Supporting Information


Gas Diffusion, Energy Transport, and Thermal Accommodation in Single-Walled Carbon Nanotube Aerogels

Scott N. Schiffres, Kyu Hun Kim, Lin Hu, Alan J. H. McGaughey, Mohammad F. Islam, and Jonathan A. Malen*
Supporting Information

Gas diffusion, energy transport, and thermal accommodation in single-walled carbon nanotube aerogels

Scott N. Schiffres,1 Kyu Hun Kim,2 Lin Hu,1 Alan J. H. McGaughey,1 Mohammad F. Islam,2

Jonathan A. Malen*1,2

a)

b)
**Figure S1.** Results of SWCNT nitrogen adsorption isotherms and BET derived specific pore diameters. (a) Nitrogen adsorption isotherms. (b) This specific pore volume versus pore diameter plot shows that the aerogel contains predominantly mesopores (2-50 nm diameter).

![Nitrogen adsorption isotherms and BET derived specific pore diameters](image)

**Figure S2.** (a) Near-infrared fluorescence spectra from a dispersion recreated from SWCNT aerogels with *deoxycholic acid (DOC)* indicating that SWCNTs remain intact during the synthesis of SWCNT aerogels. The color bar indicates emission intensity in arbitrary units. (b) Raman spectra from pristine SWCNT aerogels (top, red) and SG76 powder (bottom, black). RBMs of the Raman spectra and the similar peak intensity ratios of D to G bands, $I_{D,aerogel}/I_{G,aerogel}=0.120$ and $I_{D,powder}/I_{G,powder}=0.128$, suggest that SWCNTs remain undamaged by the SWCNT aerogel synthesis.
Figure S3. An energy dispersive spectroscopy (EDX) spectra from the SWCNT aerogel shows no peak for sodium (Na) and a small peak for Sulfur (S), which are chemical components of SDBS surfactant. These results indicate that the SDBS surfactant was completely removed, and thus, the aerogel is free of surfactant. Note that the quantitative value for sulfur (0.5 wt%) is below the 1% quantitative analysis limit of EDX.
**Figure S4.** Plot of effective total thermal conductivity for sample 2 versus gas pressure. Fits to kinetic theory model (eq 5) are indicated with solid lines.
Table S1. 12-6 Lennard-Jones parameters used in the MD simulations for predicting the accommodation coefficients.

<table>
<thead>
<tr>
<th></th>
<th>$\sigma$ (Å)</th>
<th>$\varepsilon$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-C$^1$</td>
<td>3.4</td>
<td>2.4</td>
</tr>
<tr>
<td>Ar-Ar$^1$</td>
<td>3.4</td>
<td>10.61</td>
</tr>
<tr>
<td>Ne-Ne$^1$</td>
<td>2.75</td>
<td>3.07</td>
</tr>
<tr>
<td>He-He$^2$</td>
<td>2.56</td>
<td>0.88</td>
</tr>
</tbody>
</table>


Mixing rules for LJ parameters: $\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$, $\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}}$
Alternative Derivation Relating $r_s$, $r_e$, and $\alpha$

As an alternative to the recursive derivation presented in the main text, the relationship between $r_e$, $r_s$, and $\alpha$ can be derived by taking $r_e$ to be a sum that captures the total distance traveled by the energy of one molecule.

The contribution to $r_e$ from the first collision with the solid is

$$ar_s,$$  

(S1)

from the second collision is

$$\alpha(1 - \alpha)2r_s,$$  

(S2)

and from the $n^{th}$ collision is

$$\alpha(1 - \alpha)^{n-1}nr_s.$$  

(S3)

Combining these gives

$$r_e = ar_s + \alpha(1 - \alpha)2r_s + ... + \alpha(1 - \alpha)^{n-1}nr_s.$$  

(S4)

We are interested in the limit of $n \to \infty$, where

$$\lim_{n \to \infty} \frac{r_e}{r_s} = \frac{1}{\alpha}.$$  

(S5)

This result is the same as eq 9.