Electronic Supplementary Information: Coordination Number Model to Quantify Packing Morphology of Aligned Nanowire Arrays

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§ NECSTlab

Table S1 Triangle areas, and volume fractions for all coordinations.

<table>
<thead>
<tr>
<th>N</th>
<th>$A_{\triangle,N}(P_N)$</th>
<th>$V_{f,N}(D,P_N)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$\frac{\sqrt{3}}{4} P_N^2$</td>
<td>$\frac{\sqrt{3}\pi}{6} \left( \frac{D}{P_N} \right)^2$</td>
</tr>
<tr>
<td>4</td>
<td>$\frac{1}{4} P_N^2$</td>
<td>$\frac{\pi}{4} \left( \frac{D}{P_N} \right)^2$</td>
</tr>
<tr>
<td>5</td>
<td>$\cos \left( \frac{3\pi}{10} \right) \sin \left( \frac{3\pi}{10} \right) P_N^2$</td>
<td>$\frac{\pi}{8 \cos \left( \frac{3\pi}{10} \right) \sin \left( \frac{3\pi}{10} \right)} \left( \frac{D}{P_N} \right)^2$</td>
</tr>
<tr>
<td>6</td>
<td>$\frac{\sqrt{3}}{4} P_N^2$</td>
<td>$\frac{\sqrt{3}\pi}{6} \cos \left( \frac{3\pi}{10} \right) \sin \left( \frac{3\pi}{10} \right) \left( \frac{D}{P_N} \right)^2$</td>
</tr>
</tbody>
</table>

Fig. S1 Illustration of component triangles for each coordination at the maximum theoretical volume fractions (wire walls are touching). Since the unit cell inter-wire spacing, $S_N$, is zero in this case, $P_N$, is equal to the wire diameter, $D$, in all coordinations.
Table S2  Lattice constant, Chi parameter, and average inter-wire spacing for all coordinations.

<table>
<thead>
<tr>
<th>( N )</th>
<th>( a_N(D, V_f) )</th>
<th>( \chi_N )</th>
<th>( \Gamma_N(D, V_f) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>( \sqrt{3}D\left(\sqrt{\frac{V_{\text{max}}}{V_f}}\right) )</td>
<td>( \sqrt{3} )</td>
<td>( D\left(\sqrt{\frac{\sqrt{3}+1}{2}}\sqrt{\frac{V_{\text{max}}}{V_f}}-1\right) )</td>
</tr>
<tr>
<td>4</td>
<td>( \sqrt{2}D\left(\sqrt{\frac{V_{\text{max}}}{V_f}}\right) )</td>
<td>( \sqrt{2} )</td>
<td>( D\left(\sqrt{\frac{\sqrt{2}+1}{2}}\sqrt{\frac{V_{\text{max}}}{V_f}}-1\right) )</td>
</tr>
<tr>
<td>5</td>
<td>( 2\cos\left(\frac{3\pi}{10}\right)D\left(\sqrt{\frac{V_{\text{max}}}{V_f}}\right) )</td>
<td>( 2\cos\left(\frac{3\pi}{10}\right) )</td>
<td>( D\left(\sqrt{\frac{2\cos\left(\frac{3\pi}{10}\right)+1}{2}}\sqrt{\frac{V_{\text{max}}}{V_f}}-1\right) )</td>
</tr>
<tr>
<td>6</td>
<td>( D\left(\sqrt{\frac{V_{\text{max}}}{V_f}}\right) )</td>
<td>1</td>
<td>( D\left(\sqrt{\frac{V_{\text{max}}}{V_f}}-1\right) )</td>
</tr>
</tbody>
</table>

Table S3  Deviation factor for all coordinations.

<table>
<thead>
<tr>
<th>( N )</th>
<th>( \delta_N(D, V_f) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>( \frac{\sqrt{3}+1}{2} )</td>
</tr>
<tr>
<td>4</td>
<td>( \sqrt{\frac{3}{2}}\left(\frac{\sqrt{2}+1}{2}\right) )</td>
</tr>
<tr>
<td>5</td>
<td>( \sqrt{3}\left(\frac{2\cos\left(\frac{3\pi}{10}\right)+1}{2}\right) )</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
</tr>
</tbody>
</table>
Fig. S2 Plot of the deviation factor from hexagonal packing, $\delta_N$, as a function of nanowire coordination number, $N$, using the functional form given in Eq. 8.
Final form of the average inter-wire spacing equation for $3 \leq N \leq 6$:

$$\Gamma_N(D, V_f) = D \left( (11.77(N)^{-3.042} + 0.9496) \sqrt{\frac{0.9069}{V_f}} - 1 \right)$$  \hfill (S1)

Correction equation for average inter-wire spacings extracted from HRSEM micrographs:

$$\Gamma_N(D, V_f) = \frac{\Gamma_{SEEN}^N}{\cos\left(\arctan\left(\frac{\ell_{SEEM}}{\Gamma_{SEEM}^N}\right)\right)}$$  \hfill (S2)

**Fig. S3** HRSEM micrograph for a 1.0 volume % CNT forest with lines drawn perpendicular to the CNT primary axis. The average inter-CNT spacing in the forest was then determined by counting only the bright in-focus CNTs underneath each line.