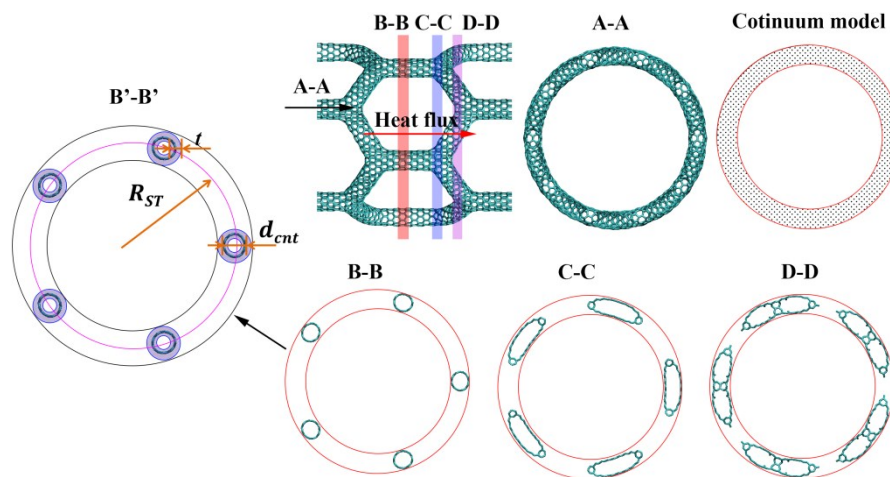# Supplementary Information

Carbon Nanotube-based Super Nanotube: Tailorable Thermal Conductivity at Three-dimensional

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S1. Schematic view of the ST's cross-section.

Above figure clearly shows that the cross-section of the ST changes along the heat flux direction (the B-B, C-C and D-D view of the cross-section). Due to the highly porous nature of the structure, it is hard to get an exact cross-sectional area. Therefore, current work adopted a continuum model to estimate the cross-sectional area, which will greatly increase the cross-sectional. Although such approximation will lead to an extremely small thermal conductivity value, it will not influence the discussions as we focus on the relative thermal conductivity of various ST.

A simple example is given to show how the estimation of the cross-sectional area will impact the calculated thermal conductivity. As illustrated in the B'-B' view, suppose that the constituent CNT has a thickness $t = 0.34\ nm$, then the cross-sectional area of the continuum and discrete (B'-B') model can be estimated as $A1 = 2\pi R_{ST}(d_{cnt} + t)$,

$$A_r = \frac{A1}{A2} = \frac{2R_{ST}(d_{cnt} + t)}{5d_{cnt}t}$$

and $A2 = 5\pi d_{cnt}t$, respectively. Thus, we have . Recall the ST(5,0)@(8,0)-γ model with $2R_{ST}\sim 6\ nm$, $d_{cnt}\sim 0.63\ nm$, A_r is estimated around 5.4. In other words, the absolute thermal conductivity would be 5.4 larger if we adopt the discrete (B'-B') model to estimate the cross-sectional area. It is evident from such

approximation that larger ST's radius will lead to bigger difference for the estimated thermal conductivity between the continuum model and the discrete model (B'-B').

S2. Atomic configurations of the junction units ST(6,0)@(6,6)-a and ST(6,0)@(6,6)-b.

(a)   (b)
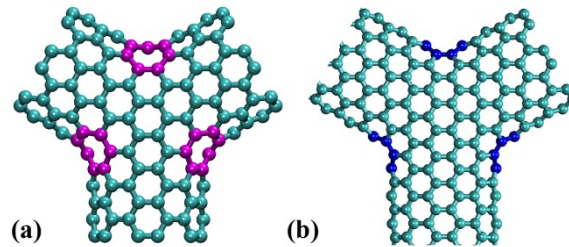
S3. Stress-strain curves of the ST under tension (T) and compression (C) using different potential cut-off distances.
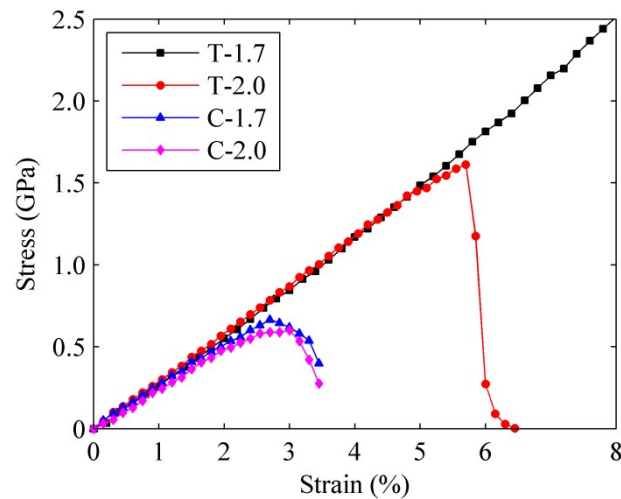
To examine the strain influence, the ST was elongated along length direction under a constant strain rate of 0.0002 ps^{-1}. To notice that the original AIREBO potential would result in spuriously high tensile force when the C-C bonds are stretched beyond 1.7 Å. Researchers have suggested that a 2.0 Å cutoff distance can be chosen to overcome such abnormal phenomenon.[1] As compared in above figure, the chosen of different cutoff distance will not alter the elastic deformation of the ST, and the emphasis of this paper is the impacts from the elastic strain. Thus, the original cutoff distance of 1.7 Å is chosen to achieve a pre-strained structure for the consistency with the thermal conductivity calculation.

References:
(1)   Shenderova, O. A.; Brenner, D. W.; Omeltchenko, A.; Su, X.; Yang, L. H., Atomistic Modeling of the Fracture of Polycrystalline Diamond. *Phys. Rev. B* **2000,** *61*, 3877-3888.