Supporting Information

Uncovering the rupture mechanism of carbon nanotube filled cis-1,4-polybutadiene via molecular dynamics simulation

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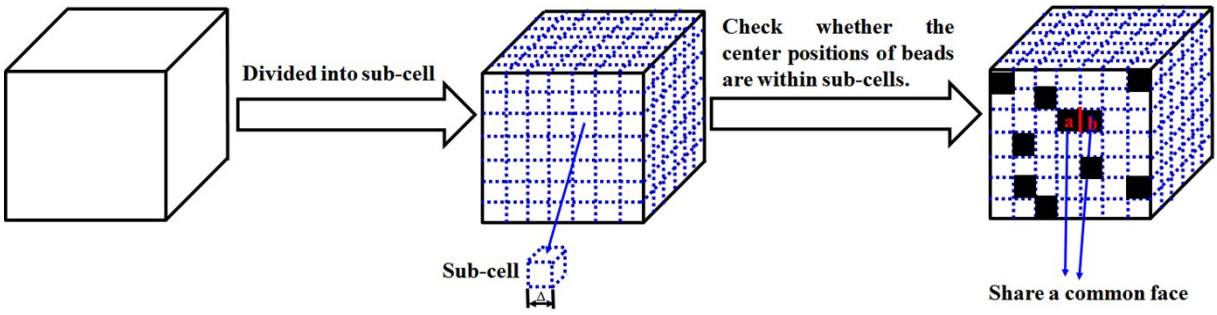

Fig. S1 Illustration of the method on defining the number and positions of voids. It is noted that the black sub-cell stands for the unoccupied sub-cell (void). In addition, the unoccupied sub-cells can appear within the inner box. For convenient, the unoccupied sub-cells on the surface of box are used as examples. The sub-cells (a) and (b) share a common face (denoted by the red line), which belong to the same void.

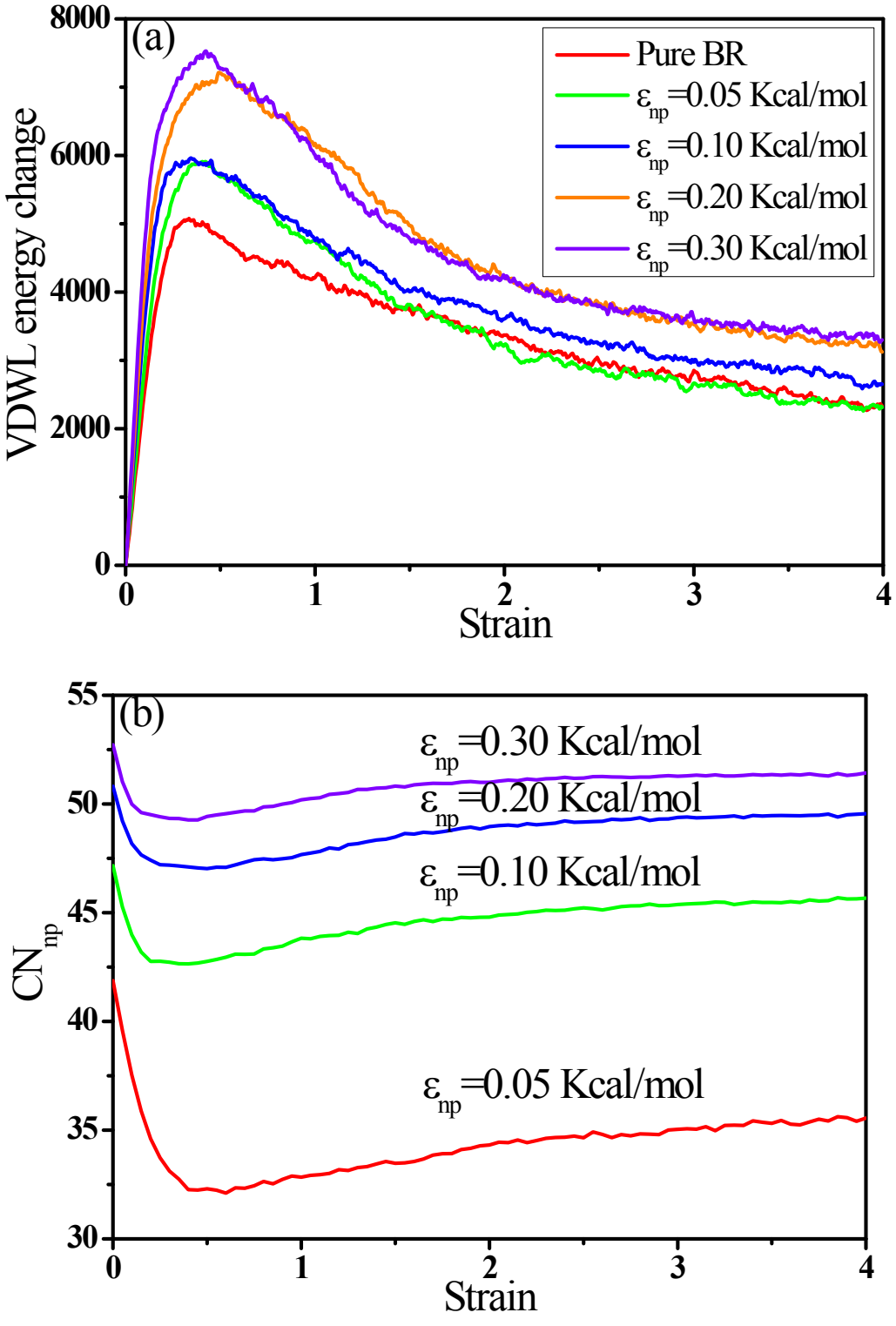

Fig. S2 (a) VDWL energy change and (b) the average number of neighbor polybutadiene beads per carbon nanotube (CNT) bead (CN_{np}) with respect to the strain for pure system and the CNT filled systems with different interactions ε_{np} .

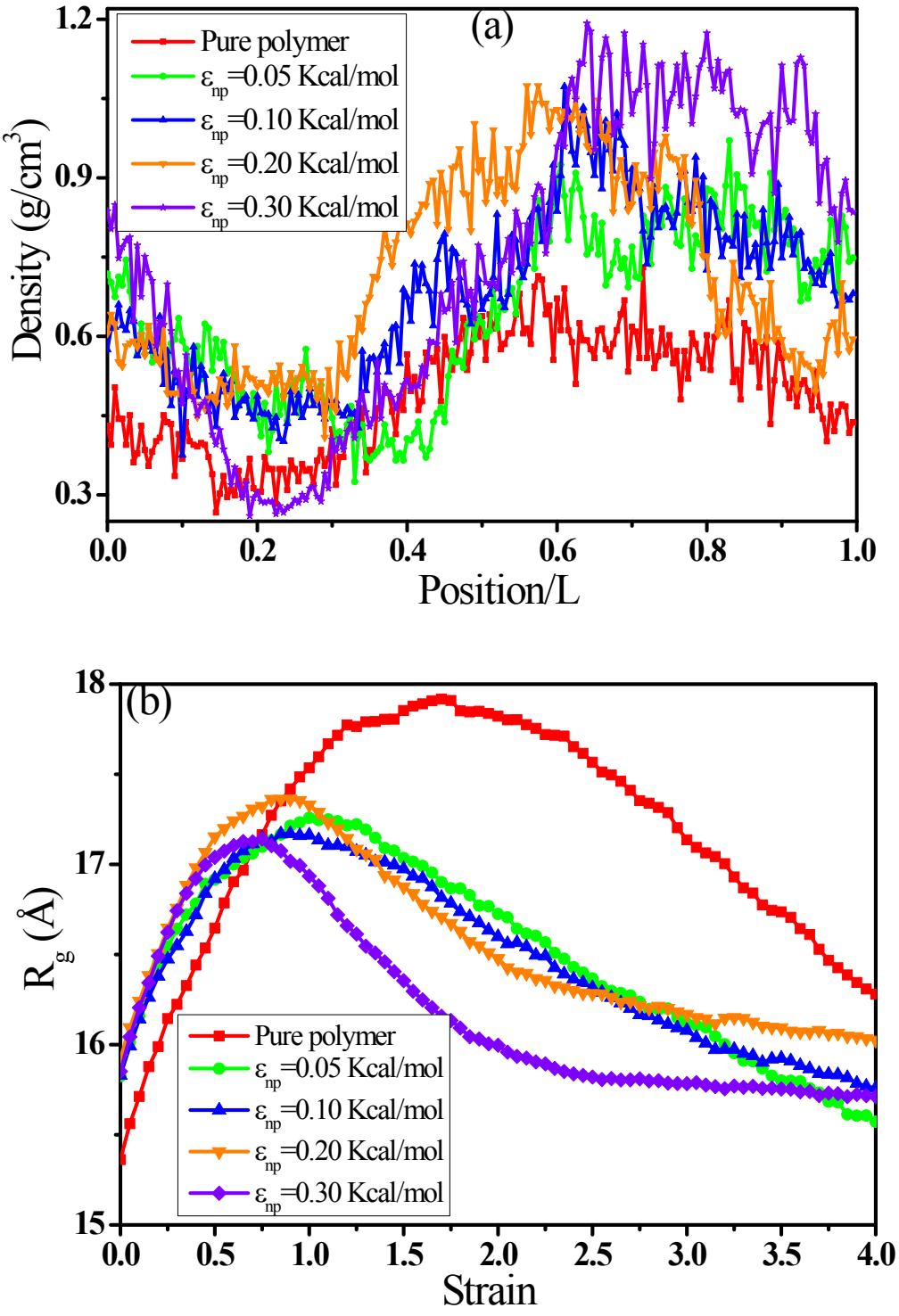

Fig. S3 (a) Density distribution of all polybutadiene beads along the tensile direction (L is the length of box along the tensile direction) at strain=0.5. (b) The root mean squared radius of gyration of chains R_g with respect to the strain for pure system and the CNT filled systems with different interactions ε_{np} .

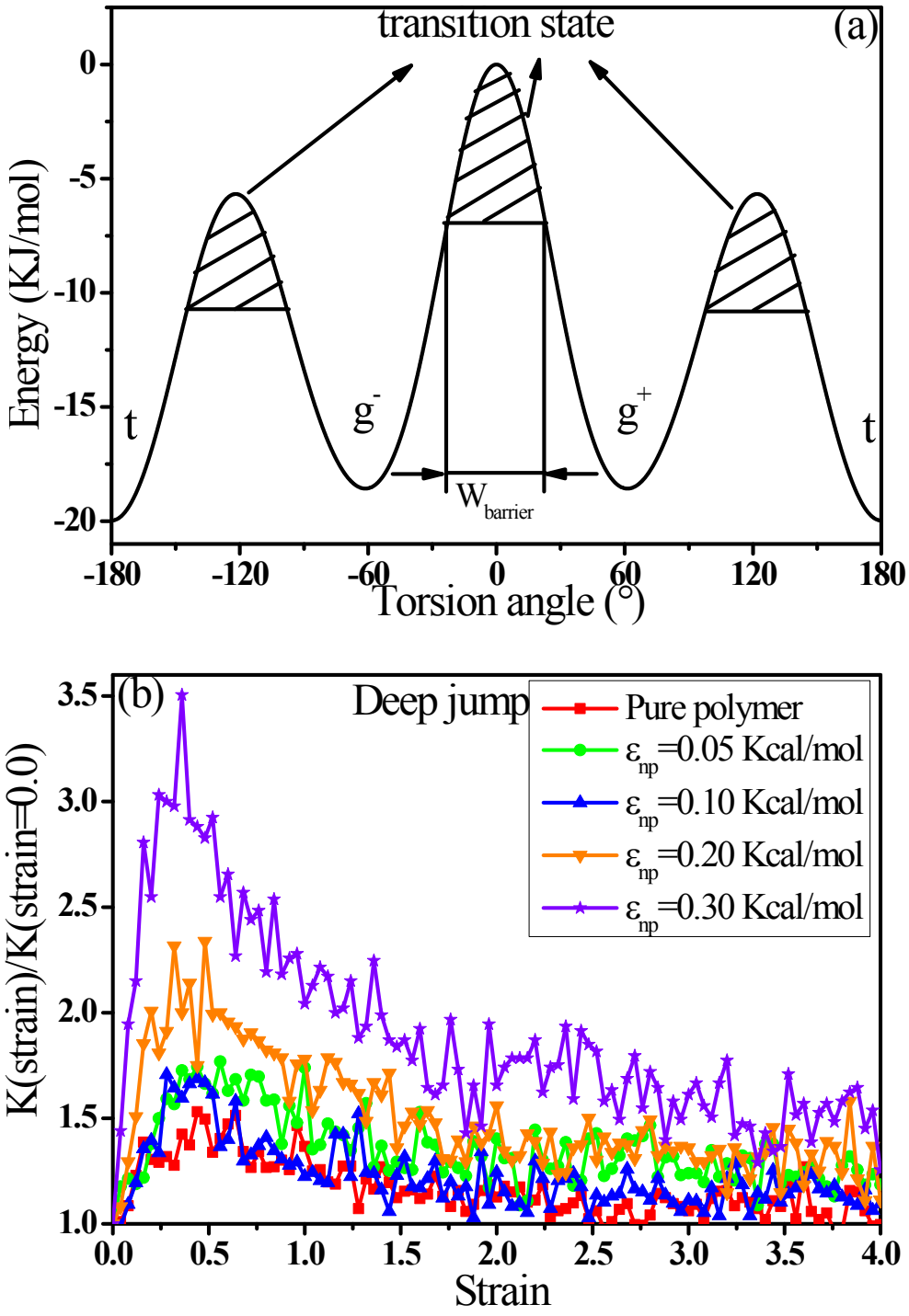

Fig. S4 (a) The illustration of the transition state and the conformational state for the torsion angle φ_3. Minimum of the energy curve is one of the t, g^+, and g^- conformational state. $W_{barrier}$ is the width of the barrier. (b) The ratio of the conformational transition rate at some strain to that at the strain=0.0 K(strain)/K(strain=0.0) for the deep jump with respect to the strain.

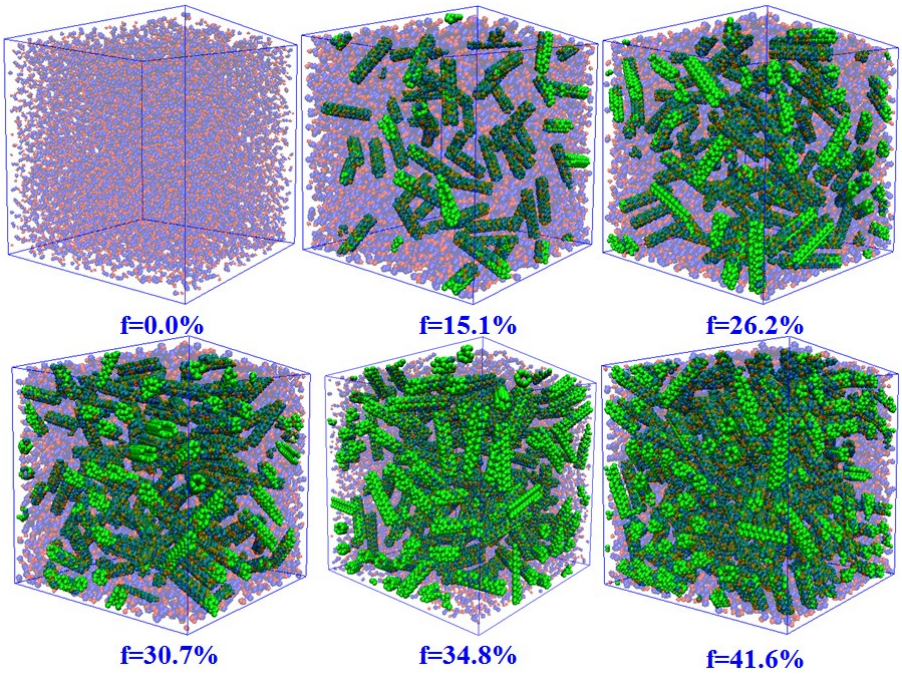

Fig. S5 (a) United atom models for cis-1,4-polybutadiene (PB); (b) Snapshots of pure system and the carbon nanotube (CNT) filled systems with different mass fractions of CNTs (f). The blue and red beads denote the PB chains, while the green beads denote the CNTs.

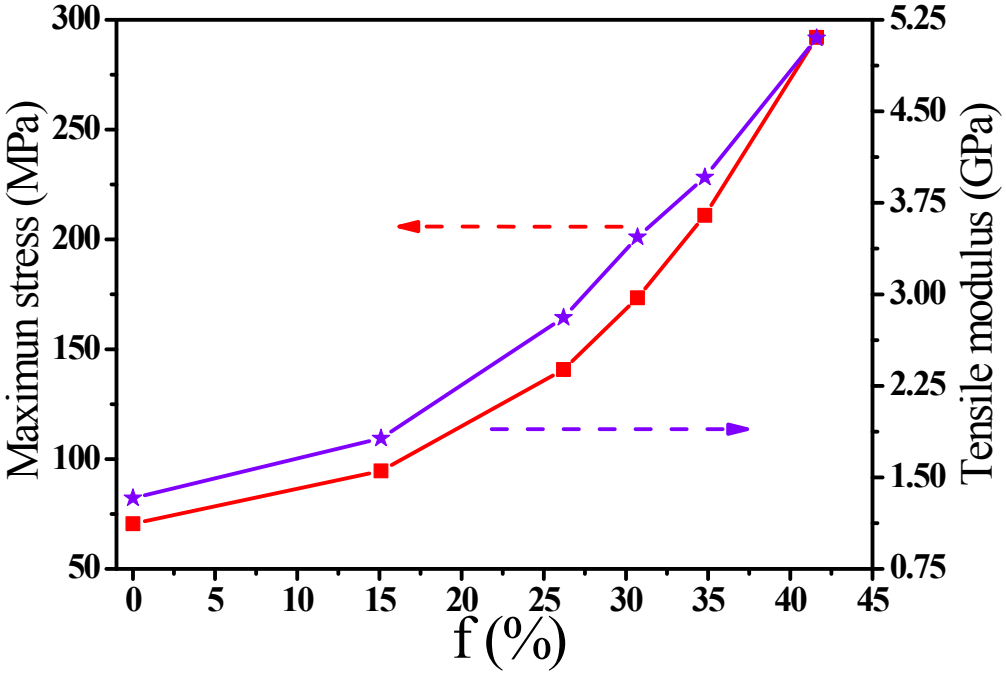

Fig. S6 The left axis denotes the maximum stress, while the right axis represents the tensile modulus with respect to the mass fraction of carbon nanotube (f).

Table SI The force-field parameters for the carbon nanotube filled polybutadiene model

(a)

Bond stretching	k_b (Kcal·(mol·Å^2)$^{-1}$)	r_0 (Å)
CH_2-CH_2	331.5	1.54
CH_2-CH	384.5	1.50
CH=CH	516.5	1.34

(b)

Bond angle bending	k_θ (Kcal·mol^{-1})	θ_0 (deg)
CH_2-CH_2-CH	57.5	111.65
CH_2-CH-CH	44.7	125.89

(c)

Torsion	k_1 (Kcal· mol^{-1})	k_2 (Kcal· mol^{-1})	k_3 (Kcal· mol^{-1})	k_4 (Kcal· mol^{-1})	k_5 (Kcal· mol^{-1})	k_6 (Kcal· mol^{-1})
CH_2-CH=CH-CH_2 φ_1	-	12.1	-	-	-	-
CH_2-CH_2-CH=CH φ_2	0.5165	-0.236	0.2777	0.1315	0.173	0.082
CH-CH_2-CH_2-CH φ_3	-0.444	0.3095	-1.8195	-0.033	-0.1235	-0.095

(d)

Non-bonding		ε (Kcal·mol^{-1})	σ (Å)	r_{cutoff}(Å)
CH_2	CH_2	0.0936	4.009	10.023
CH_2	CH	0.1015	3.793	9.483
CH	CH	0.1000	3.385	8.463
CNT	CH_2	0.05-0.3	3.385	8.463
CNT	CH	0.05-0.3	3.385	8.463
CNT	CNT	0.1000	3.385	3.791