Supporting Information for

"Ice Nanoribbons Confined in Uniaxially Distorted Carbon Nanotubes"

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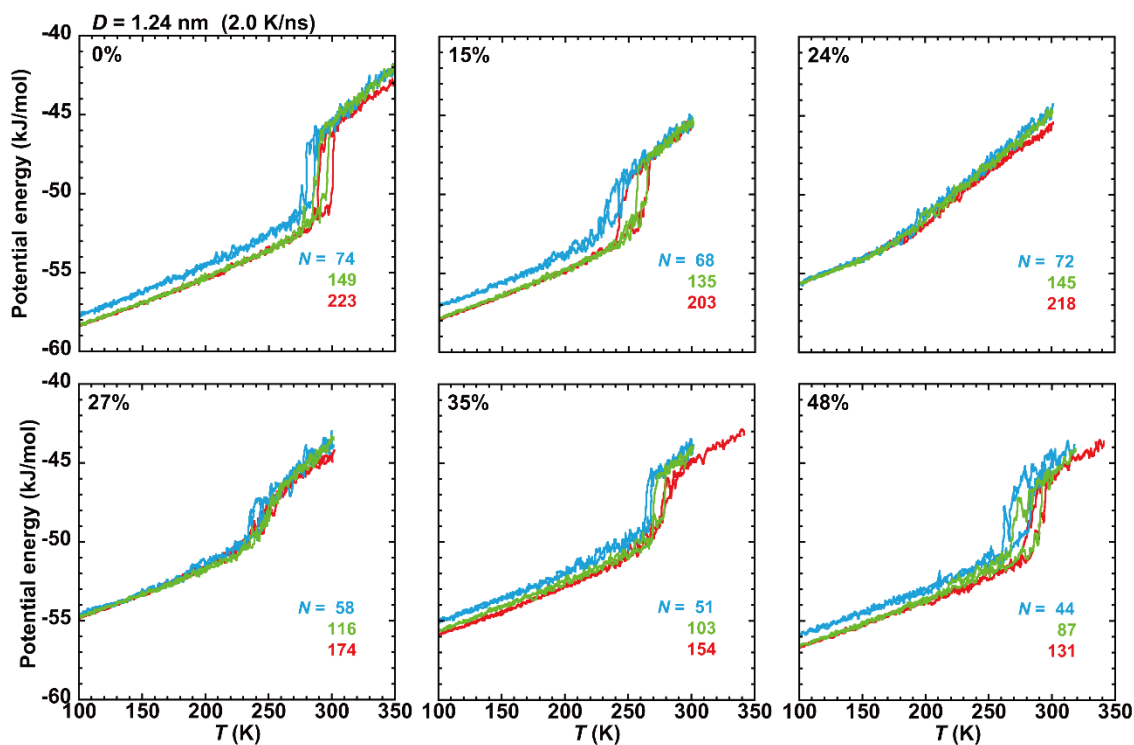
Figure S1. System size dependence of potential energy of water confined in the 1.24 nm SWCNTs with γ = 0, 15, 24, 27, 35, and 48%. N represents the number of water molecules in the system. The length of the SWCNT was fixed. Although a smaller number of water molecules N tends to have a lower transition temperature, essentially the same low-T structures were obtained as shown in Fig. S2.
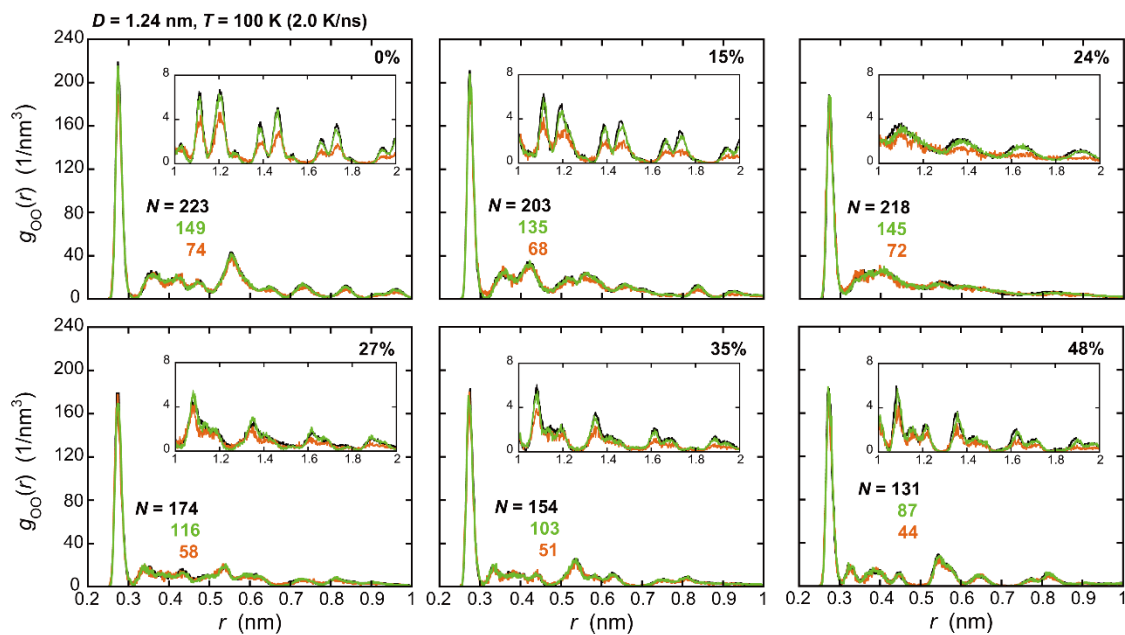
Figure S2. System size dependence of $g_{oo}(r)$ calculated at 100 K of water confined in the 1.24 nm SWCNTs with γ = 0, 15, 24, 27, 35, and 48%. Insets show larger r regions. N represents the number of water molecules in the system. The length of the SWCNT was fixed.
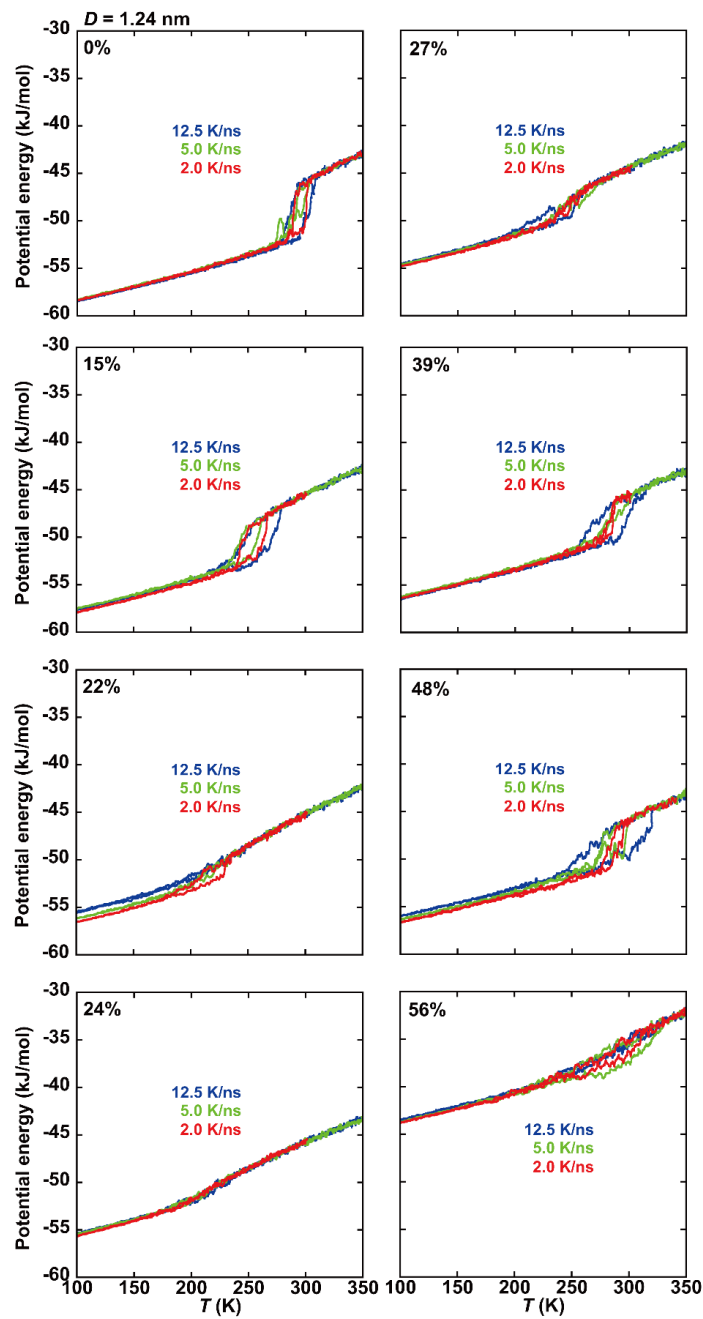
Figure S3. Effects of heating/cooling rates on the potential energy per water molecules in the compressed 1.24 nm SWCNTs with γ = 0, 15, 22, 24, 27, 39, 48, and 56%. The cooling/heating rates were 12.5 K/ns, 5.0 K/ns, and 2.0 K/ns.
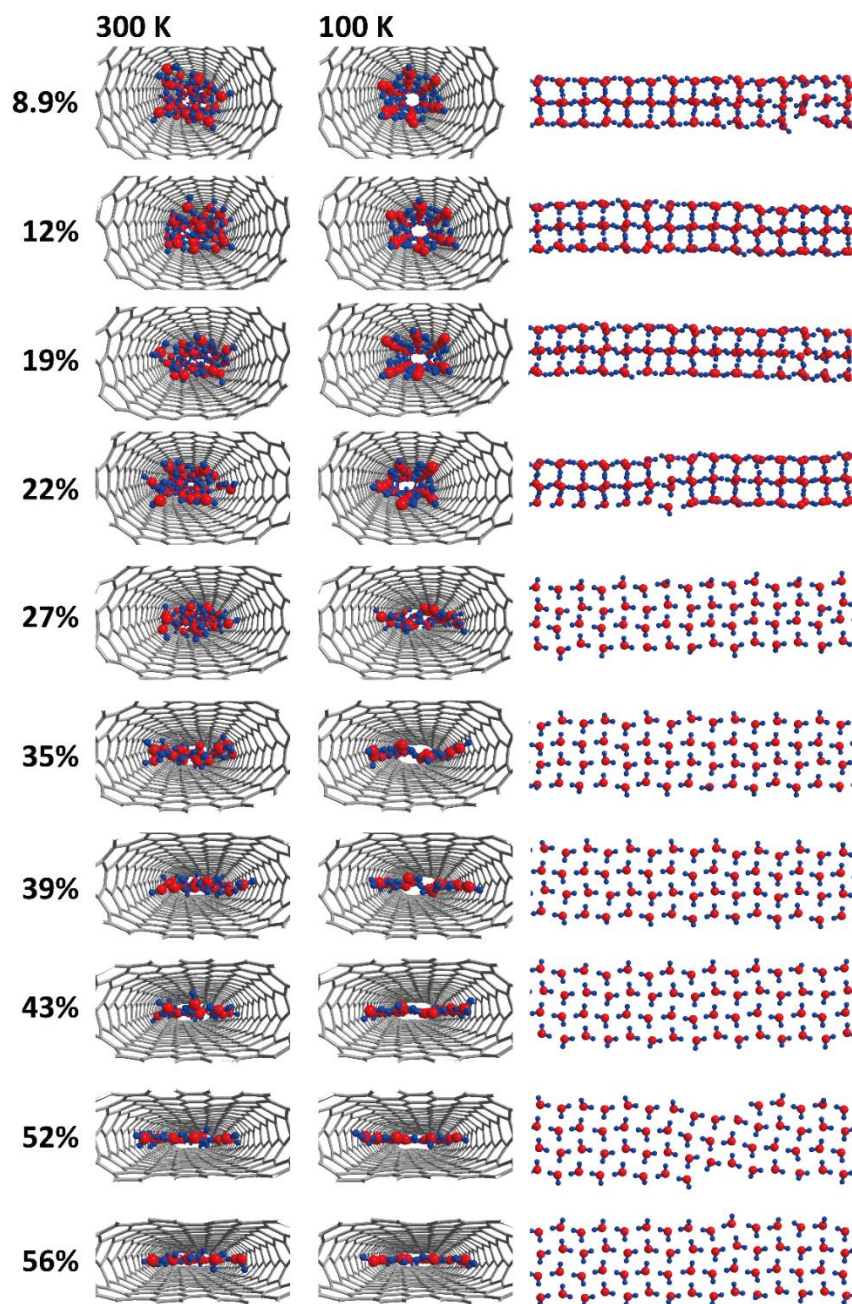
Figure S4. *S*napshot structures at 300 K and 100 K of water confined in the 1.24 nm SWCNTs with γ = 8.9, 12, 19, 22, 27, 35, 39, 43, 52, and 56%. Cooling/heating rates of the simulation were set to 2.0 K/ns.
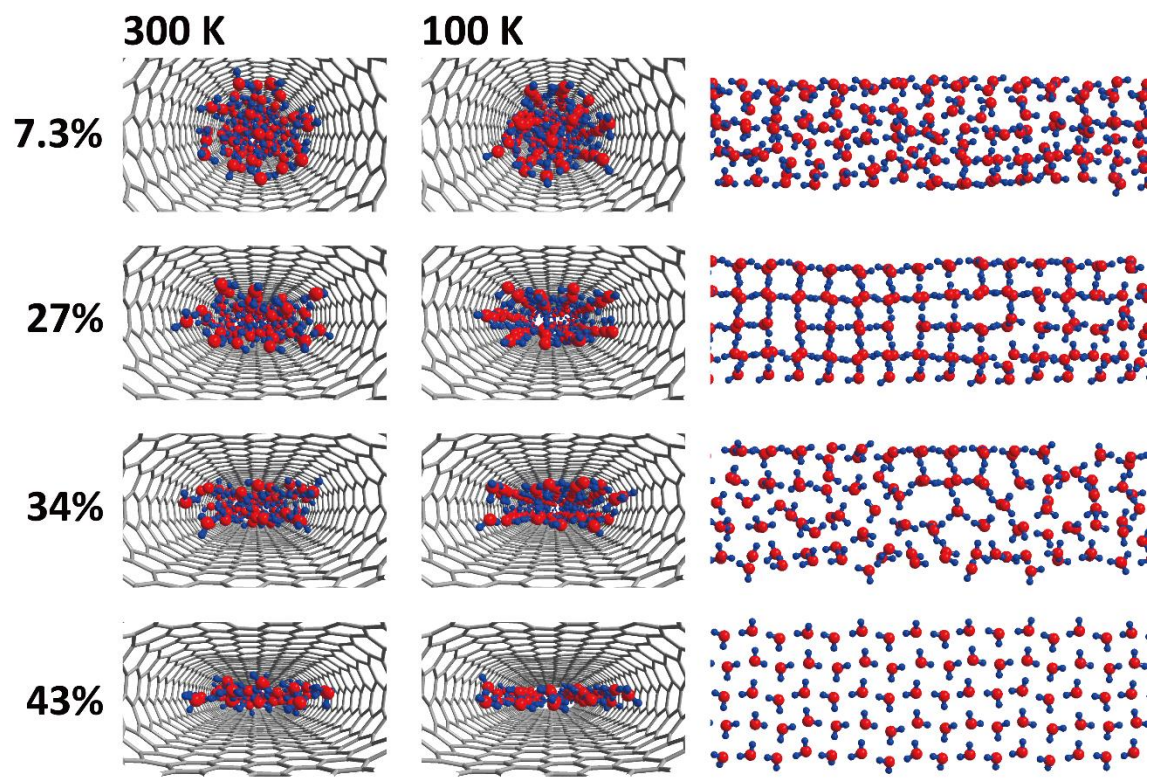
Figure S5. Snapshot structures at 300 K and 100 K of water confined in the 1.51 nm SWCNTs with γ = 7.3, 27, 34, and 43%. Cooling/heating rates of the simulation were set to 2.0 K/ns.
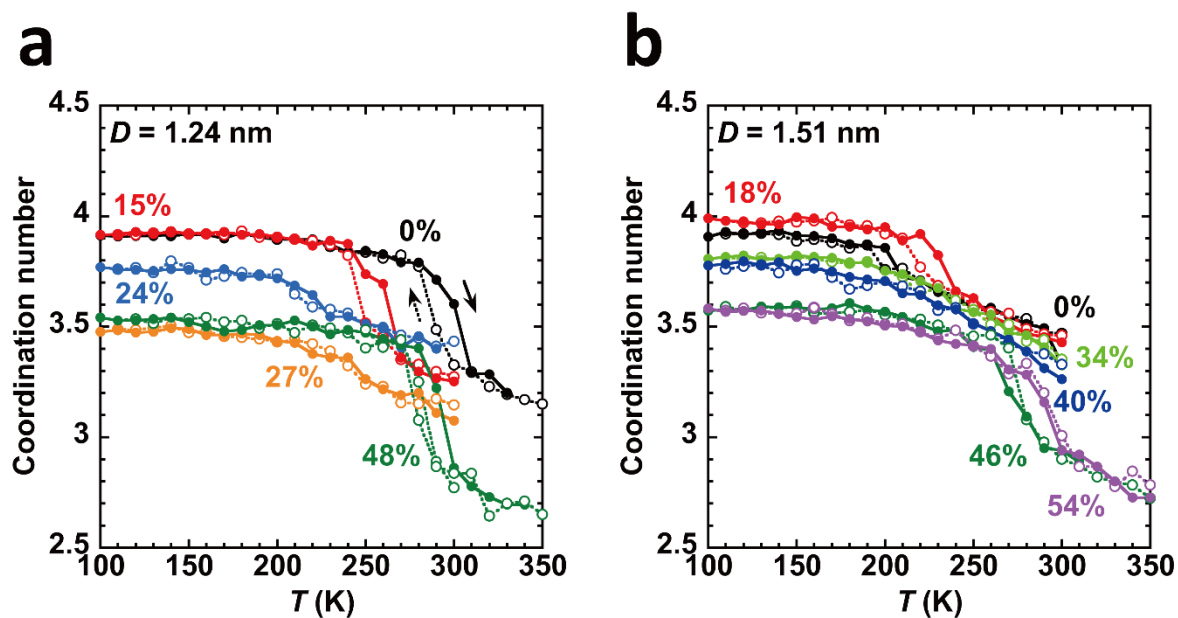
Figure S6. Temperature dependence of coordination numbers of water molecules inside (a) the 1.24 nm SWCNTs and (b) the 1.51 nm SWCNTs. The molecules within the O–O distance of 0.32 nm were taken into account as the coordinated molecules.
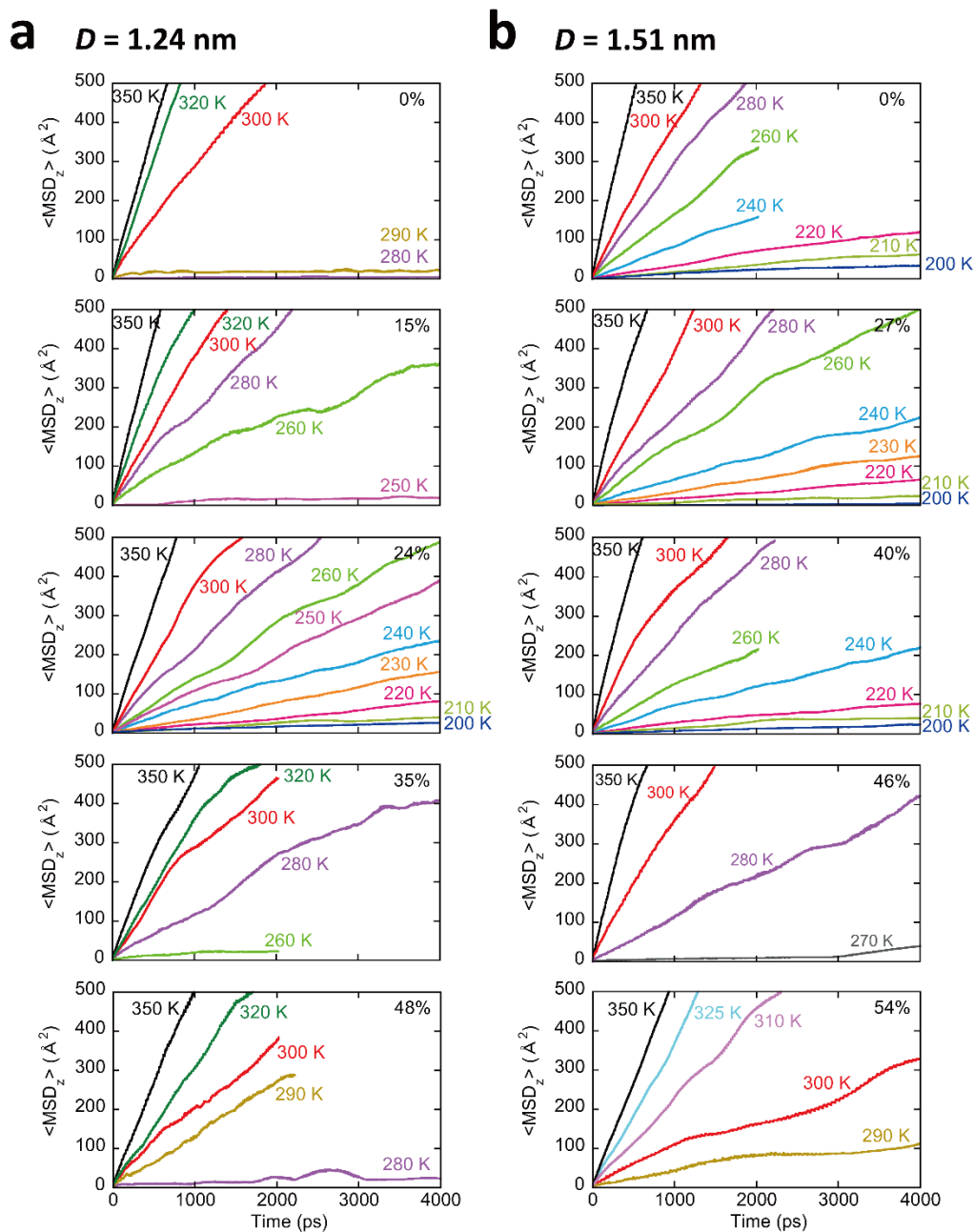
Figure S7. Mean square displacements of oxygen atoms in water along the SWCNT axis, $\langle MSD_z \rangle$, as a function of the elapsed time t for several temperatures in the 1.24 nm SWCNTs and 1.51 nm SWCNTs. Results for $\gamma = 0$, 15, 24, 35, and 48% in the 1.24 nm SWCNTs and for $\gamma = 0$, 27, 40, 48, and 54% in the 1.51 nm SWCNTs are shown from the top to bottom.