Supplemental Material: Thermal Conduction and Rectification Phenomena in Nanoporous Silicon Membranes

Konstanze R. Hahn, Claudio Melis, and Luciano Colombo

Department of Physics, University of Cagliari,

Cittadella Universitaria, 09042 Monserrato (CA), Italy

METHODS

In order to obtain a properly relaxed nonequilibrium steady state condition, the modulus of the heat fluxes into and out of the thermostats should be equal. The difference between the two has been carefully monitored through the calculation and the criterion for convergence has been set to 2% for $\frac{|J_{cold}|-|J_{hot}|}{|J_{cold}|}$. In addition, the change in (relative) heat flux J with time $\mathrm{d}J/J\mathrm{d}t$ has been monitored and its steady state has been used as an additional criterion for convergence. Steady state has been defined when $\mathrm{d}J/J\mathrm{d}t \leq 10^{-7}$1/fs. Fig. S1 shows the heat flux in reverse bias for the cold thermostat and its numerical time derivative while the heat transferred from and to the thermostats and the corresponding flux for both reservoirs as a function of simulation time are shown in Fig. S2 together with the error $\frac{|J_{cold}|-|J_{hot}|}{|J_{cold}|}$ for sample 12x18 (Φ_{tot}=0.03, $\Phi_{\perp}$=0.22) with ordered pore distribution.

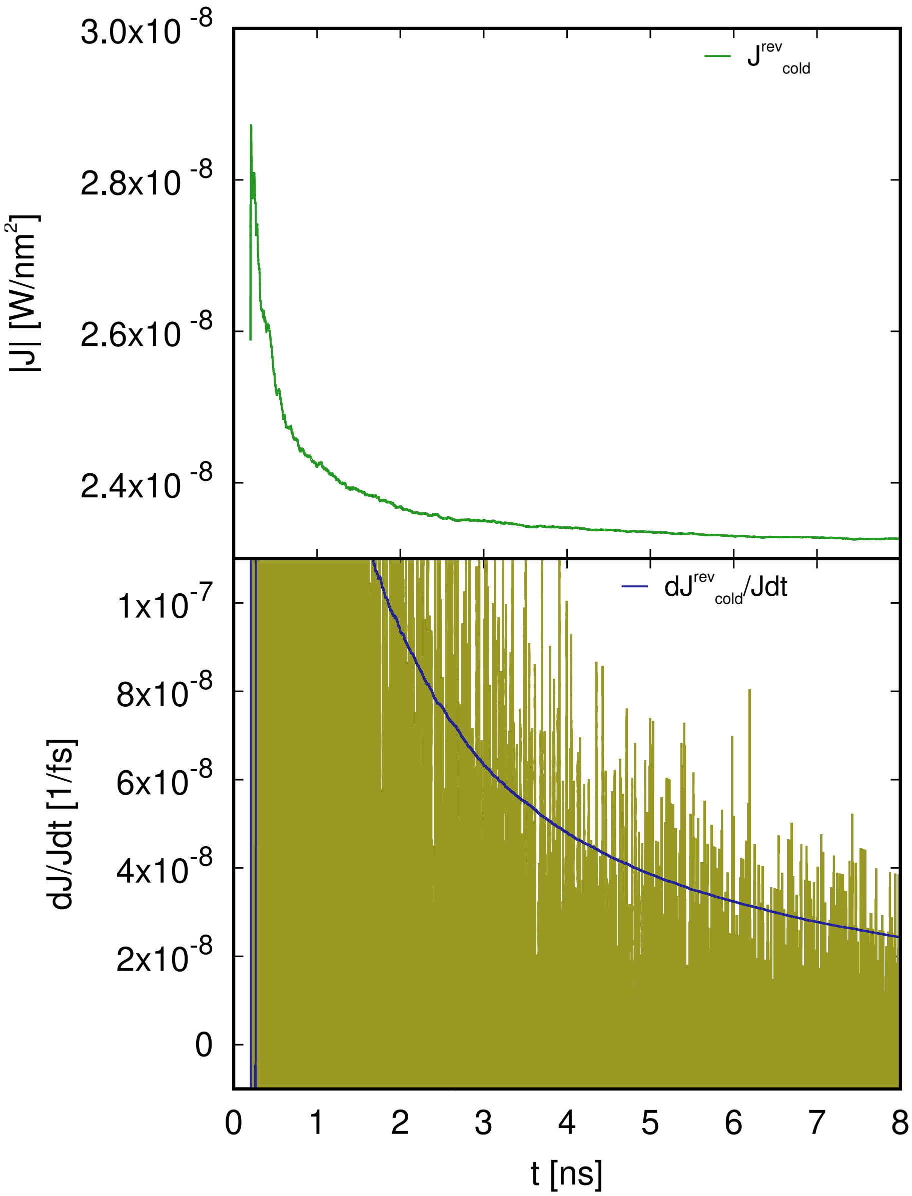

FIG. S1. Heat flux (top), numerical derivative of the heat flux (center) and error between flux of hot and cold reservoir (bottom) in a sample with ordered pore distribution, 12x18.

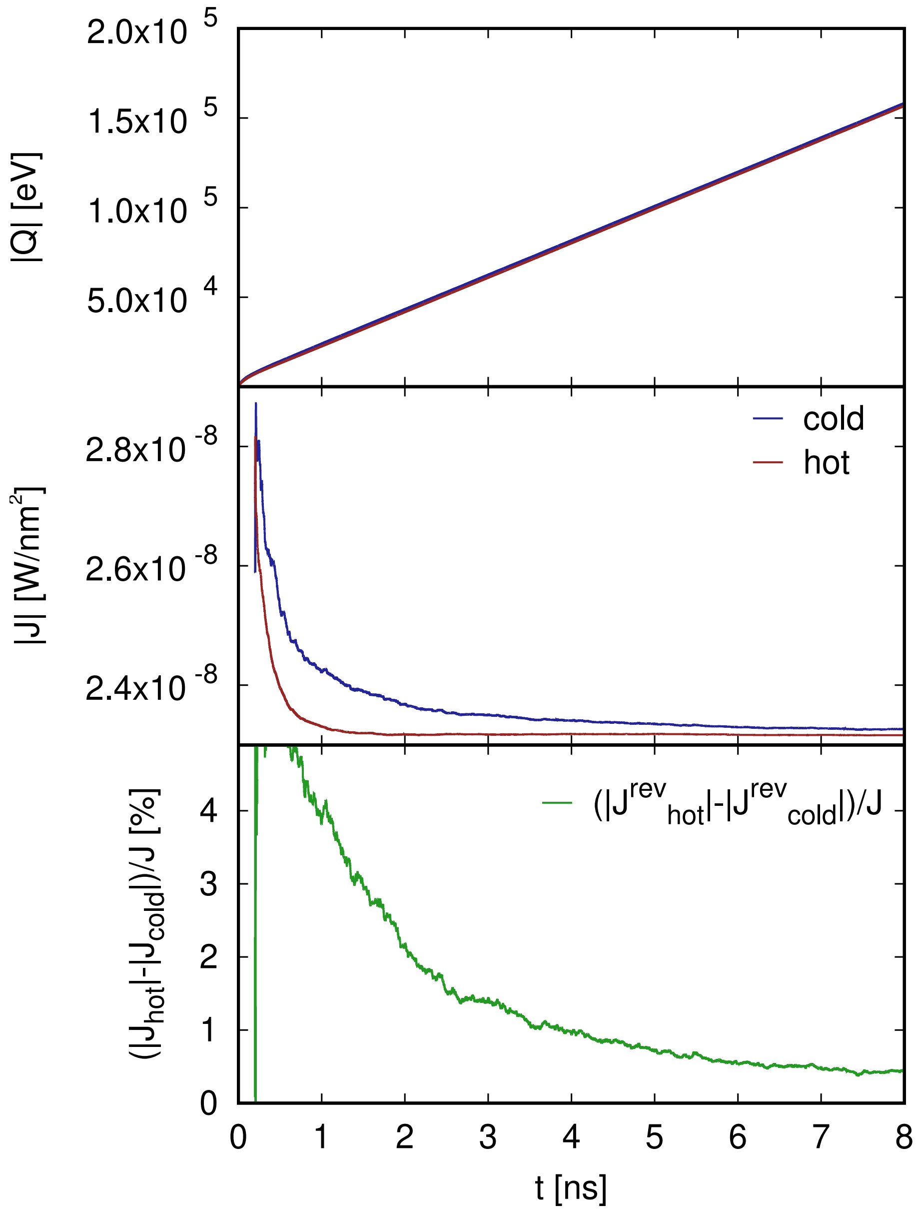

FIG. S2. Heat transfer into (hot) and out of (cold) the system via the thermostats (top), the corresponding flux calculated from the numerical time derivative of the transferred heat per cross-section area (center) and error between flux of hot and cold reservoir (bottom) in a sample with ordered pore distribution, 12x18.

RESULTS

Effect of pore distribution

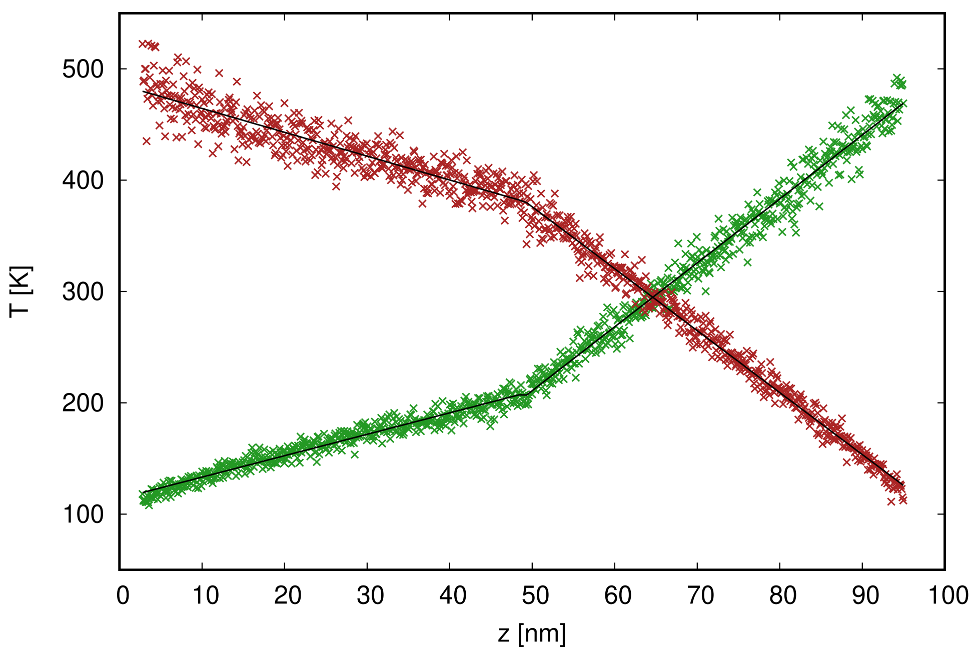

FIG. S3. Temperature profile in direction of the heat flow for a step-like ordered distrubution of pores with $n_{p,\perp}$=12 and Φ_{tot}=0.03.

Effect of interface thermal resistance

In the case of $n_{p,||}$=4 ($\Phi_{tot} = 0.014$), four segments can be identified where the thermal conductivity of each segment has been approximated with the thermal conductivity of a crystalline Si membrane at the average temperature of each segment. The overall thermal conductivity in forward bias can thus be written as

$$\frac{1}{\kappa^{fwd}} = \frac{\alpha_1}{\kappa_{\mathrm{Si}}(T_1)} + \frac{R_{ITR}^{fwd,I}}{L_z} + \frac{\alpha_2}{\kappa_{\mathrm{Si}}(T_1)} + \frac{R_{ITR}^{fwd,II}}{L_z} + \frac{\alpha_3}{\kappa_{\mathrm{Si}}(T_3)} + \frac{R_{ITR}^{fwd,III}}{L_z} + \frac{\alpha_4}{\kappa_{\mathrm{Si}}(T_4)} \tag{1}$$

and accordingly in reverse bias

$$\frac{1}{\kappa^{rev}} = \frac{\alpha_1}{\kappa_{\mathrm{Si}}(T_1)} + \frac{R_{ITR}^{rev,I}}{L_z} + \frac{\alpha_2}{\kappa_{\mathrm{Si}}(T_1)} + \frac{R_{ITR}^{rev,II}}{L_z} + \frac{\alpha_3}{\kappa_{\mathrm{Si}}(T_3)} + \frac{R_{ITR}^{rev,III}}{L_z} + \frac{\alpha_4}{\kappa_{\mathrm{Si}}(T_4)}. \tag{2}$$

The thermal conductivity has directly been taken from the fitted temperature gradient for each segment where the temperature profile was linear. The values obtained using this method are shown in Table S2 together with the values for the interface thermal resistance $R_{ITR}^{fwd/rev,ij}$ and the average temperature T_i of each segment.

TABLE S1. Average temperatures T_i, fitted thermal conductivity κ_i and interface thermal resistance R_{ITR} for segments i in forward and reverse bias for ordered pore distribution with $\Phi_{tot} = 0.014$.

	forward	reverse
T_1 [K]	150.5	442.6
T_2 [K]	261.1	327.1
T_3 [K]	367.3	222.0
T_4 [K]	447.0	148.3
κ_1 [W/mK]	9.85	8.89
κ_2 [W/mK]	13.23	12.73
κ_3 [W/mK]	11.54	11.80
κ_4 [W/mK]	7.41	7.99
R_{ITR}^{I} [m^{2}K/W]	$6.49{\cdot}10^{-10}$	$6.28{\cdot}10^{-10}$
R_{ITR}^{II} [m^{2}K/W]	$6.43{\cdot}10^{-10}$	$5.92{\cdot}10^{-10}$
R_{ITR}^{III} [m^{2}K/W]	$6.85{\cdot}10^{-11}$	$5.89{\cdot}10^{-10}$

TABLE S2. Average temperatures T_i and interface thermal resistance R_{ITR} for segments i in forward and reverse bias for ordered pore distribution with $\Phi_{tot} = 0.021$.

	forward	reverse
T_1 [K]	134.2	463.6
T_2 [K]	212.1	378.8
T_3 [K]	288.7	300.4
T_4 [K]	357.2	234.9
T_5 [K]	415.1	181.4
T_6 [K]	460.0	136.0
R_{ITR}^{I} [m^{2}K/W]	$5.78{\cdot}10^{-10}$	$8.46{\cdot}10^{-10}$
R_{ITR}^{II} [m^{2}K/W]	$5.95{\cdot}10^{-10}$	$5.33{\cdot}10^{-10}$
R_{ITR}^{III} [m^{2}K/W]	$6.08{\cdot}10^{-11}$	$6.18{\cdot}10^{-10}$
R_{ITR}^{IV} [m^{2}K/W]	$5.44{\cdot}10^{-11}$	$6.18{\cdot}10^{-10}$
R_{ITR}^{V} [m^{2}K/W]	$4.07{\cdot}10^{-11}$	$5.20{\cdot}10^{-10}$