Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information for

Insights into the Mechanical Stability of Tetrahydrofuran Hydrates from Experimental, Machine Learning, and Molecular Dynamics Perspectives

Characterizations

X-ray diffraction (XRD) patterns were measured by a Bruker D8 ADVANCE X-ray diffractometer using Cu Kα radiation. The data were collected at ambient temperature from 2θ values between 5.0 and 50.0° at a continuous scan rate of 11.0°/min, with a revolution period of 5 min. As shown in Figure S1, the characteristic peaks of ice at 22.7°, 24.1° and 25.8°, correspond to the (100), (002) and (101) planes. These characteristic peaks sharply decrease in the diffractograms for the M1-3 samples.

The mesoscopic structure of THF hydrates with different ice contents are carried out by X-ray microscope/micrometer microcomputed tomography (CT) equipment which the equipment model is Xradia 610.

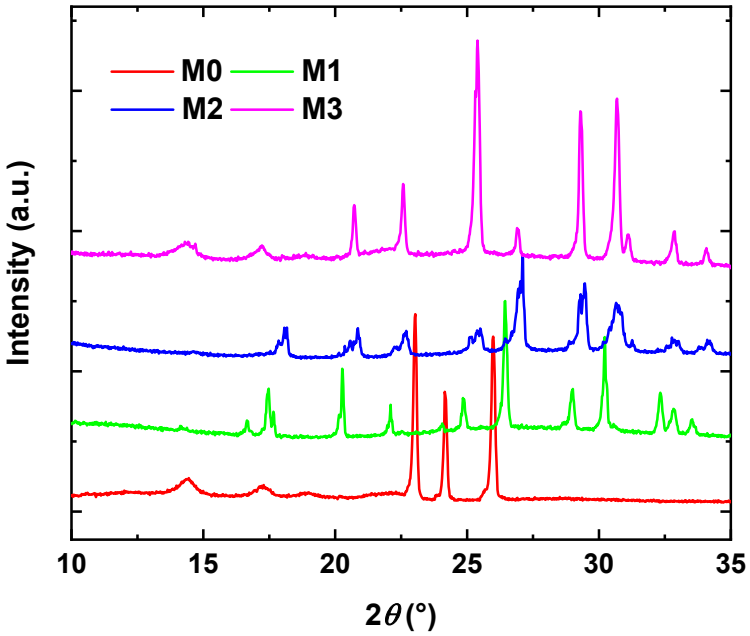

Figure S1 XRD diffracttogram of the M0-3 samples.

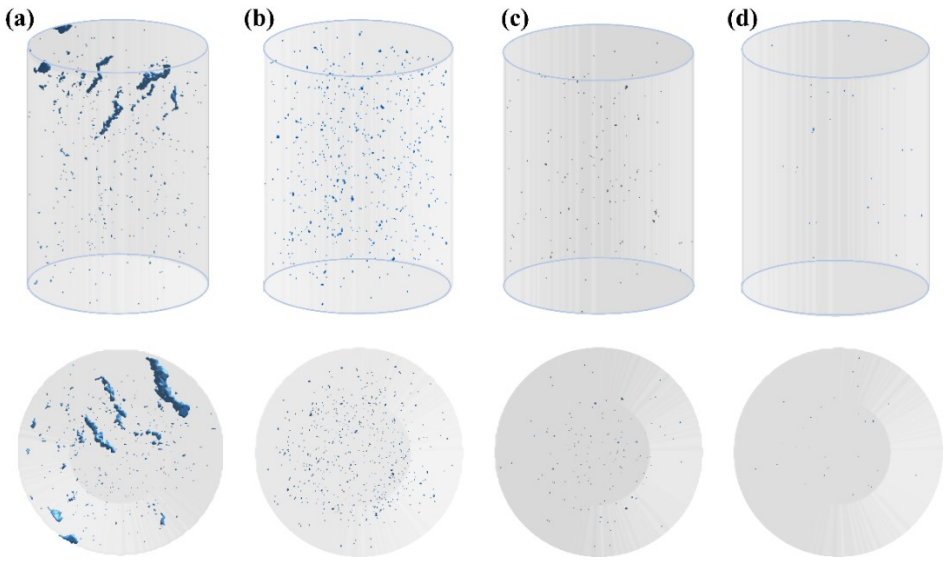

Figure S2 The 3D images of (a) M0, (b) M1, (c) M2 and (d) M3 samples obtained by the computed tomography (CT) technology at -20°C. The pore size of the samples increases with increasing ice content.

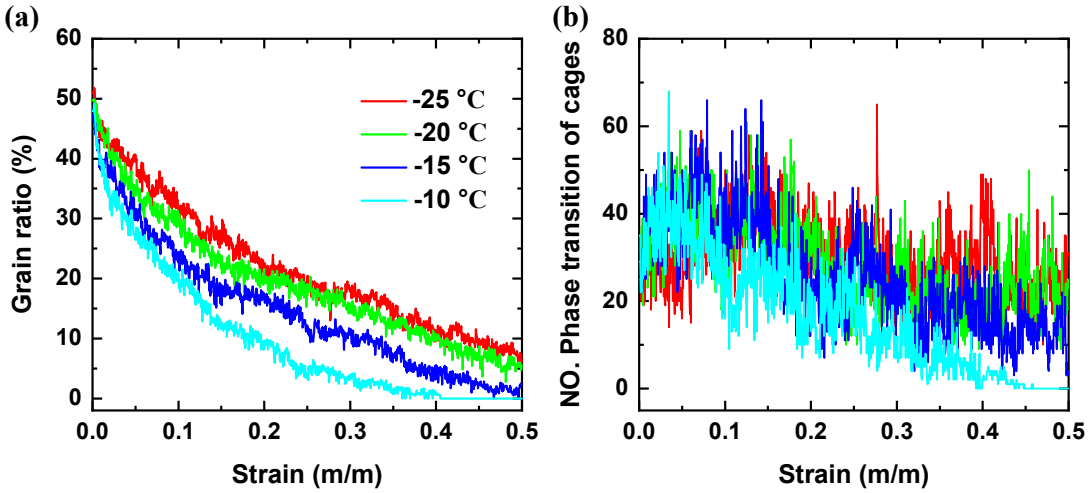

Figure S3 (a) Variations of the ratios of the hydrate grains occupancy in system with strain under different temperatures. (b) Phase transition of the 5^{12} and $5^{12}6^4$ clathrate cages from sII hydrate grains to the GBs during compressive process.

Table S1 The number of times transformation between $5^{12}/5^{12}6^4$ and other cages during the compressive tests.

Temperatures/Cage transformation	248 K	253 K	258 K	263 K
$5^{12} \rightarrow 4^2 5^8 6^1$	23	14	15	11
$5^{12} \rightarrow 4^2 5^8 6^2$	9	11	4	10
$5^{12} \rightarrow 4^1 5^{10} 6^2$	2	1	4	4
$4^2 5^8 6^1 \rightarrow 5^{12}$	13	4	14	9
$4^2 5^8 6^2 \rightarrow 5^{12}$	5	--	4	6
$4^1 5^{10} 6^2 \rightarrow 5^{12}$	3	2	4	--
$5^{12} 6^4 \rightarrow 4^1 5^{10} 6^5$	6	6	4	4
$5^{12} 6^4 \rightarrow 4^1 5^{10} 6^6$	1	2	--	3
$4^1 5^{10} 6^5 \rightarrow 5^{12} 6^4$	8	3	2	2
$4^1 5^{10} 6^6 \rightarrow 5^{12} 6^4$	--	1	1	1