



**My current research status**

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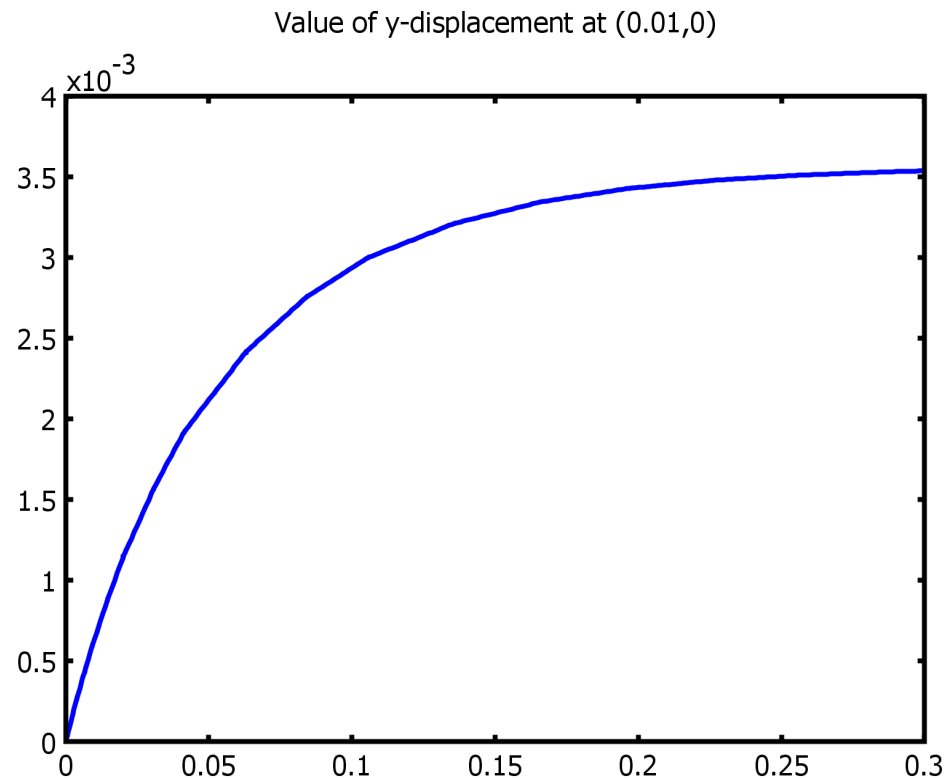
01/16/2007

## Previous status (in December)



- I had started modeling electrochemical reactions with FEM
- I had almost finished modeling of bending mechanism

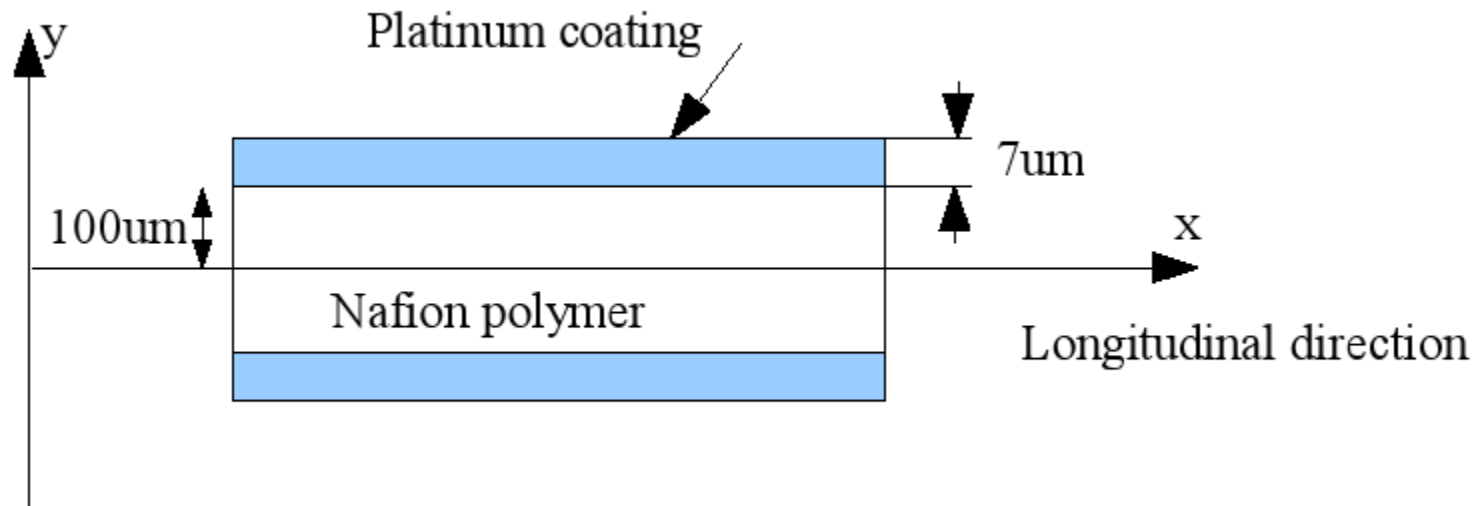
$$F_{local} = A \cdot (c_{Na} - c_{SO})$$



# Changes in bending model



- As I use FEM, I thought it would be nice to use three layer model for simulations (not to consider Pt only as boundary layer)



## Changes in bending model (2)



- Previously I defined local force inside the polymer:

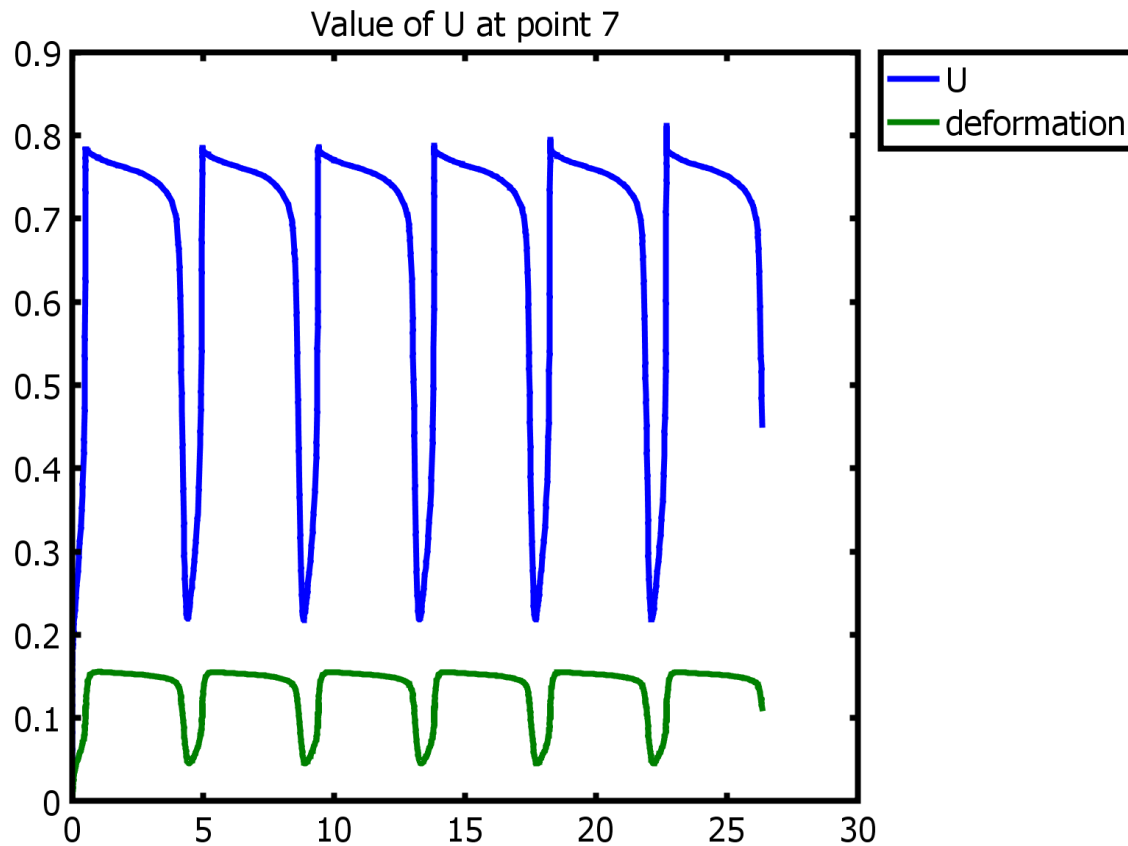
$$F_{local} = A \cdot (c_{Na} - c_{SO})$$

- Now I have tried to simulate:

$$F_{local} = A \cdot (c_{Na} - c_{SO}) + B \cdot \text{sgn}(c_{Na} - c_{SO}) \cdot (c_{Na} - c_{SO})^2$$

- The problem with those simulations are that each simulation takes at least 10min (to simulate 0.2s). So it is quite time consuming
- **Conclusion:** Three layer model or not, it's all about constants A and B

- For reminding: I try to model electrochemical oscillations using FEM approach



- Previously I had equations:

$$\dot{\theta}_{CO} = R \cdot k_2 \cdot (1 - \theta_{CO} - \theta_{OH}) - k_4 \cdot \theta_{CO} \cdot \theta_{OH}$$

$$\dot{\theta}_{OH} = k_3 \cdot (1 - \theta_{CO} - \theta_{OH}) - k_3 \cdot \theta_{OH} - k_4 \cdot \theta_{CO} \cdot \theta_{OH}$$

$$\dot{E} = I_{th} + (I - I_{th}) \cdot R \cdot \text{sgn}(c_{HCHO} - c_{HCHO2M}) - j \cdot (k_1 \cdot (1 - \theta_{OH} - \theta_{CO}) + k_4 \cdot \theta_{CO} \cdot \theta_{OH})$$

$$R = \frac{C_{HCHO}}{C_{HCHO2M}}$$

- Simulations show, that this **R** in the first equations produces some instabilities, though there are couple of articles where this first equation is really dependent of concentration of HCHO
- For SPIE, I think I leave this R out from first equations, but a bit better model should be developed in close future.

- Some facts
  - There is small potential inside the polymer – it is quite uniform throughout the polymer (simulation supports it and also literature).
  - There are currents nearby layers (simulation).
  - Electric field inside the polymer is ~ zero/very small
- One idea of explaining the phenomenon.
  - Applied voltage causes processes in the polymer – electronic current, breaking some hydrogen bonds or etc.
    - a. Anyway, reorientation of polymer chains/molecules is fast process, measured in milliseconds. But softening lasts seconds.
  - Maybe the slowness of the softening could be explained by stretching of IPMC:
    - a. Initial processes cause softening.
    - b. Stretching makes IPMC thinner --> causes stronger electric field / change of voltage inside the polymer
    - c. Stronger fields could cause more currents/disorientations inside the molecule
  - Fields inside the IPMC could be simulated with FEM (ASAP)

## Other activities



- Writing manuscript for SPIE (almost done now)
- Had an exam in December.
- Small vacation in Estonia