

Supplemental Material for “Superheating and Homogeneous Single Bubble Nucleation in a Solid-State Nanopore”

Gaku Nagashima, Edlyn V. Levine, David P. Hoogerheide, Michael M. Burns, and Jene A. Golovchenko

This document provides supplemental information regarding the COMSOL calculation used to determine the temperature of the electrolyte in the solid-state nanopore during the nanopore heating experiments.

The calculation required solving the heat equation in the nanopore with inclusion of a Joule heating source term, appropriate boundary conditions and temperature dependent material properties of the electrolyte and membrane. The heat equation must be coupled with charge continuity and Ohm’s law to determine the source term. This is done using the Joule Heating (jh) and Electric Currents (ec) modules in COMSOL. The equations take the form

$$\begin{aligned}\nabla \cdot \mathbf{J} &= \nabla \cdot (\sigma \mathbf{E}) = 0 \\ \mathbf{J} &= \sigma \mathbf{E} \\ \mathbf{E} &= -\nabla V \\ \rho C_p \frac{\partial T}{\partial t} &= \nabla \cdot (\kappa \nabla T) + \mathbf{J} \cdot \mathbf{E}\end{aligned}$$

where T is the temperature, V is the electrical potential, \mathbf{E} is the electric field, and \mathbf{J} is the current density. The membrane is assumed to be non-conducting and the applied voltage is specified on the boundary far from the pore. The temperature condition imposed on the boundary was $T = T_0$, where T_0 is the ambient temperature measured at the start of the experiment. The initial condition was $T = T_0$ everywhere. The density, ρ , heat capacity at constant pressure, C_p , thermal conductivity, κ , and electrical conductivity, σ , are all temperature dependent properties of the electrolyte. Material data for superheated aqueous 3M sodium chloride solution at atmospheric

pressure is not available for the extremely high temperature regime that we reach experimentally. Therefore, we used values for the density, heat capacity and thermal conductivity available from the IAPWS-95 formulation for the equation of state of water [1-3].

Experimental data for the electrical conductivity at such high temperatures under atmospheric pressure is not available either. We therefore fit the electrical conductivity to the experimentally measured conductance curve using two free parameters. Our resulting conductivity curve is compared to those reported by Bannard [4] in Figure 1. The high temperature behavior is understood to arise from the temperature dependent behavior of the solvent, water, as described in Quist and Marshal's paper [5] on the subject.

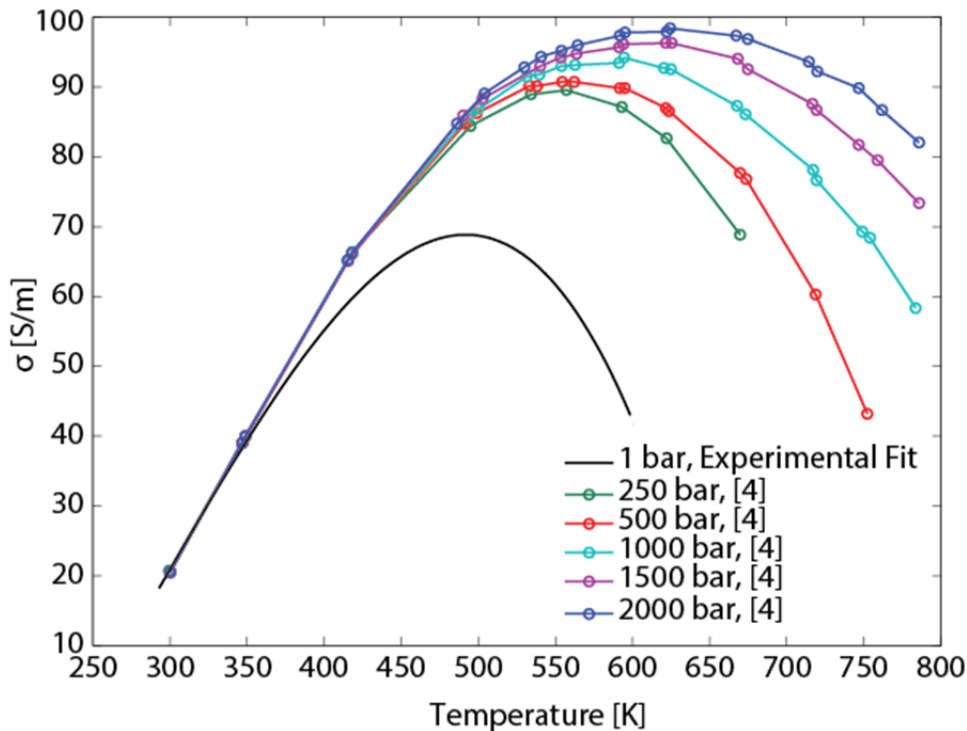


Figure 1. The electrical conductivity of aqueous 3M NaCl solution as a function of temperature. The data points are those reported in Figure 7 of [4] and are shown here for reference. The conductivity curve we fit to our experimental results and used for temperature calculations is also shown.

[1] W. Wagner and A. Pruß, *J. Phys. Chem. Ref. Data* **31**, 387 (2002).

- [2] *Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use*, (The International Association for the Properties of Water and Steam, Doorwerth, The Netherlands, September, 2009, <http://www.iapws.org/relguide/IAPWS-95.html>).
- [3] *Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance* (The International Association for the Properties of Water and Steam, Plzen, Czech Republic, pp. 1–15, September, 2011, <http://www.iapws.org/relguide/ThCond.html>).
- [4] J. Bannard, *J. Appl. Electrochem* **5**, 43 (1975).
- [5] A. S. Quist and W. L. Marshall, *J. Phys. Chem* **72**, 684 (1968).