Strong Localization and Rapid Time Scales of Superheating in Solid-State Nanopores

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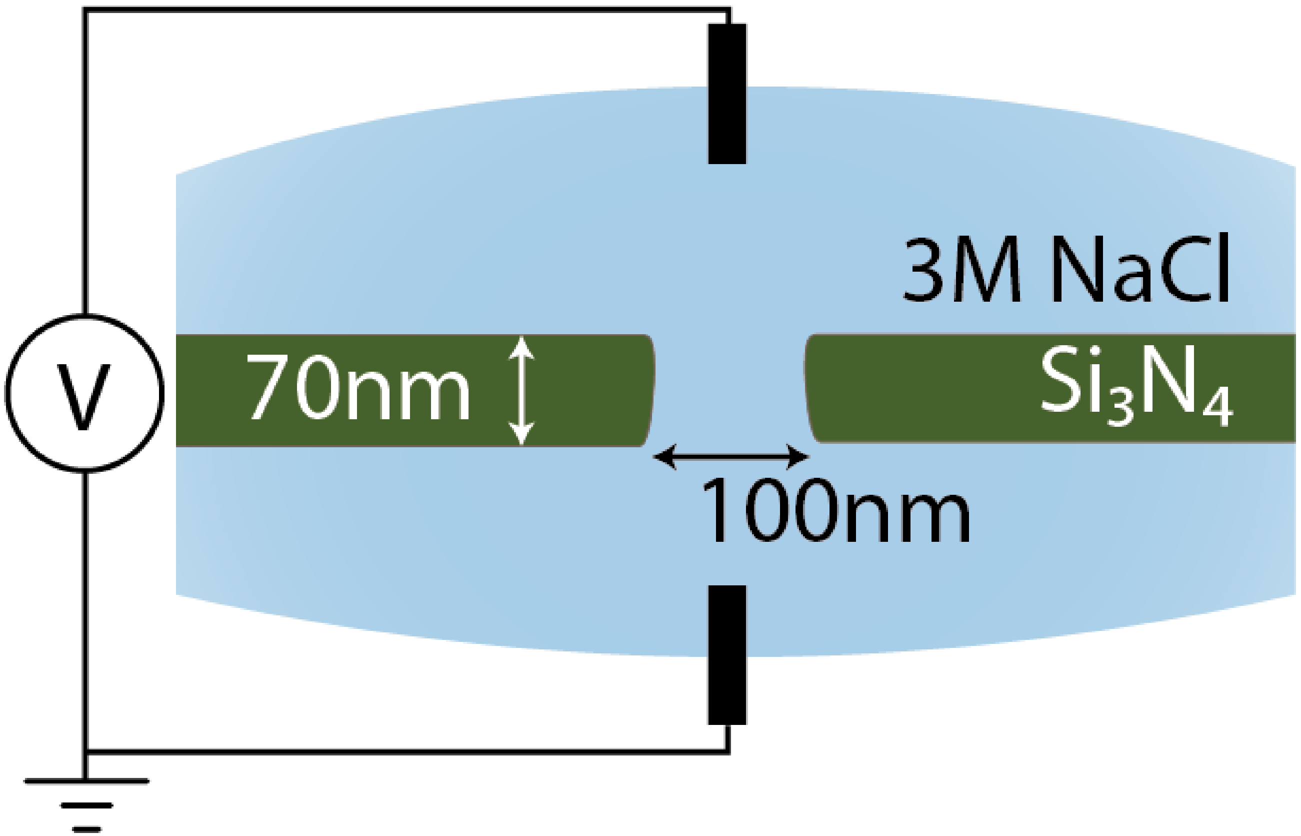
October 9, 2014

HARVARD
School of Engineering
and Applied Sciences

COMSOL CONFERENCE
2014 BOSTON

Nanopore Heating



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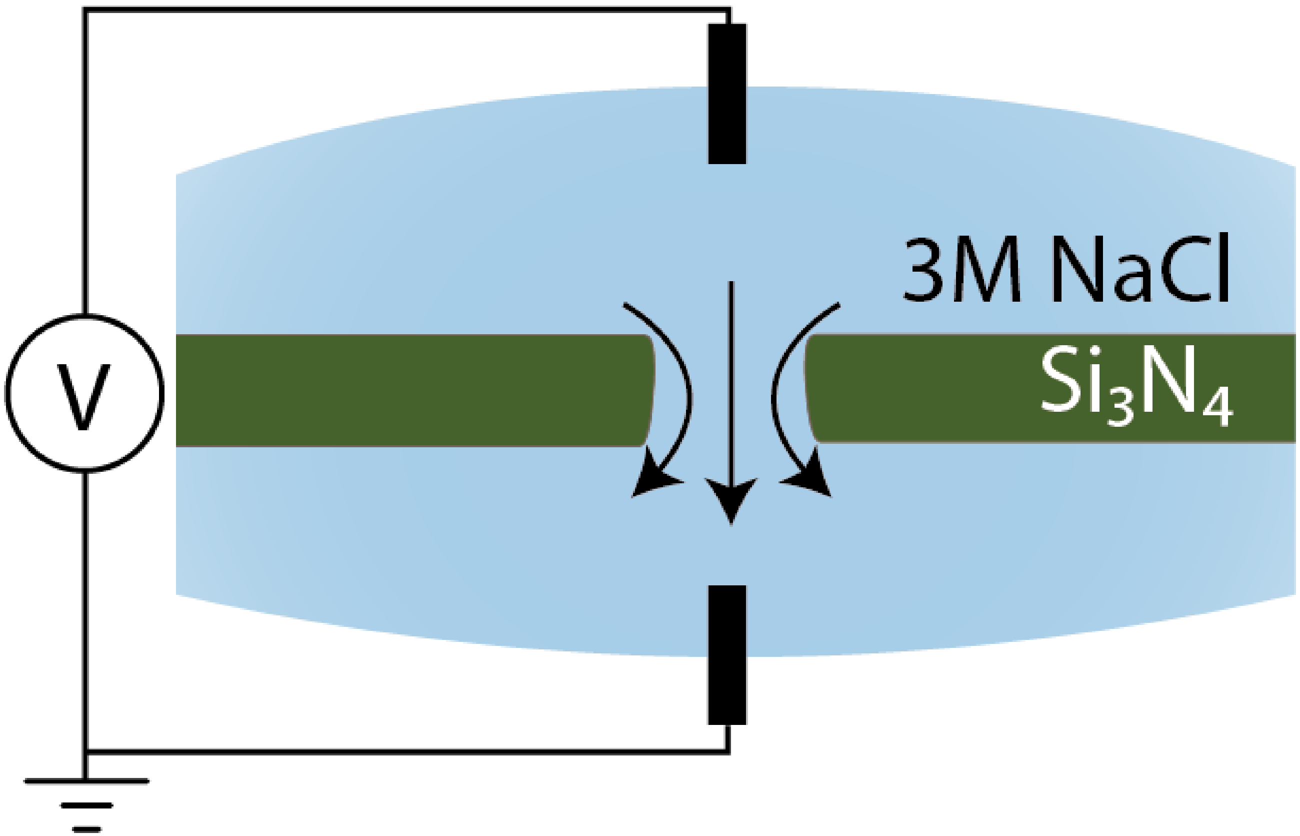

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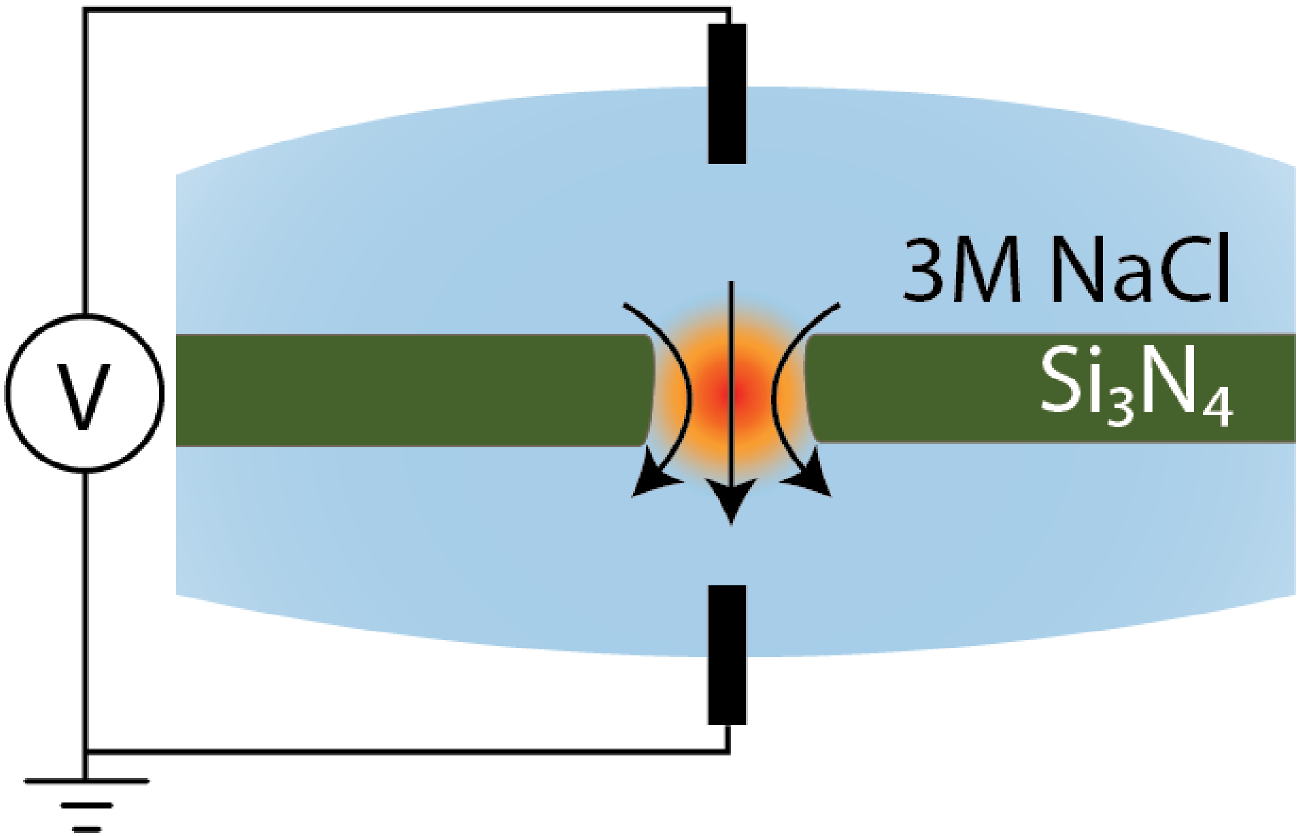

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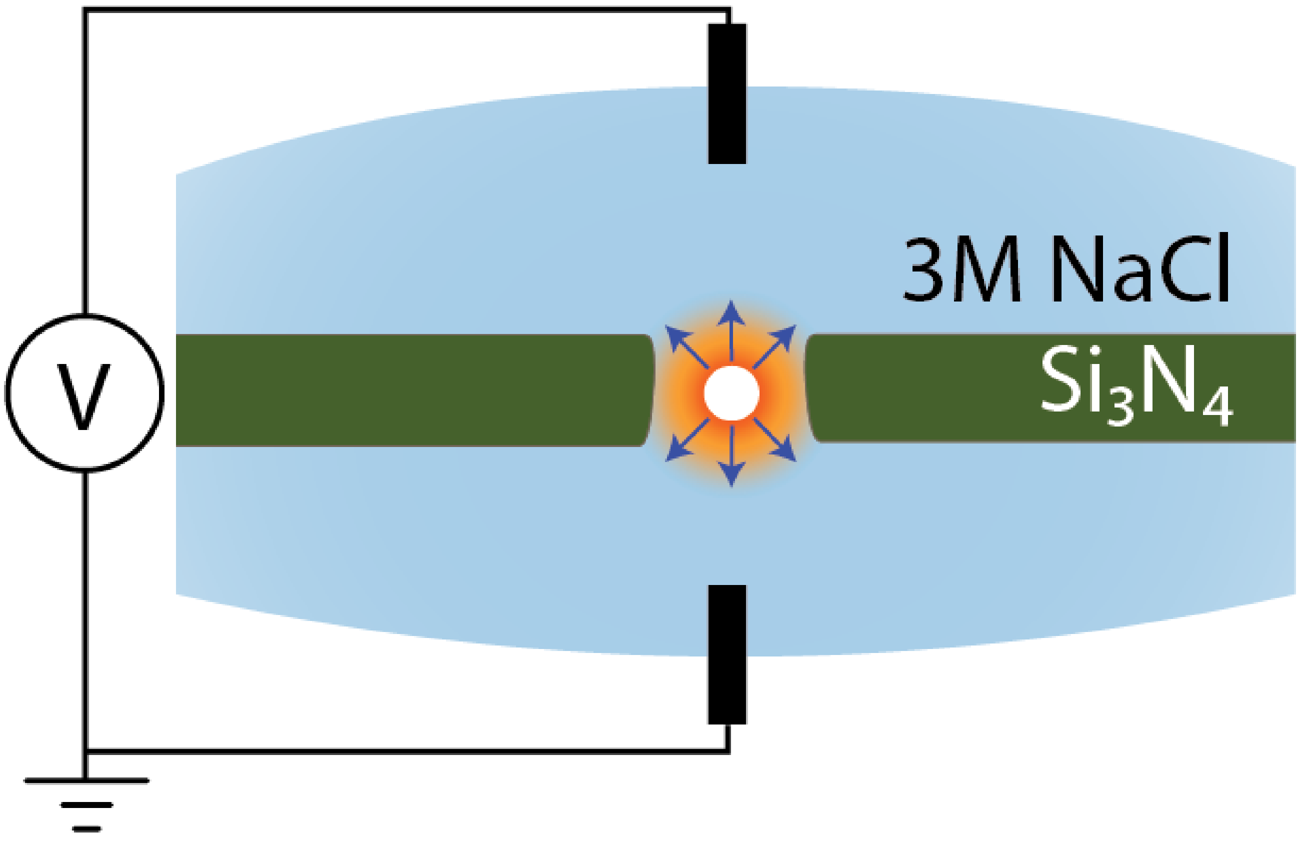
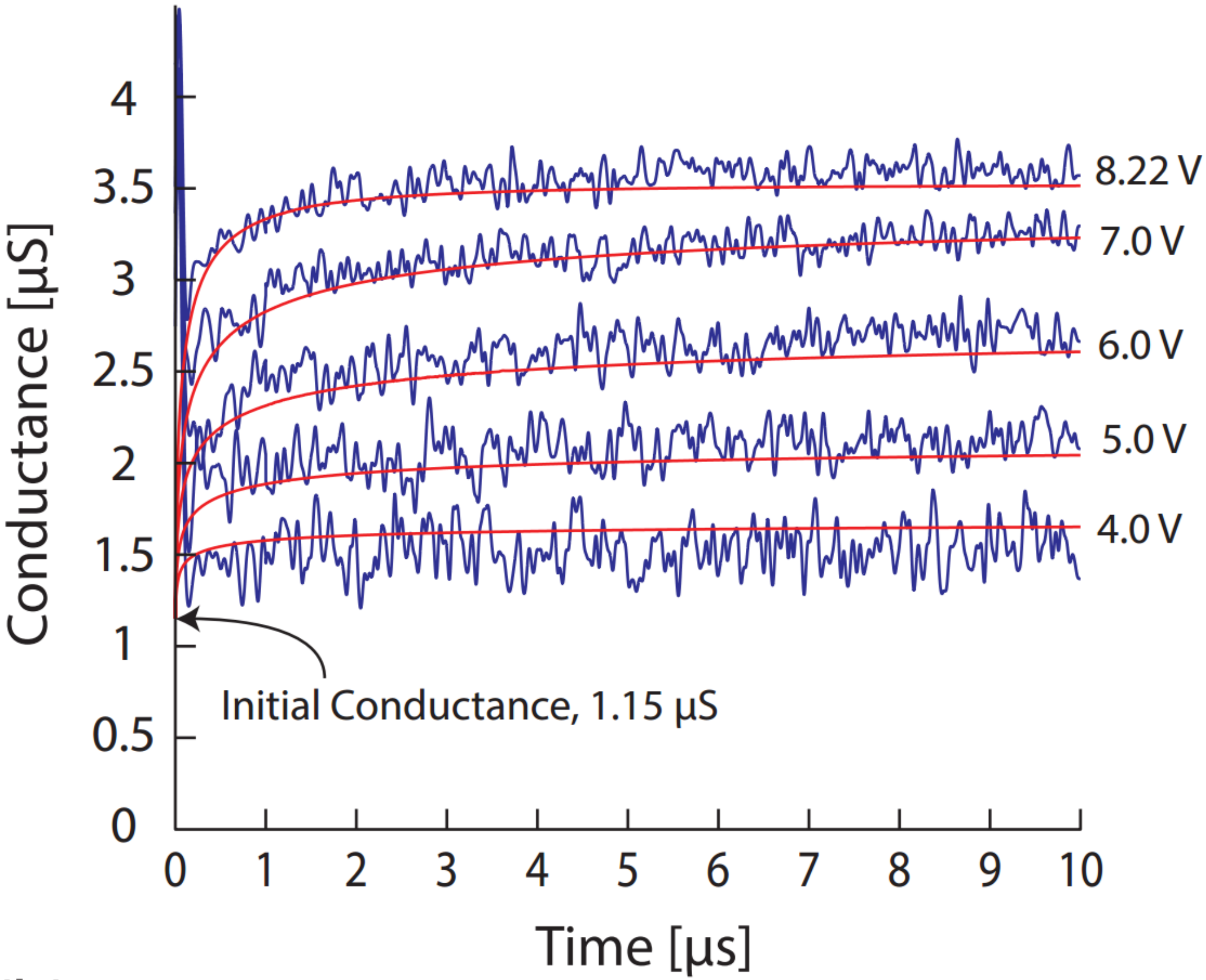


Experimental Results: Pore Conductance



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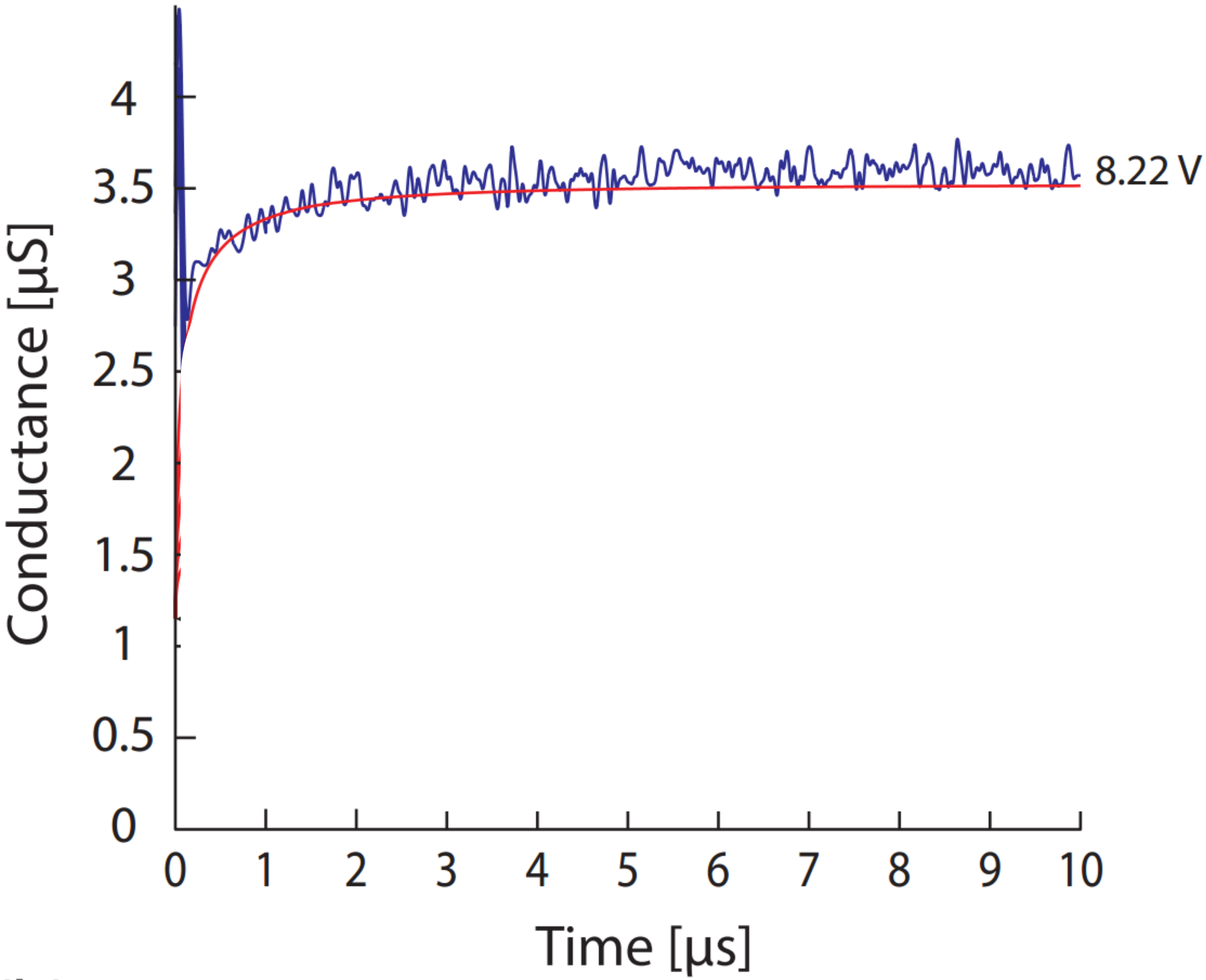

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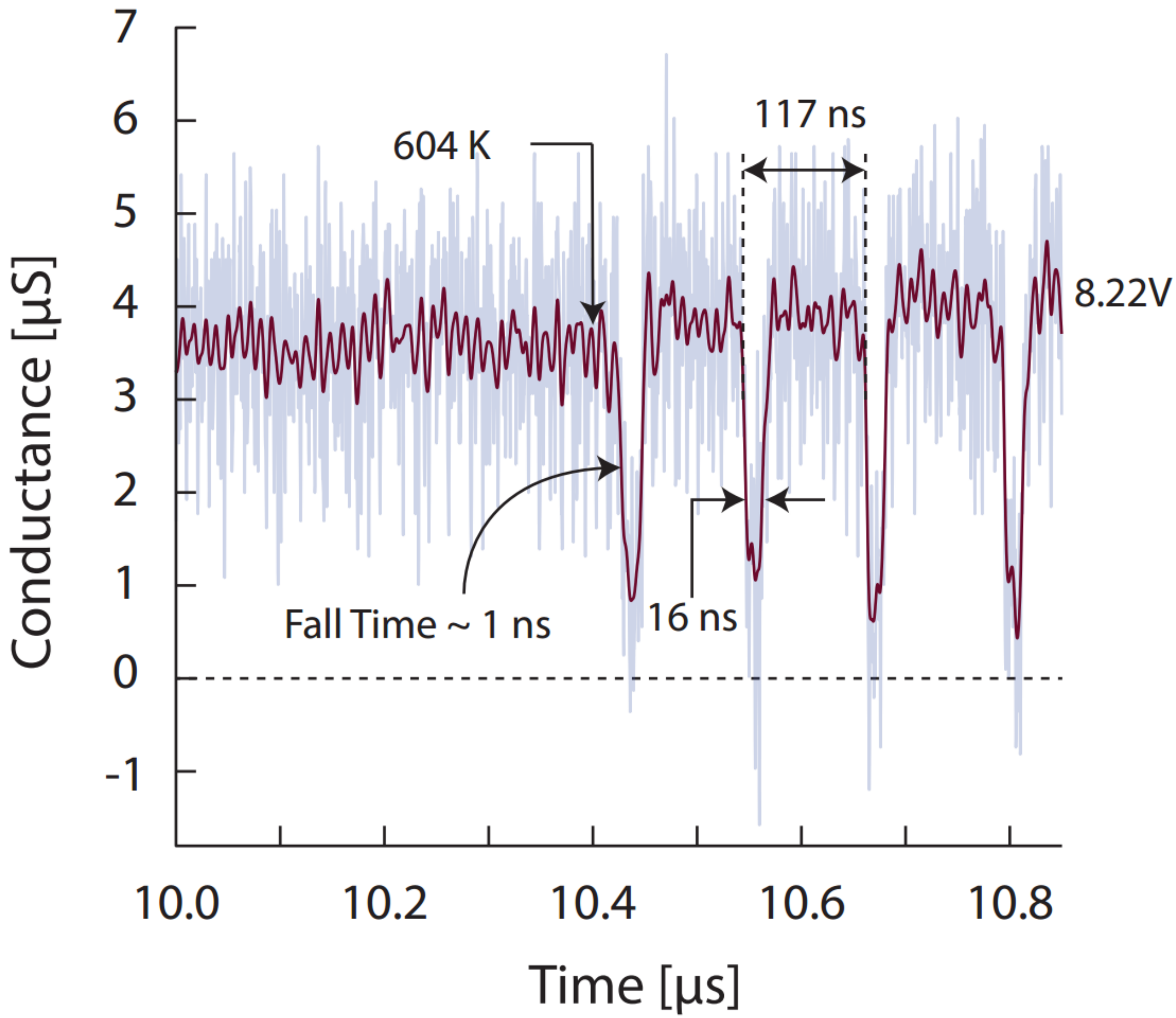

Motivating Question

How hot is the pore center?

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Can heating dynamics explain nonlinear conductivity measured before a nucleation event?

COMSOL Modeling

- Geometry
- Governing Equations: Joule Heating
- Material Properties
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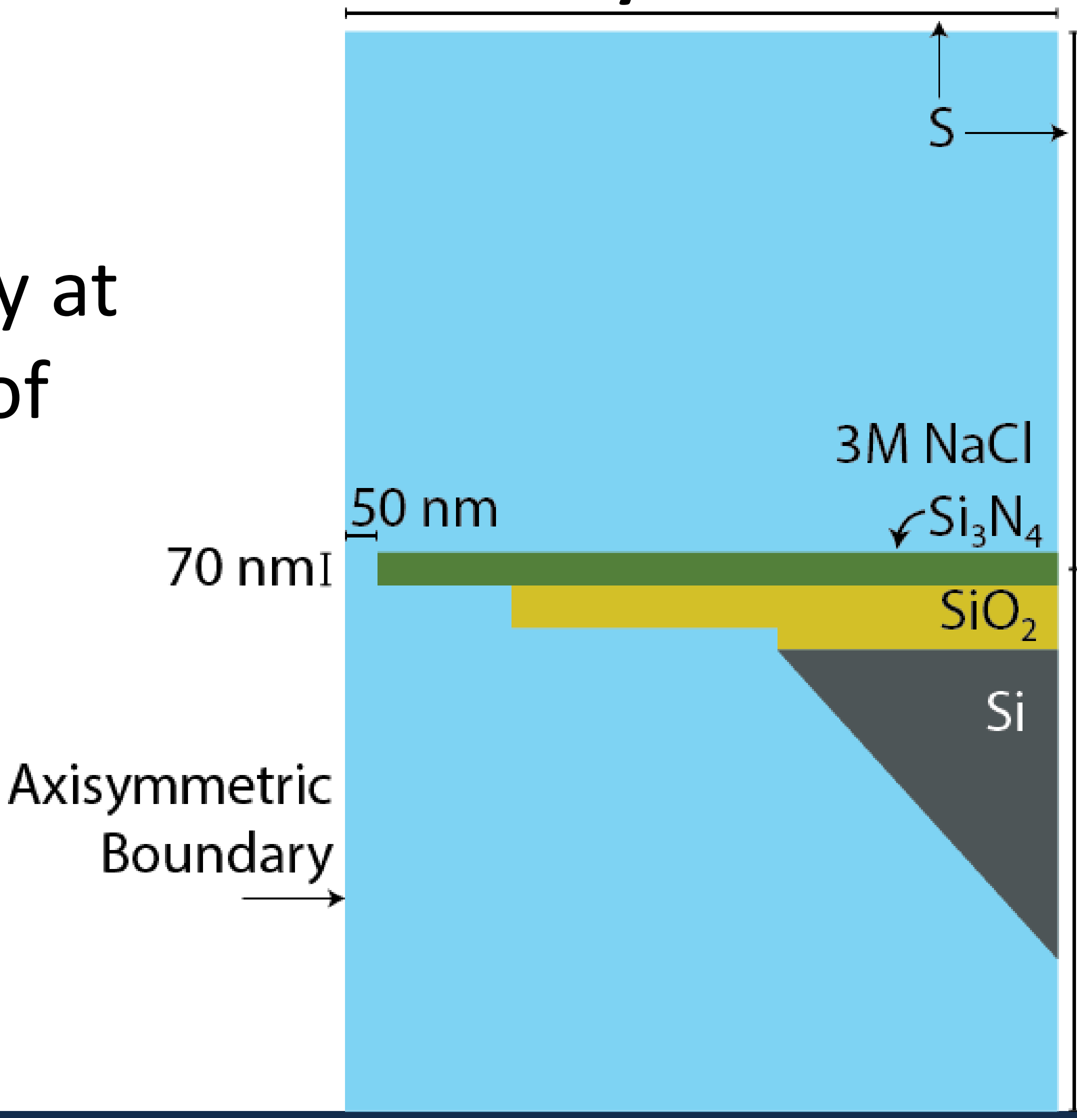
Nanopore Geometry

- 2D Axisymmetry
- External boundary at S is on the order of 200 microns



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Source Term: $Q = \boldsymbol{J}_t \cdot \boldsymbol{E}$

Continuity Equation: $\nabla \cdot \boldsymbol{J}_t = \underbrace{q_i}_{\text{Distributed Current Source } [A/m^3]}$

$$\boldsymbol{J}_t = \underbrace{\sigma \boldsymbol{E}}_{\text{Ohm's Law}} + \underbrace{\epsilon_0 \epsilon_r \frac{\partial}{\partial t} \boldsymbol{E}}_{\text{Displacement Current}} + \underbrace{\boldsymbol{J}_{ex}}_{\text{External Current Density } [A/m^2]}$$

$$\boldsymbol{E} = -\nabla V$$

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Heat Equation: $\rho C_p \frac{\partial}{\partial t} T = \nabla \cdot [\kappa \nabla T] + Q$

Source Term: $Q = \boldsymbol{J}_t \cdot \boldsymbol{E}$

Continuity Equation: $\nabla \cdot \boldsymbol{J}_t = q_i$ ($q_i = 0$)

$$\boldsymbol{J}_t = \sigma \boldsymbol{E} + \epsilon_0 \epsilon_r \frac{\partial}{\partial t} \boldsymbol{E} + \boldsymbol{J}_{ex}$$

($\boldsymbol{J}_{ex} = 0$)

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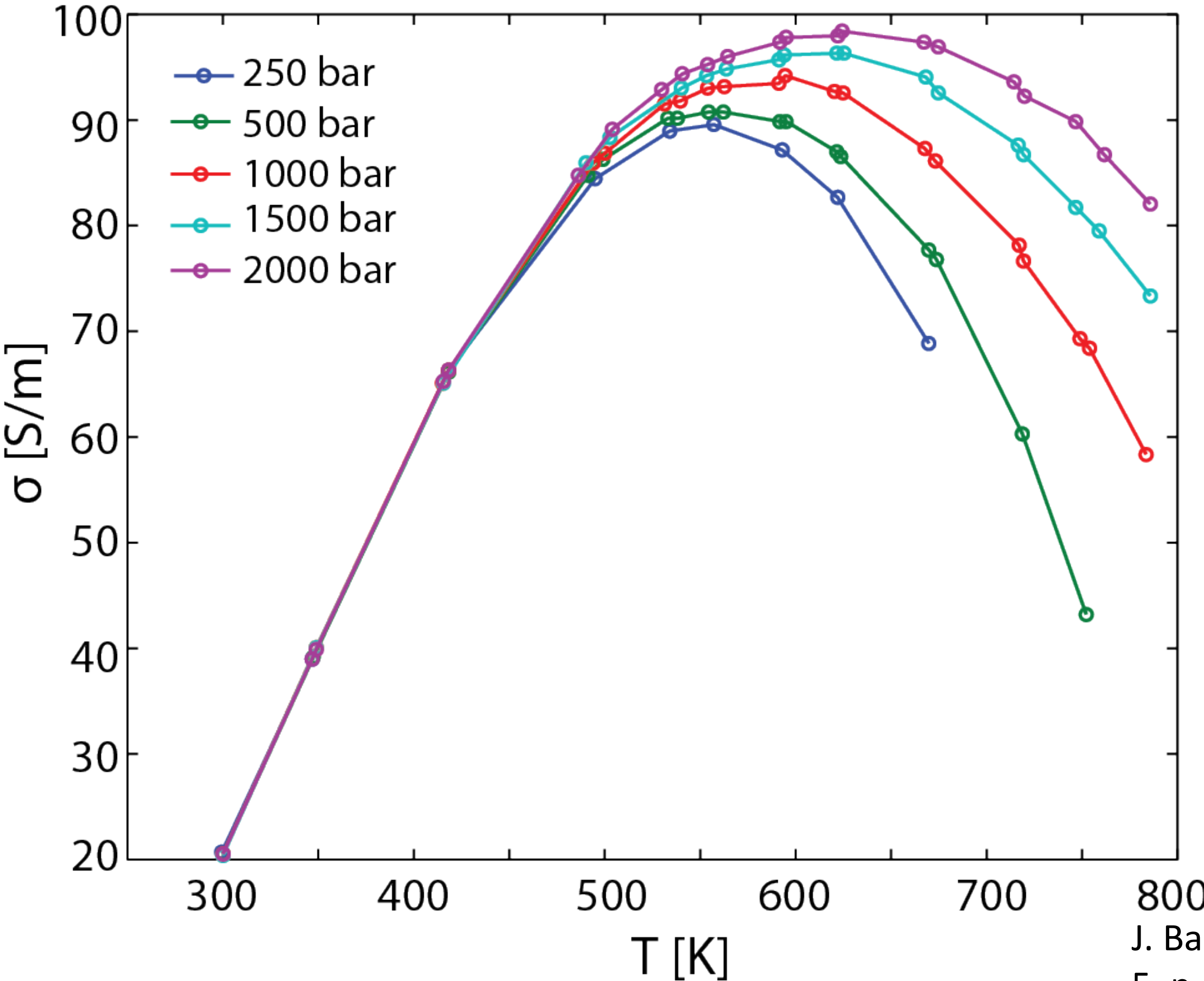
- What about electrical conductivity of 3M NaCl solution?

Conductivity 3M NaCl Solution



Joule Heating:

$$\sigma(T)E^2$$

J. Bannard, J. Appl. Electrochem., vol. 5, p. 43–53, 1975.

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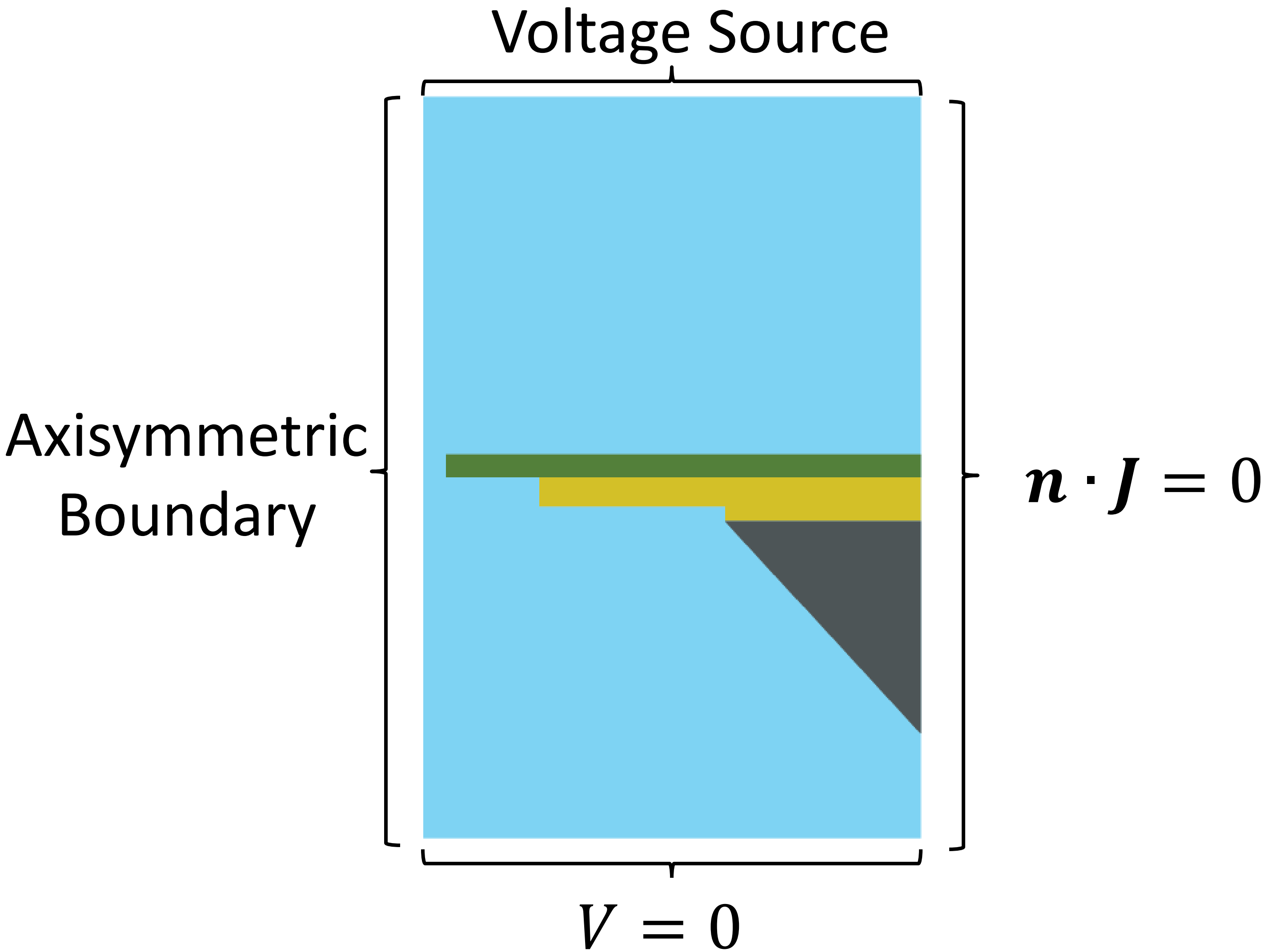
Boundary Conditions



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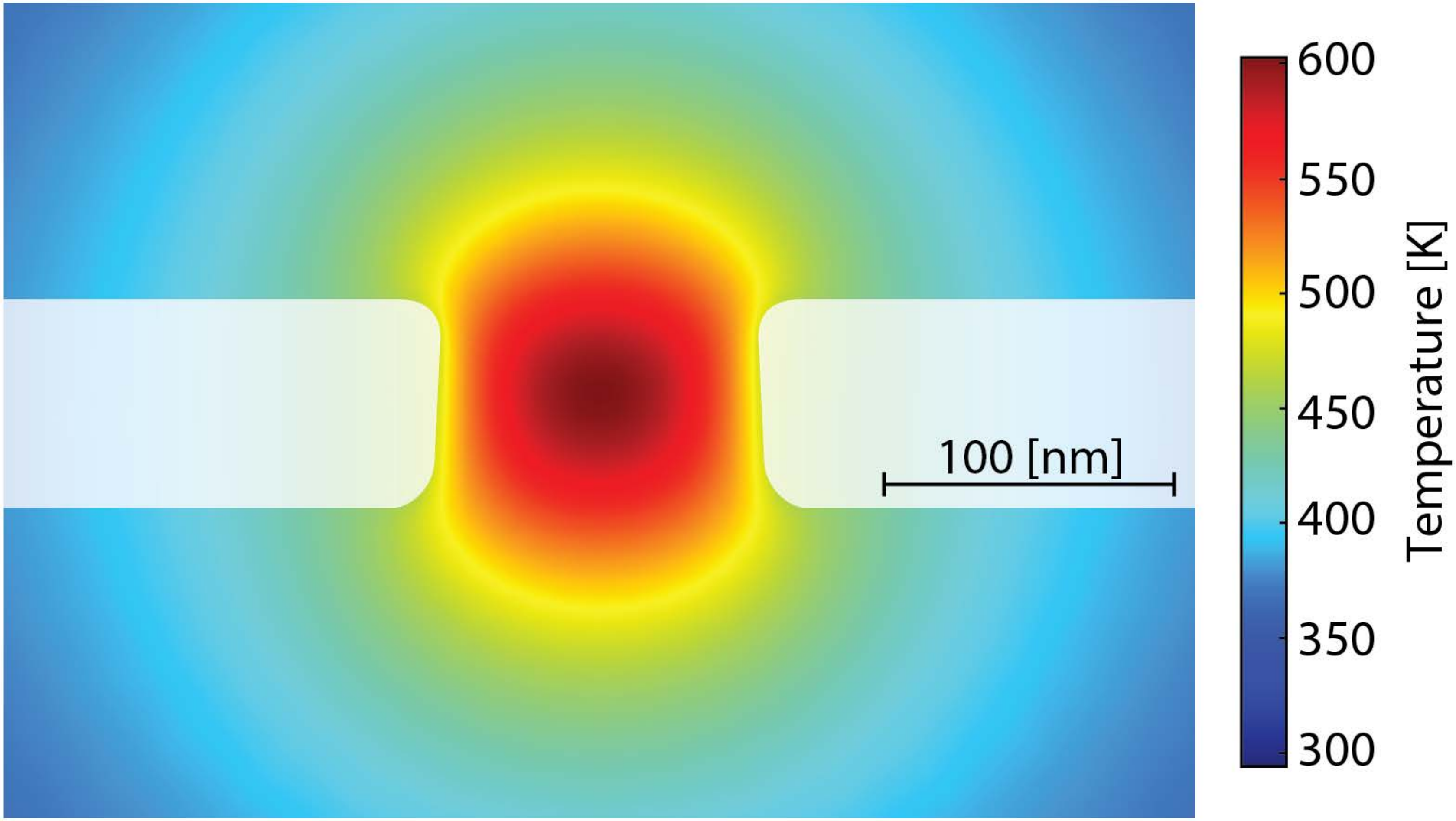
Nanopore Heating

8.22V pulse applied for 10.4μs



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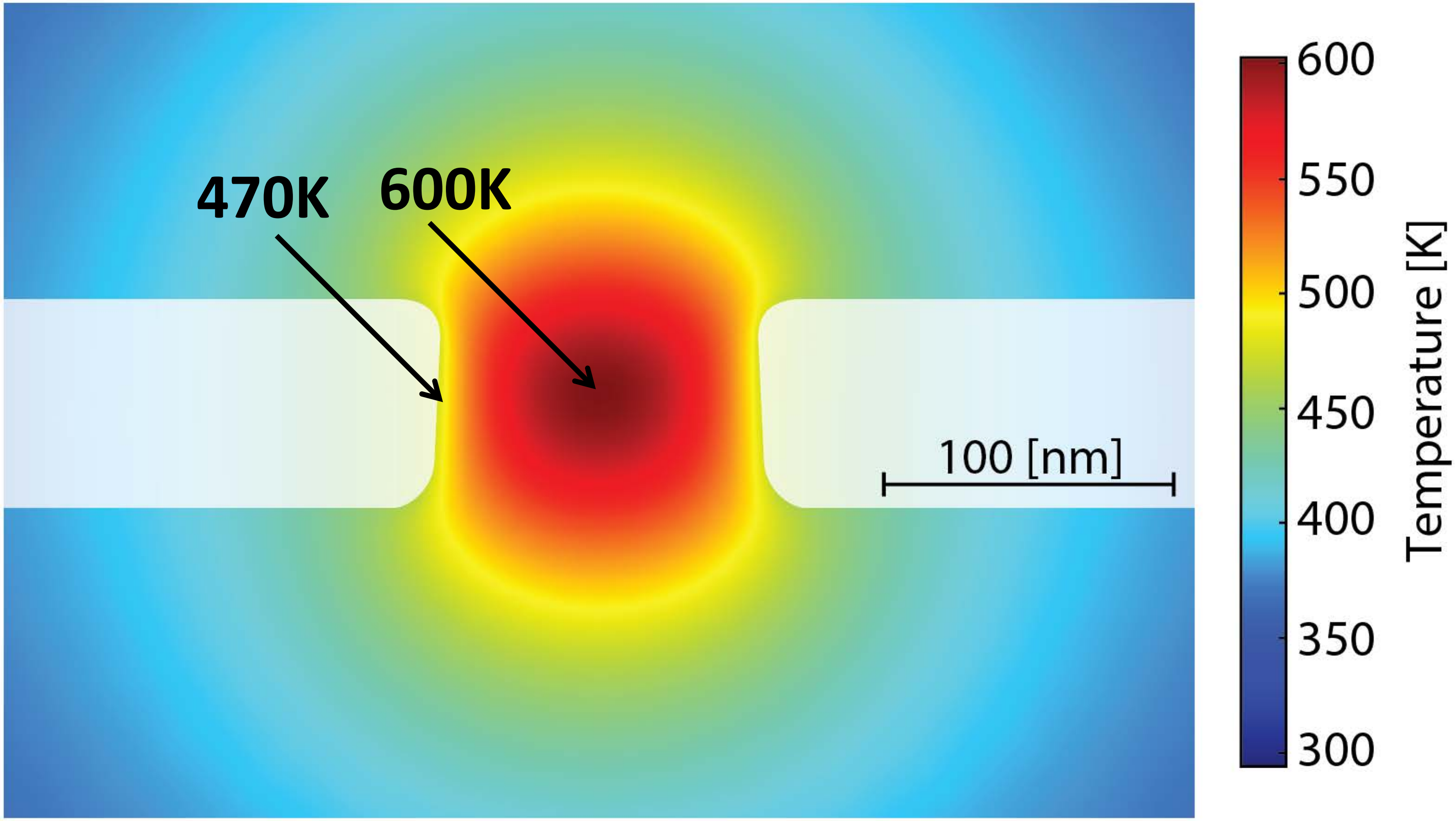

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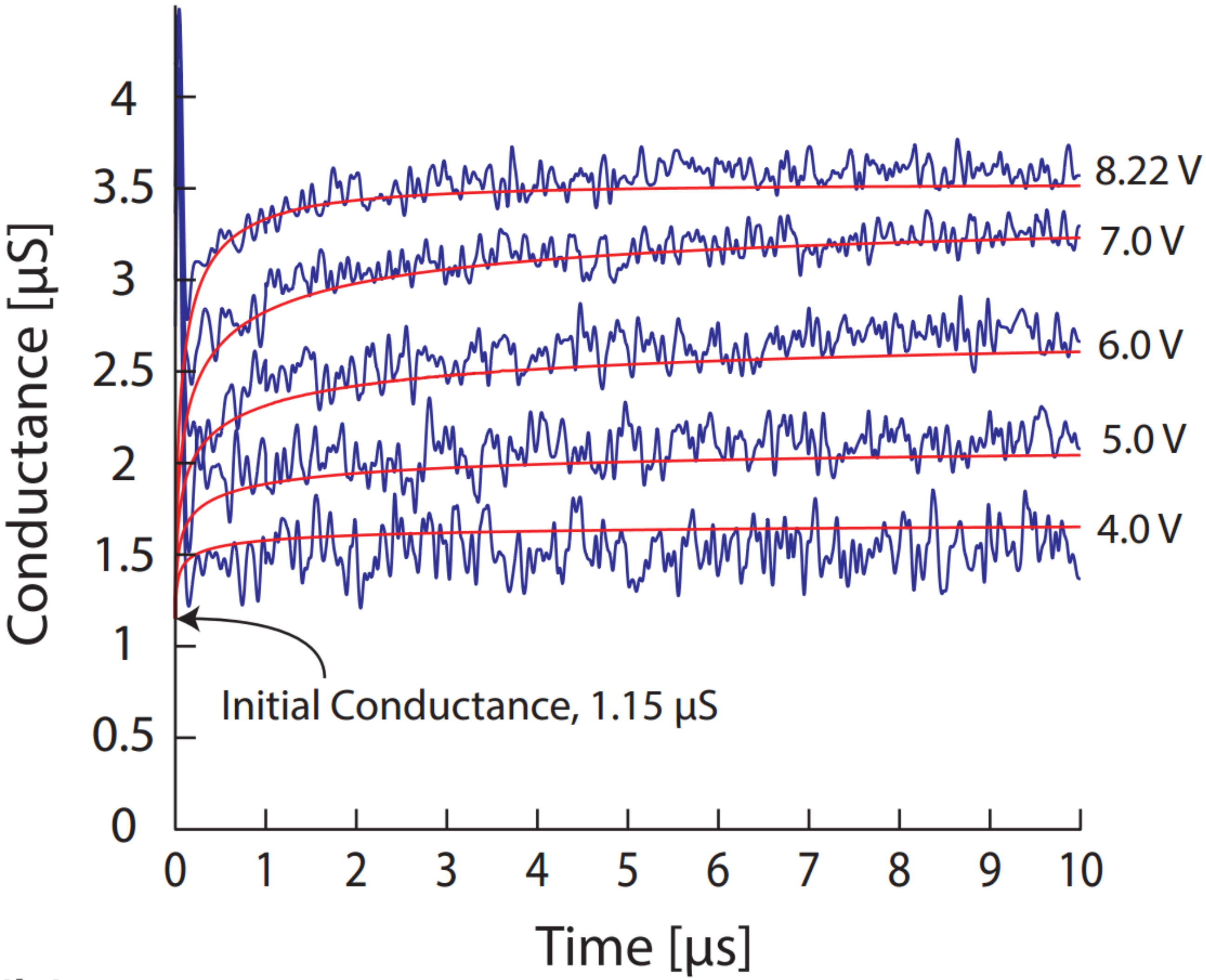

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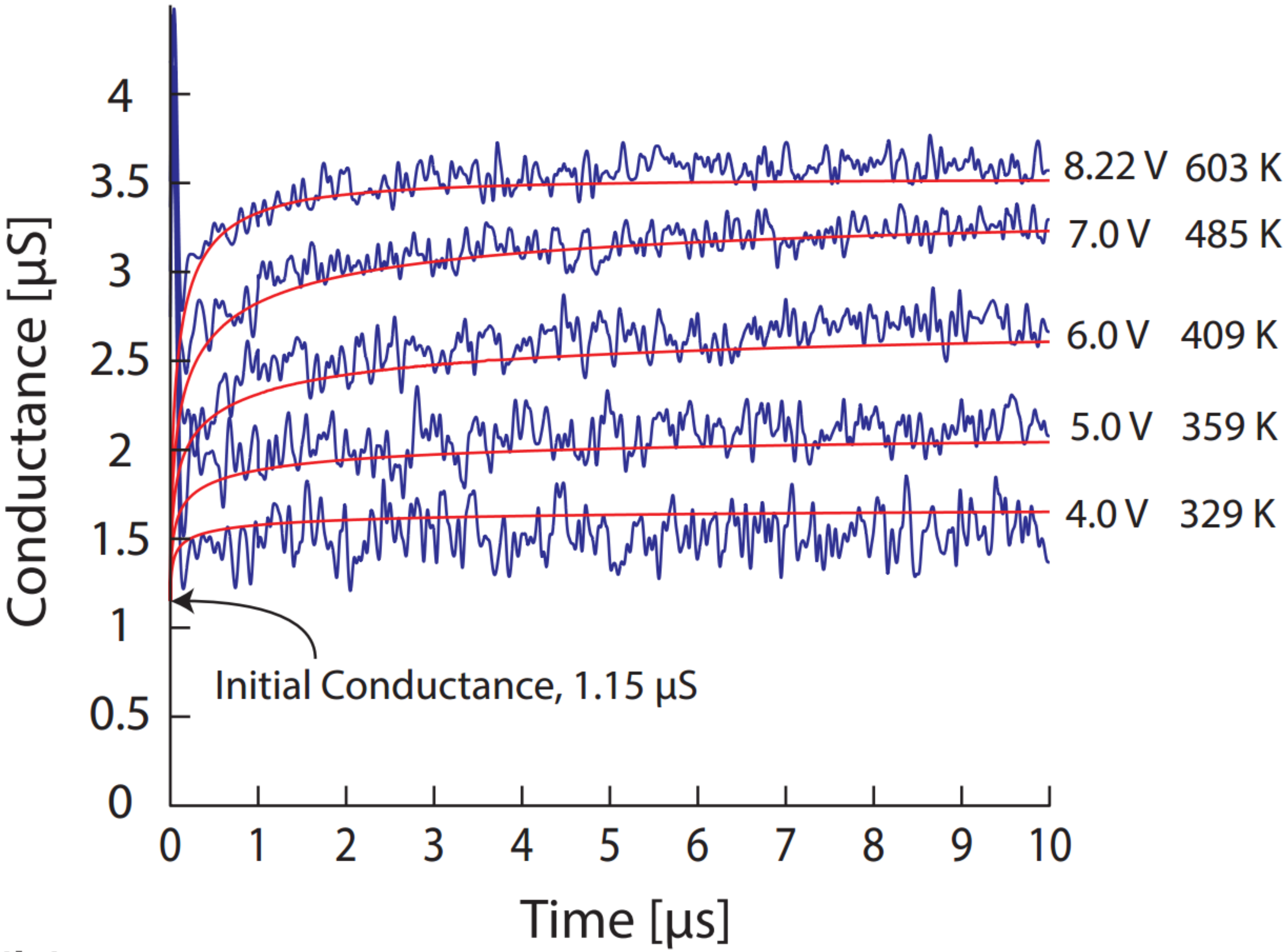

Conclusions

- Nanopore heating experiments
  - Temperature at the center of the pore: 600K
  - Close to kinetic limit of superheat
  - Not possible to experimentally measure
- Modeled using COMSOL Joule Heating Module
  - Flexibility to incorporate specialized material data

Acknowlegements

- Group
  - Prof. Jene Golovchenko
  - Gaku Nagashima
  - Dr. Dave Hoogerheide
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  - Golovchenko Group
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G. Nagashima, E.V. Levine, D.P. Hoogerheide, M.M. Burns, J.A. Golovchenko, "Superheating and Homogeneous Single Bubble Nucleation in a Solid-State Nanopore", PRL 113, July 9, 2014.

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$$\nabla \cdot \left(\sigma \boldsymbol{E} + \frac{\partial}{\partial t} \mathbf{D} \right) = \nabla \cdot (\sigma \boldsymbol{E}) + \frac{\partial \rho}{\partial t} = 0$$

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↑

Not zero!