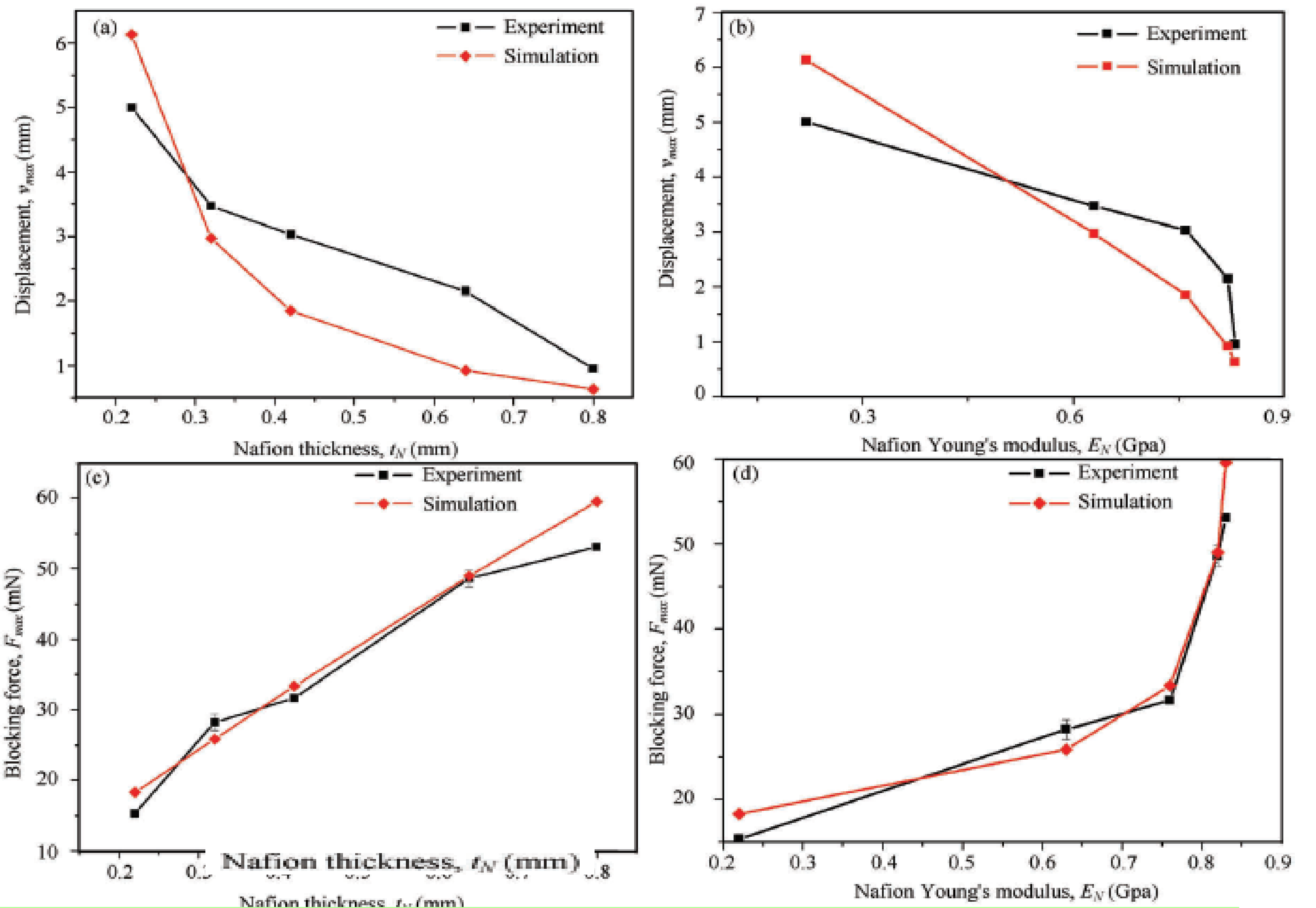

The **Scheme** of the **distributed mesh** employed with a dense mesh distribution at the interface Nafion-Electrode

<u>The most efficient strategy for the computation:</u>
solving the 1D (PNP) equation set first followed by solving the 3D Structural Mechanics (SM) using the 1D PNP solution as an input for the 3D problem.




The diagram of the simulated cation concentration, c, in dependence on the distance from the **Pt cathode** for various times. The insets show the **cation concentration** in the regions close to the electrodes.

# Data comparison



# Conclusion

Not bad agreement between the simulated and measured maximum displacement and blocking force

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