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Supplementary Information for Torsional Fracture of Carbon Nanotube Bundles: A Reactive Molecular Dynamics Study

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I. STRESS ANALYSIS

To shear stress in CNTBs during the torsional loading can be analyzed by calculating the von Mises stress σ^k_{vMS} [1]. Importantly, the σ^k_{vMS} values provide useful information on the fracture dynamics from the starting twisting regime up to complete structural failure (fracture) of the CNTB. Also, they allow identifying the point from which the fracture starts. In this way, for each k-atom of the system, σ^k_{vMS} is given by

$$\sigma^k_{\text{vMS}} = \sqrt{\frac{(\sigma_{xx}-\sigma_{yy})^2 + (\sigma_{xx}-\sigma_{zz})^2 + (\sigma_{yy}-\sigma_{zz})^2 + 6\cdot\left(\sigma^2_{xy}+\sigma^2_{xz}+\sigma^2_{yz}\right)}{2}}, \tag{1}$$

where σ_{ij}, when $i = j$, corresponds to the uniaxial stress tensor components. When $i \neq j$, σ_{ij} corresponds to the shear stress tensor components. Each virial strees component [2] is given by

$$\sigma_{ij} = \frac{1}{V}\sum_{k}^{N}\left(m_k \cdot v_{k_i} \cdot v_{k_j}\right) + \frac{1}{V}\sum_{k}^{N}\left(r_{k_i} \cdot f_{k_j}\right), \tag{2}$$

where N is the number of atoms, V is the total system volume, and m_k, v_k, r_k, and f_k represent the mass, velocity, position, and force of k-atom, respectively. Below, we present the σ^k_{vMS} distribution for the cases presented in Figures 2 and 3 of the main text.

Figure S1 shows representative MD snapshots for the twisting process of a CNTB formed with CNTs(3,3) at 300 (referred to as CNTB@CNT(3,3) in our work) with the von Mises stress distribution. We analyzed this case in Figure 2 of the main text. Figure S1 illustrates the MD simulation for the CNTB@CNT(3,3) subjected to a twisting angle or cycle (cyc.) of (a) 0° or 0 cycle, (b) 360° or 1 cycle, (c) 720° or 2 cycles, (d) 1005° or 2.8 cycles, (e) 1260° or 3.5 cycles, and (f) 1440° or 4 cycles. In the color scheme of this figure, the blue and red colors denote the regions with low and high accumulation of stress, respectively. Figure S1(a) shows the structure equilibrated at 300 with no stress accumulation (blue color). After one twisting cycle (Figure S1(b)), one can note that the CNTB starts to accumulate a considerable amount of stress and the blue regions vanish almost completely (white and red colors dominate). The blue regions in the edges are the fixed atoms used for twisting the CNTB. Figure

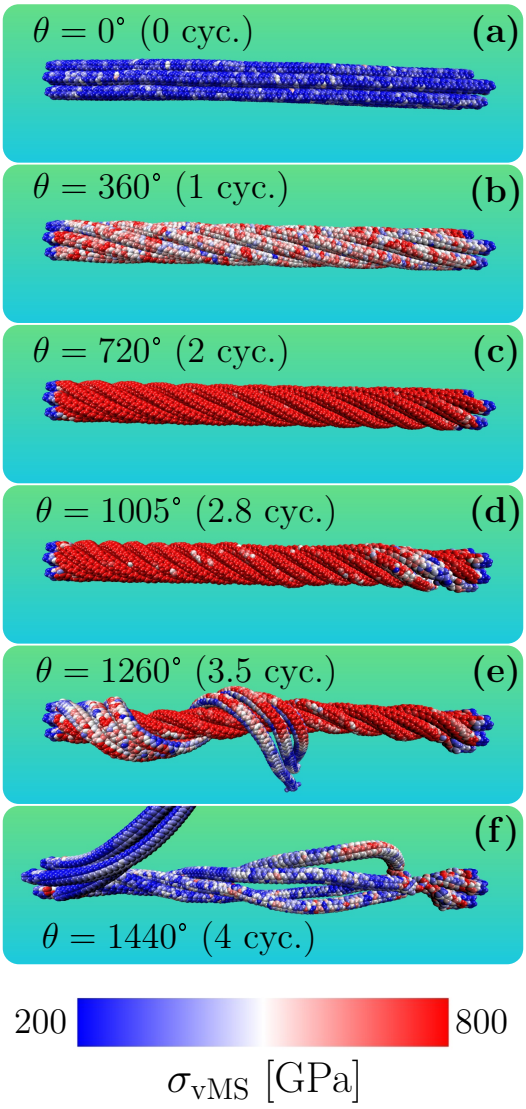

FIG. S1. von Mises stress distribution for the representative MD snapshots presented in Figure 2 of the main text. This figure illustrates the MD simulation for the CNTB@CNT(3,3) case at 300 K.

S1(c) shows that the von Mises stress is more uniformly distributed (or accumulated) for high values (red color). In 2.8 cycles, the stress accumulation in the CNTB structure reaches its critical value, and one of the nanotubes is fractured nearby the right edge (see Figure S1(d)), triggering the fracture process of the CNTB. After this moment, part of the fractured nanotube releases the accumulated stress, and one can note the appearance of white/blue regions. A similar fracture process occurs for other nanotubes in the CNTB structure (see Figure S1(e)). Finally, in 3.5 cycles (as shown in Figure S1(f)), large cross-section deformations take place, and the tubes remaining in the bundle collapse into a single structure that forms a defective region, i.e., the diamondoid structure. This collapsed structure

can not play the role of accumulating stress, and low-stress regions represented in blue dominate the CNTB structure.

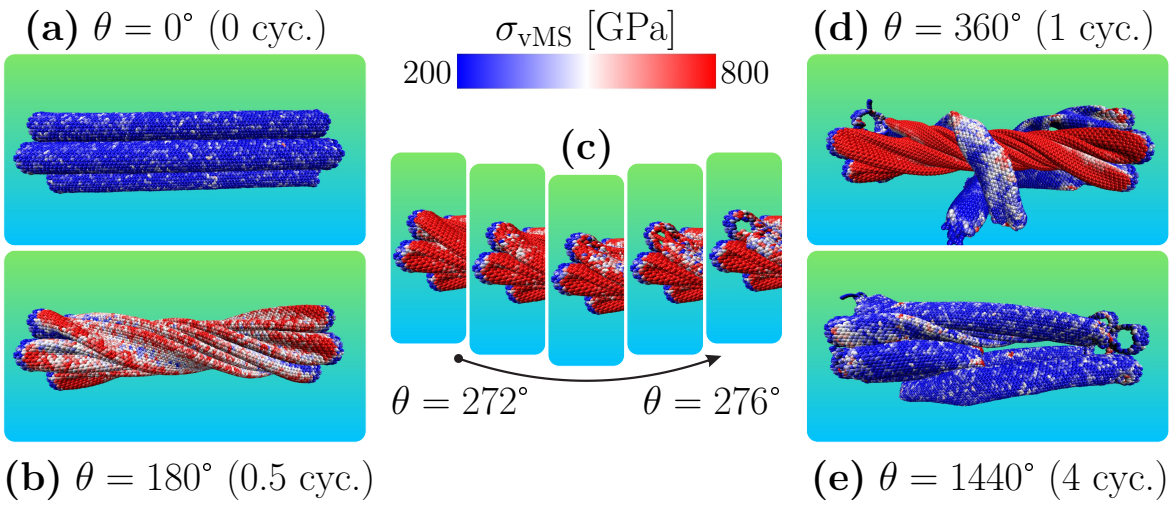

FIG. S2. von Mises stress distribution for the representative MD snapshots presented in Figure 3 of the main text. This figure illustrates the MD simulation for the CNTB@CNT(14,14) case at 300 K.

We also show the representative MD snapshots for the twisting process of a CNTB formed with CNTs(14,14) at 300 K (referred to as CNTB@CNT(14,14) in our work) with the von Mises stress distribution. We analyzed this case in Figure 3 of the main text. In this way, Figure S2 illustrates the MD simulation for the CNTB@CNT(14,14) subjected to a twisting angle or cycle (cyc.) of (a) 0° or 0 cycle, (b) 180° or 0.5 cycle, (c) between 272° and 276°, (d) 360° or 1 cycle, and (e) 1440° or 4 cycles. In the color scheme of this figure, the blue and red colors denote the regions with low and high accumulation of stress, respectively. Figure S2(a) shows the structure equilibrated at 300 with no stress accumulation (blue color). In the 0.5 twisting cycles (Figure S2(b)), the CNTB starts to accumulate stress, and the blue regions vanish almost completely (white and red colors dominate). This process occurs in the same fashion in CNTBs formed with nanotubes with smaller diameters (see Figure S1(b)). The first difference in the torsion process of CNTB@CNT(14,14), when contrasted with the CNTB@CNT(3,3) case, is presented in Figures S2(b) and S2(c). In Figure S2(c), one can note that $\theta = 274°$ is the critical twisting angle for realizing the first fracture point of the CNTB@CNT(14,14). The fracture process and the von Mises stress distribution in a nanotube that compose the CNTB@CNT(14,14) are similar to the CNTB@CNT(3,3) case. Another difference between the torsional process of CNTB@CNT(3,3) and CNTB@CNT(14,14) can be noted by contrasting their final structures, as presented in Figures S1(f) and S2(e), respectively. In the torsional dynamics of CNTB@CNT(14,14), no collapsed structure

is formed after four cycles, and low-stress regions represented in blue dominate the CNTB structure.

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