Supporting Information

Thermal Conductivity of Polyacrylamide Hydrogel at Nanoscale

Shuai Xu[†,‡], *Shengqiang Cai*[‡] *and Zishun Liu*[*,†]

[†] Inter. Center for Applied Mechanics, State Key Laboratory for Strength and Vibration of Mechanical Structures, Xi'an Jiaotong University, Xi'an, 710049, China

[‡] Mechanical and Aerospace Engineering, University of California, San Diego, CA La Jolla 92093, USA

*Corresponding author: Email: zishunliu@mail.xjtu.edu.cn

In all of the simulations, CVFF force field is adopted:

$$U(r_{ij},\theta_{ijk},\varphi_{ijkl}) = K_1(r-r_0)^2 + K_2(\theta-\theta_0)^2 + K_3[1+dcos(n\varphi)] + 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \frac{Cq_iq_j}{\epsilon r} \quad (1)$$

where K_1 and r_0 are the parameters for the Harmonic bond potential; K_2 and θ_0 are the parameters for the Harmonic angle potential; K_3, d and n are the parameters for the Harmonic torsion parameters; The nonbonded parameters ε, σ, q_i and q_j are for the LJ and Coulombic interactions. C and ϵ are energy-conversion constant and dielectric constant, respectivily. These parameters are given in Table S1-S4:

Table S1. Bond parameters

Bond	K_l [Kcal*mol^{-1}*Å^2]	r_0 [Å]
c2-c1	322.7158	1.526
c2-h	340.6175	1.105
c2-c2	322.7158	1.526
c1-c'	283.0924	1.52
c1-h	340.6175	1.105
c'-o'	615.322	1.23
c'-n2	388	1.32
n2-hn	457.4592	1.026
c1-c1	322.7158	1.526
c1-c3	322.7158	1.526
h-c3	340.6175	1.105
c2-c'	283.0924	1.52
c2-c3	322.7158	1.526
c'-n	388	1.32
c2-n	377.5752	1.46
hn-n	483.4512	1.026
o*-h*	540.6336	0.96

Table S2. Angle parameters

Angle	K_2 [Kcal*mol^{-1}*radian^{-2}]	θ_0 [degree]
c1-c2-h	44.4	110
c2-c2-c1	46.6	110.5
h-c2-h	39.5	106.4
c2-c2-h	44.4	110
c2-c1-c'	46.6	110.5
c2-c1-h	44.4	110
c2-c1-c2	46.6	110.5
c'-c1-h	45	109.5
c1-c'-o'	68	120
c1-c'-n2	53.5	114.1
o'-c'-n2	68	120
c'-n2-hn	37.5	115
hn-n2-hn	33	125
c2-c1-c1	46.6	110.5
c1-c1-c'	46.6	110.5
c1-c1-h	44.4	110
c1-c2-c1	46.6	110.5
c1-c3-h	44.4	110
h-c3-h	39.5	106.4
c'-c1-c3	46.6	110.5
h-c1-c3	44.4	110
c2-c1-c3	46.6	110.5
c2-c2-c2	46.6	110.5
c2-c2-c'	46.6	110.5
c'-c2-h	45	109.5
c2-c'-o'	68	120

c2-c'-n2	53.5	114.1
c1-c1-c3	46.6	110.5
c1-c2-c3	46.6	110.5
h-c2-c3	44.4	110
c2-c3-h	44.4	110
c'-c2-c3	46.6	110.5
c1-c'-n	53.5	114.1
o'-c'-n	68	120
c2-n-c'	111	118
c'-n-hn	37.5	115
c2-n-hn	35	122
h-c2-n	51.5	109.5
c2-c'-n	53.5	114.1
h*-o*-h*	50	104.5

Table S3. Torsion parameters

Torsion	K3 [Kcal*mol^{-1}]	d	n
h-c2-c1-c'	0.1581	1	3
h-c2-c1-h	0.1581	1	3
h-c2-c1-c2	0.1581	1	3
c2-c2-c1-c'	0.1581	1	3
c2-c2-c1-h	0.1581	1	3
c2-c2-c1-c2	0.1581	1	3
c1-c2-c2-c1	0.1581	1	3
c1-c2-c2-h	0.1581	1	3
h-c2-c2-h	0.1581	1	3
c1-c2-c1-c2	0.1581	1	3
c1-c2-c1-c'	0.1581	1	3
c1-c2-c1-h	0.1581	1	3

c1-c'-n2-hn	1.5	-1	2
o'-c'-n2-hn	1.5	-1	2
h-c2-c1-c1	0.1581	1	3
c2-c2-c1-c1	0.1581	1	3
c2-c1-c1-c2	0.1581	1	3
c2-c1-c1-c'	0.1581	1	3
c2-c1-c1-h	0.1581	1	3
c'-c1-c1-c'	0.1581	1	3
c'-c1-c1-h	0.1581	1	3
h-c1-c1-h	0.1581	1	3
c1-c2-c1-c1	0.1581	1	3
c2-c2-c2-c1	0.1581	1	3
c2-c2-c2-h	0.1581	1	3
c'-c1-c3-h	0.1581	1	3
h-c1-c3-h	0.1581	1	3
c2-c1-c3-h	0.1581	1	3
c1-c2-c1-c3	0.1581	1	3
h-c2-c1-c3	0.1581	1	3
c'-c2-c2-h	0.1581	1	3
c2-c2-c2-c'	0.1581	1	3
c2-c'-n2-hn	1.5	-1	2
c2-c2-c2-c2	0.1581	1	3
c1-c2-c2-c'	0.1581	1	3
c2-c2-c1-c3	0.1581	1	3
c1-c1-c3-h	0.1581	1	3
c2-c1-c1-c3	0.1581	1	3
c'-c1-c1-c3	0.1581	1	3
h-c1-c1-c3	0.1581	1	3
c3-c2-c1-c'	0.1581	1	3

c3-c2-c1-h	0.1581	1	3
c3-c2-c1-c2	0.1581	1	3
c1-c2-c3-h	0.1581	1	3
h-c2-c3-h	0.1581	1	3
c'-c2-c3-h	0.1581	1	3
c1-c'-n-c2	3.2	-1	2
c1-c'-n-hn	1.2	-1	2
o'-c'-n-c2	3.8	-1	2
o'-c'-n-hn	1.8	-1	2
c2-c'-n-c2	3.2	-1	2
c2-c'-n-hn	1.2	-1	2

Table S4. Nonbonded parameters

Atoms	ε [Kcal/mol]	σ [Å]	Charge [multiple of electron charge]
c2	0.039	3.875409	-0.2
c1	0.039	3.875409	-0.1
c'	0.148	3.617049	0.38
h	0.038	2.449971	0.1
o'	0.228	2.859785	-0.38
n2	0.167	3.501232	-0.56
hn	0	0	0.28
c3	0.039	3.875409	-0.3
n	0.167	3.501232	-0.5
o*	0.155416	3.16552	-0.82
h*	0	0	0.41

In this paper, we investigated the temperature profile of 3 interface models to calculate the equivalent conductivity of interface. One profile is displayed in the paper in Figure 6d, while the other two are displayed below in Figure S1.

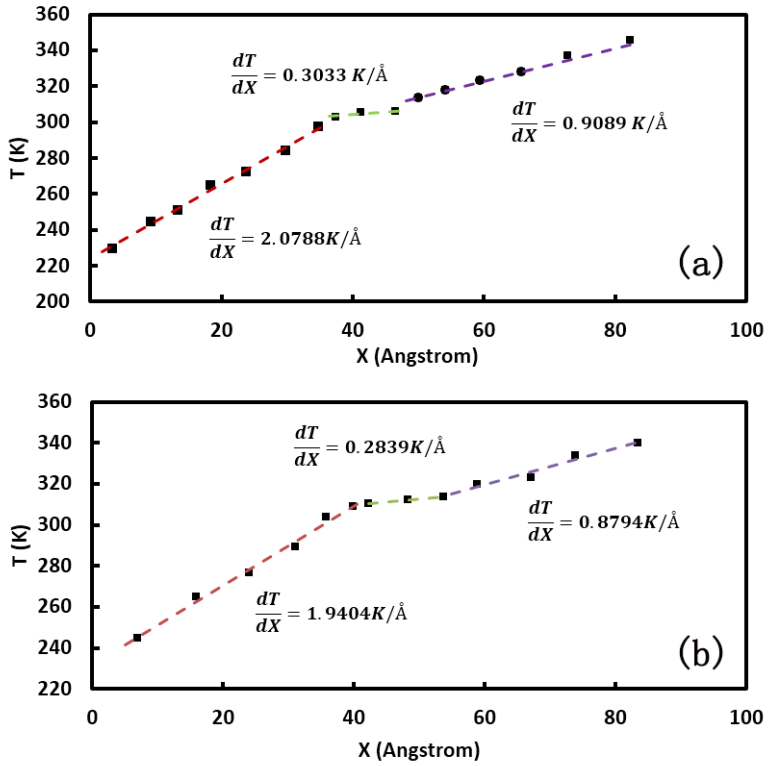

Figure S1. (a) The temperature profile of the second interface model. (b) The temperature profile of the third interface model.

The average equivalent conductivity of interface calculated by these three models is 2.0139 ± 0.0414 W m^{-1} K^{-1}.

At every water volume fractions, the fractions of polymer (V-poly), interface (V-inter) and free water (V-free) are listed below.

Table S5. Volume fractions of polymer, interface and free water

Water fraction (%)	V-poly (%)	V-inter (%)	V-free (%)
9.24	90.76	9.24	0
20.36	79.64	20.36	0
34.97	65.03	34.05	0.92
46.42	53.58	42.89	3.53
56.35	43.65	46.73	9.62
64.98	35.02	48.74	16.24
76.70	23.30	51.04	25.66
84.44	15.56	47.07	37.37
90.24	9.76	21.71	68.53