## **Supporting Information**

## Mechanical and thermal properties of carbon nanotubes in carbon nanotube fibers under tension-torsion loading

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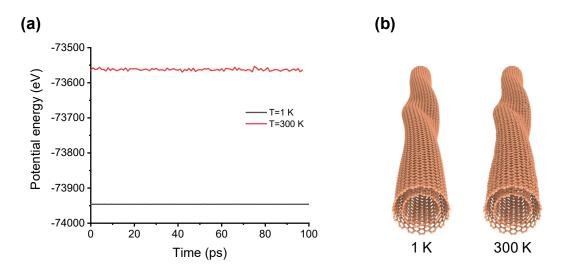
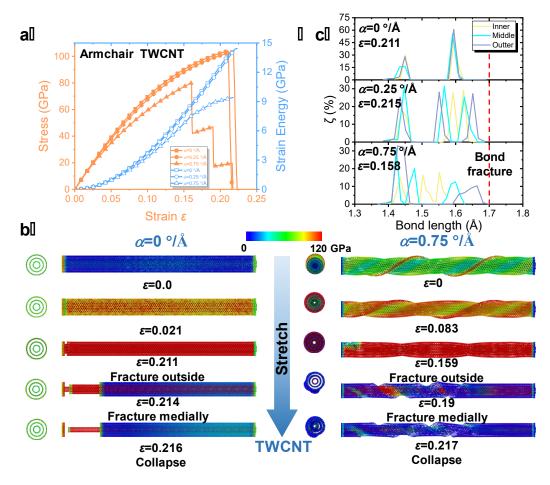


Figure S1 (a) Potential energy of representative DWCNT with  $\alpha$ =0.25 °/Å during relaxation process; (b) Snapshots of fully relaxed DWCNT under temperature 1 K and 300 K.



**Figure S2.** (a) Stress and strain energy versus strain curves of TWCNT; (b) Snapshot of tensile process of TWCNT under  $\alpha$ =0 °/Å and  $\alpha$ =0.75 °/Å, atoms are colored by von mises stress; (c) The corresponding diagram of different bond length distribution of TWCNT in (a).