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Supporting Information

Molecular dynamics simulation of rupture mechanism in nanorod filled polymer nanocomposites

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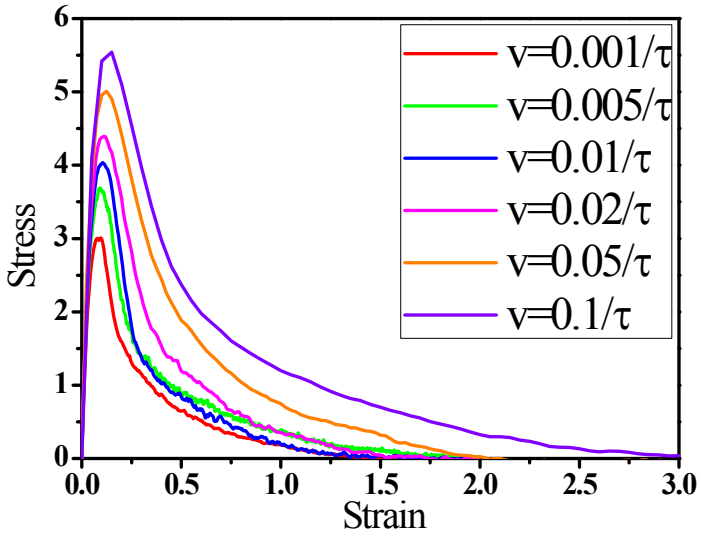


Fig. S1 Stress versus strain curves using different strain rates.

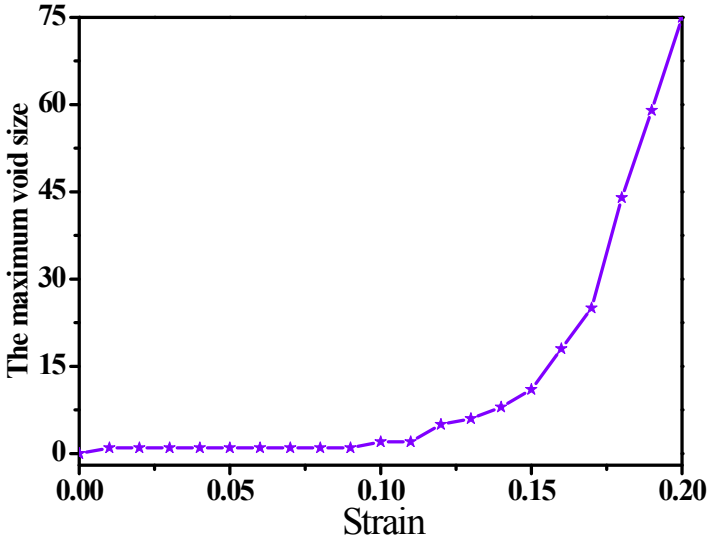
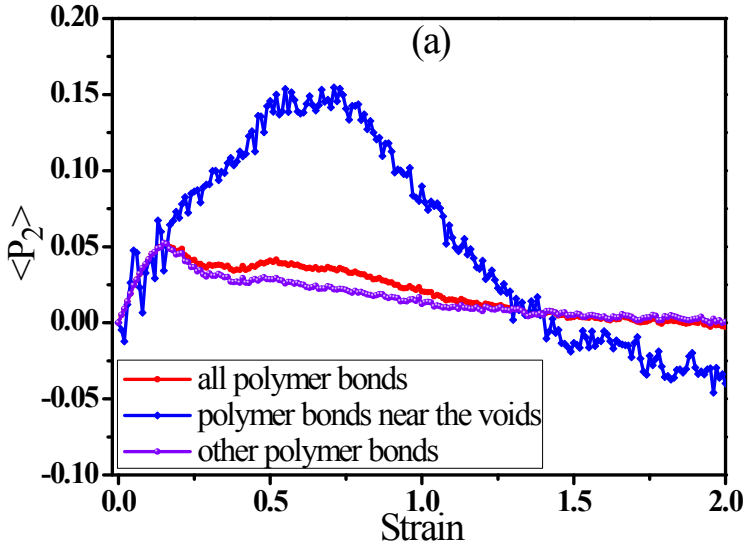


Fig. S2 The maximum void size versus strain.

We examined further the structural properties of polymer nanocomposites by calculating their orientational order parameter. The order parameter is defined by $S = 0.5(3\cos^2\theta - 1)$, where θ is the angle between the bond vector and the tensile direction. Its lower bound is S=-0.5 and corresponds to an ensemble of chains whose bonds vector are all perpendicular to the tensile direction. The upper bound S=1 corresponds to a perfectly stretched sample along the tensile direction, while S=0 for a random, isotropic arrangement. Fig. S3(a) showed the order parameter S as a function of the strain for all polymer bonds, the polymer bonds near the voids and other polymer bonds. At first, the bonds exhibit random distribution. With the increase of the strain, the polymers are stretched along the tensile direction and the value of S increases. Further separation of material leads to a higher orientation until the big voids appear. Accordingly, the order parameter S reaches a maximum and then decreases. It is interesting to find that the peak of S of the polymer bonds near the voids is roughly close to that of radius of gyration $\langle R_g \rangle$, while the peak of S of other polymer bonds is consistent with that of VDWL energy. When small voids grow and merge into big voids, the inner chains begin to contract, which leads to the decrease of S of other polymer bonds. And when the material completely ruptures, namely the polymer bundles begin to get separated, the chains near the voids begin to contract, leading to the decrease of S of the polymer bonds near the voids. The number of bonds near the void is less compared with the total number of bonds, so the bond orientation of S of all polymer bonds is similar to that of other polymer bonds.

The rupture behavior can be understood better by analyzing the various energy

contributions inside our system. The total kinetic energy comprises kinetic contributions of all individual beads, which is constant during the simulation because of the thermostating. The evolution of the energy (total potential energy, VDWL energy, bond energy and angle energy) during the rupture process was presented in Fig. S3(b) as a function of the strain. The bond and angle energies are roughly constant since bonds and angles cannot break in our model. The VDWL energy dominates the process.



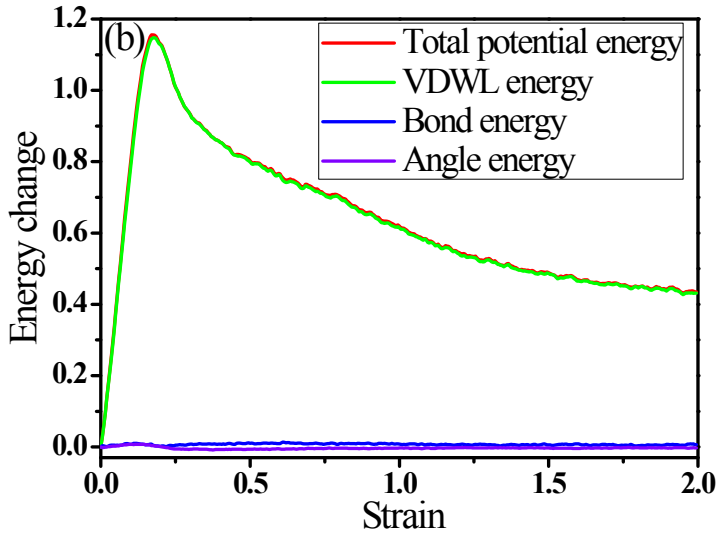


Fig. S3(a) The order parameter S for all polymer bonds, the polymer bonds near the voids and other polymer bonds. (b) The energy change (total potential energy, VDWL energy, bond energy and angle energy) as a function of strain.

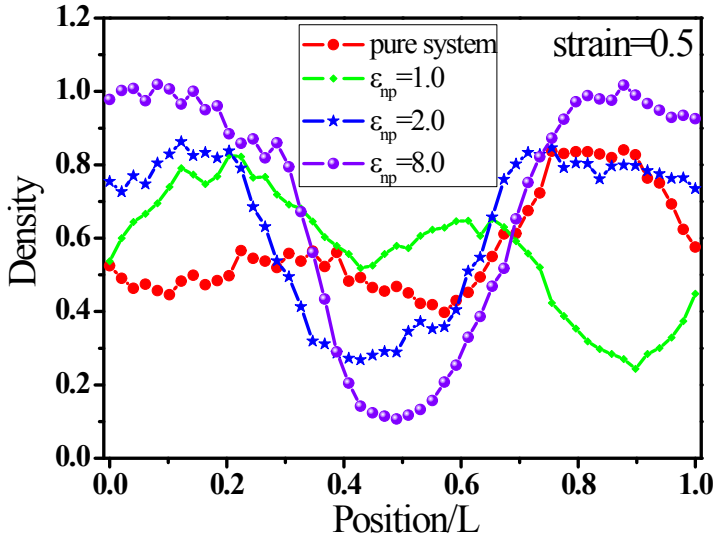
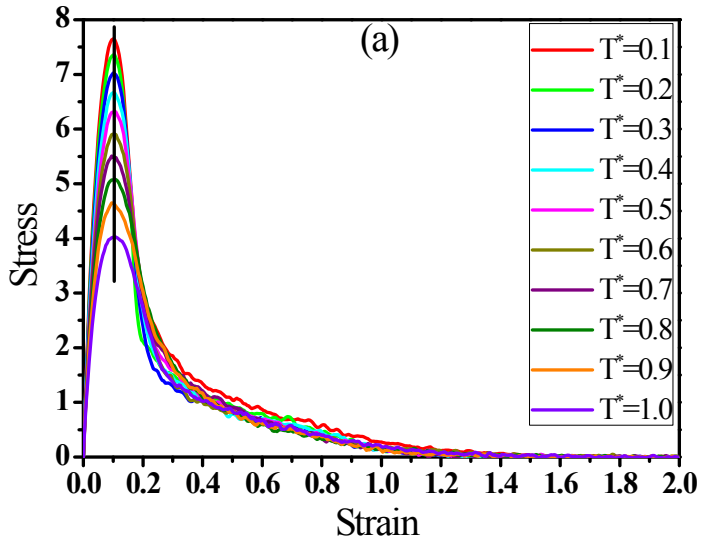


Fig. S4 Distribution of all beads along the tensile direction (L is the length of box along the tensile direction) at strain=0.5.



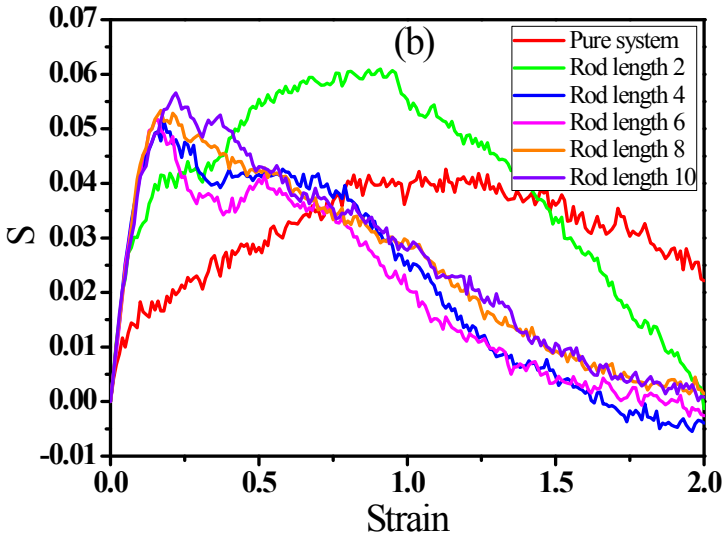


Fig. S5(a) Stress-strain curves obtained for different simulated temperatures ($\varepsilon_{np} = 3.0$). (b) The order parameter S as a function of the strain for different rod lengths.

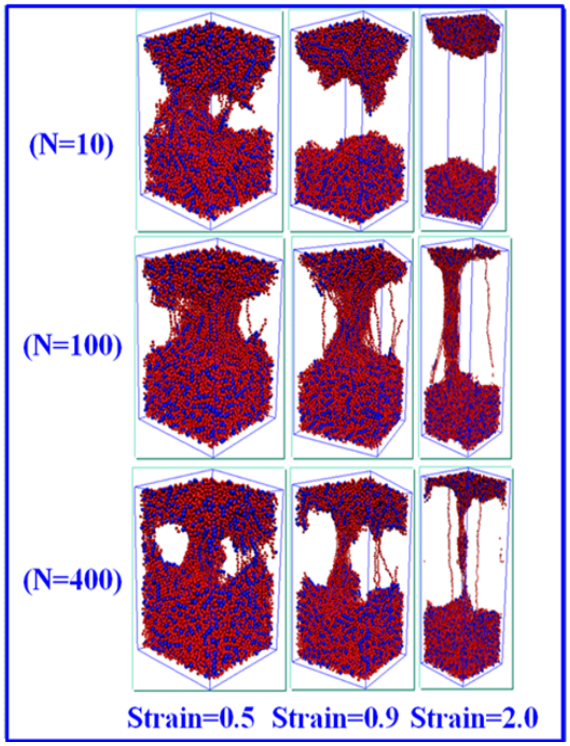
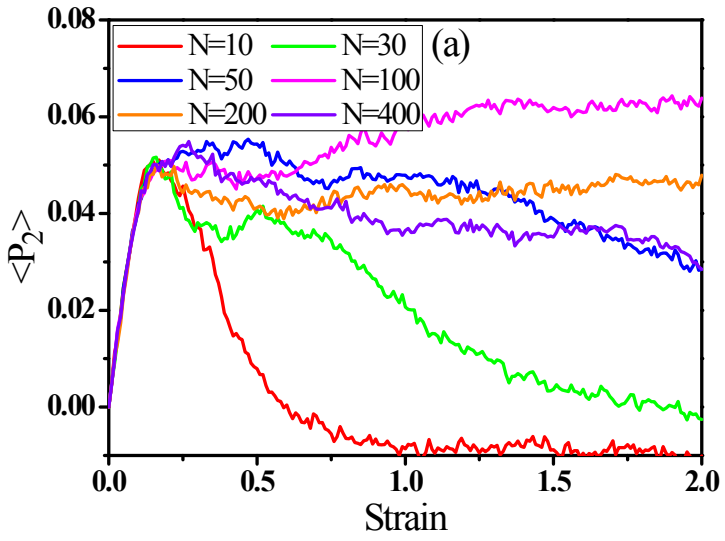


Fig. S6 The snapshots at strain=0.5, 0.9 and 2.0 for three types of chain lengths.



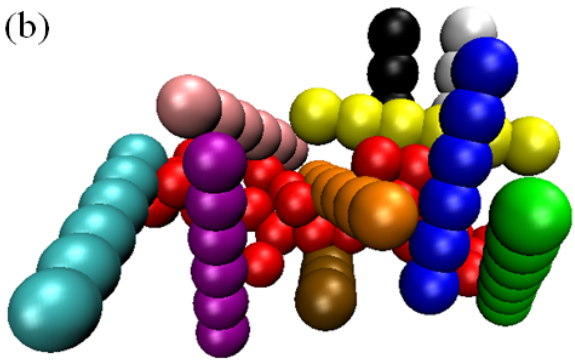
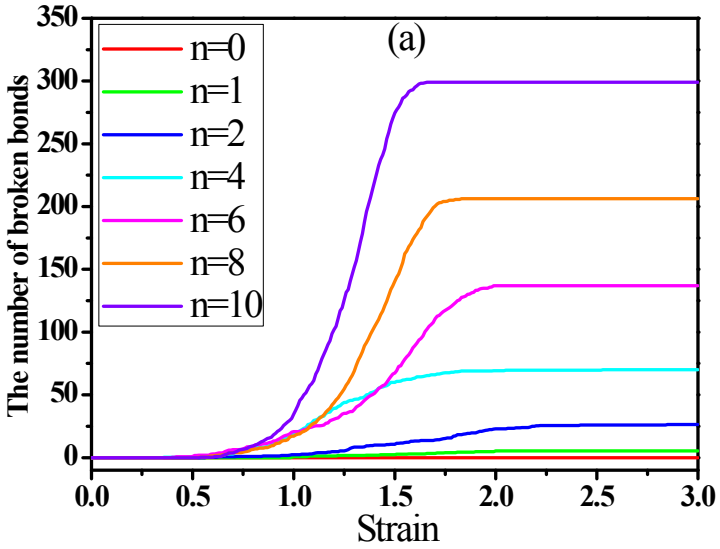


Fig. S7 (a) The order parameter S as a function of the strain for different chain lengths. (b) **The snapshots for a bridging cluster of nanorods via one polymer layer. The red beads denote one polymer chain and other color beads denote nanorods.**



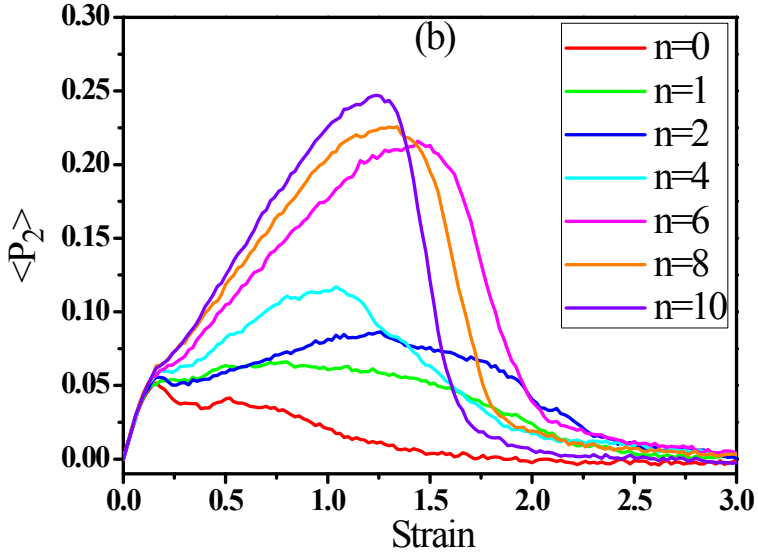


Fig. S8 (a) The number of broken bonds and (b) the order parameter S as a function of the strain for different cross-linking density n.

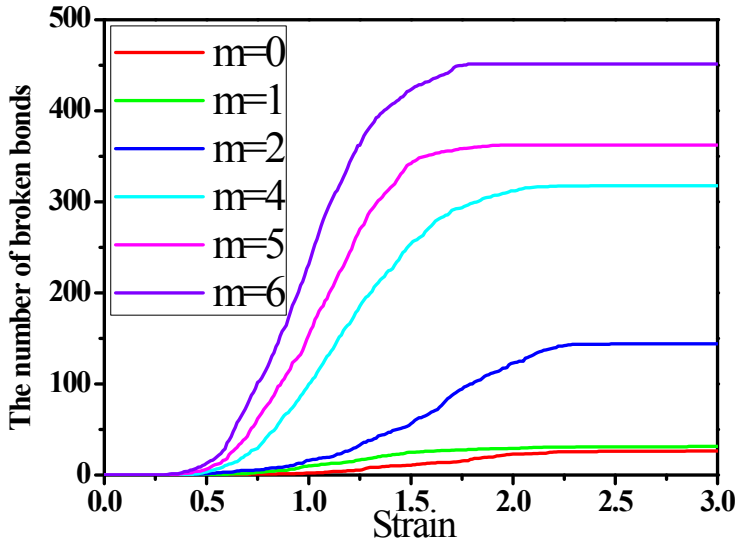


Fig. S9 The number of broken bonds as a function of the strain for different interfacial chemical bonds m.

Table I. All simulated systems

System	Chain		Interaction strength	Temperature	Nanorod		Equilibration times τ
	Number	length			Number	length	
1	600	30		1.0	0	0	50000
2	600	30	1.0	1.0	800	6	50000
3	600	30	1.5	1.0	800	6	50000
4	600	30	2.0	1.0	800	6	50000
5	600	30	3.0	1.0	800	6	50000
6	600	30	5.0	1.0	800	6	50000
7	600	30	8.0	1.0	800	6	50000
8	600	30	3.0	0.1	800	6	50000
9	600	30	3.0	0.2	800	6	50000
10	600	30	3.0	0.3	800	6	50000
11	600	30	3.0	0.4	800	6	50000
12	600	30	3.0	0.5	800	6	50000
13	600	30	3.0	0.6	800	6	50000
14	600	30	3.0	0.7	800	6	50000
15	600	30	3.0	0.8	800	6	50000
16	600	30	3.0	0.9	800	6	50000
17	600	30	3.0	1.0	2400	2	50000
18	600	30	3.0	1.0	1200	4	50000
19	600	30	3.0	1.0	600	8	50000

20	600	30	3.0	1.0	480	10	50000
21	600	30	3.0	1.0	400	12	50000
22	600	30	3.0	1.0	343	14	50000
21	600	30	3.0	1.0	300	16	50000
22	1800	10	3.0	1.0	800	6	50000
23	360	50	3.0	1.0	800	6	50000
24	180	100	3.0	1.0	800	6	50000
25	90	200	3.0	1.0	800	6	50000
26	45	400	3.0	1.0	800	6	50000
27	600	30	3.0	1.0	200	6	50000
28	600	30	3.0	1.0	500	6	50000
28	600	30	3.0	1.0	1600	6	50000
29	600	30	3.0	1.0	2000	6	50000
30	600	30	3.0	1.0	2800	6	50000