Electronic Supplementary Material (ESI) for Soft Matter.

Molecular dynamics simulation of the electrical conductive network formation of polymer nanocomposites by utilizing diblock copolymer-mediated nanoparticles

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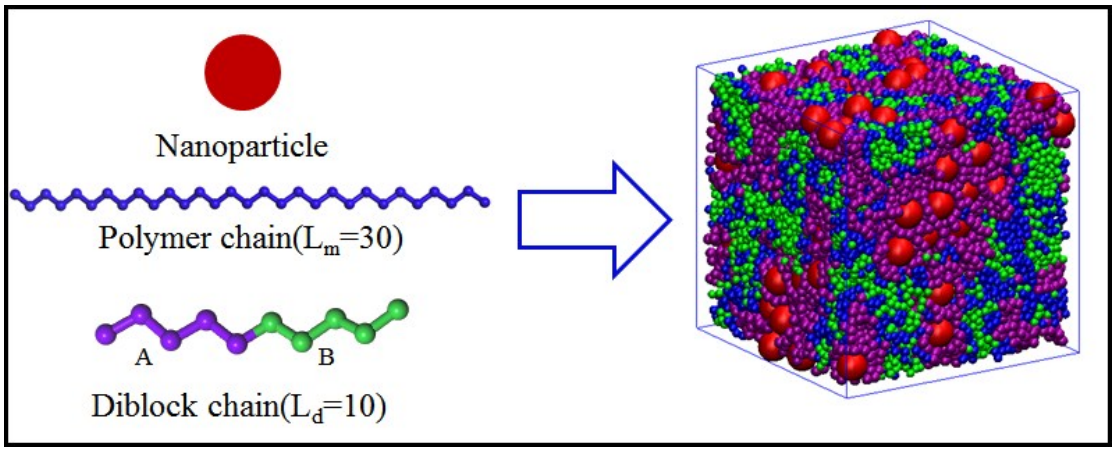


Fig. S1 Schematics of a typical system which contains nanoparticles, diblock chains and polymer chains.

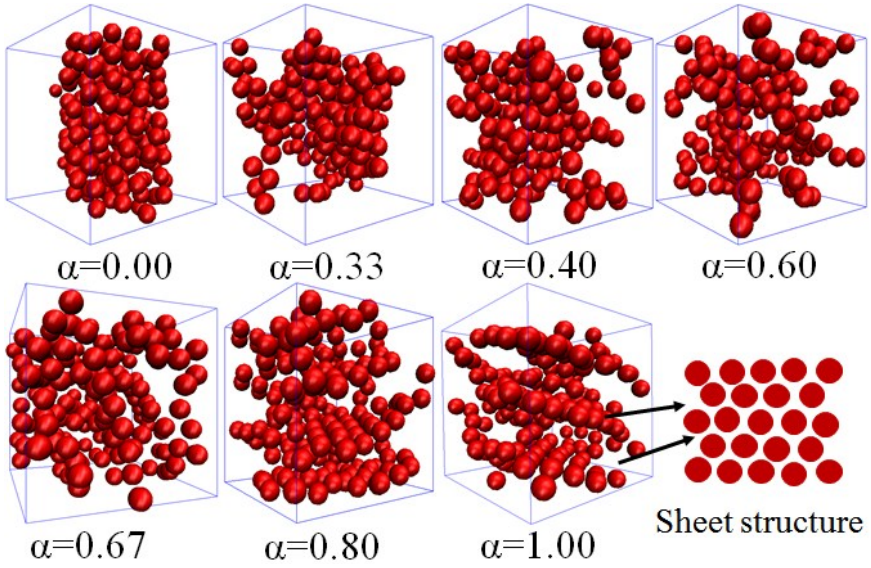


Fig. S2 The snapshots of the nanoparticles (NPs) with respect to the ratio α of the number of beads of BCPs to that of all the chains where the polymer chains are neglected for clarity at φ=15.2%. The red spheres denote the NPs. (T^*=1.0)

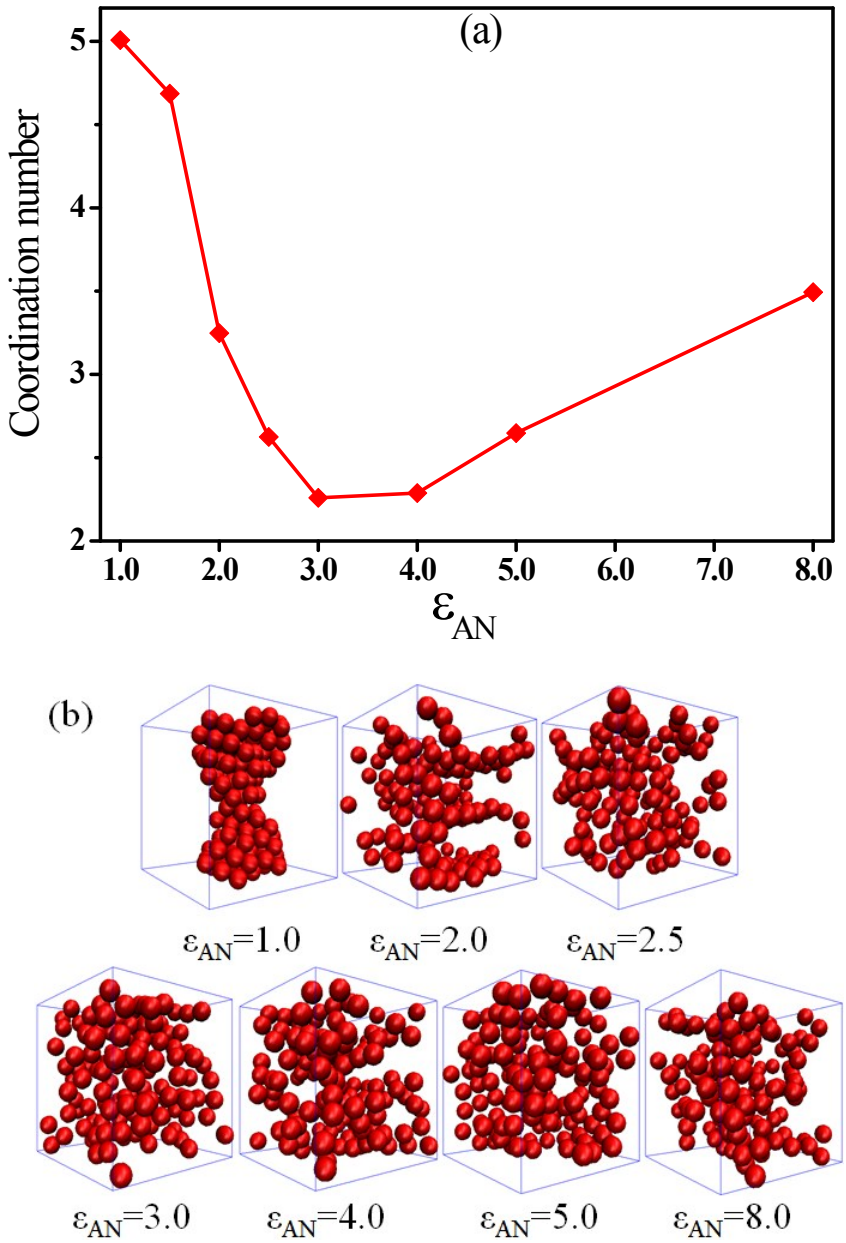


Fig. S3(a) The coordination number and (b) the snapshots of the nanoparticles (NPs) with respect to the A-Block-NP interaction ε_{AN} where the polymer chains are neglected for clarity at φ =12.4%. The red spheres denote the NPs. (T^* =1.0)

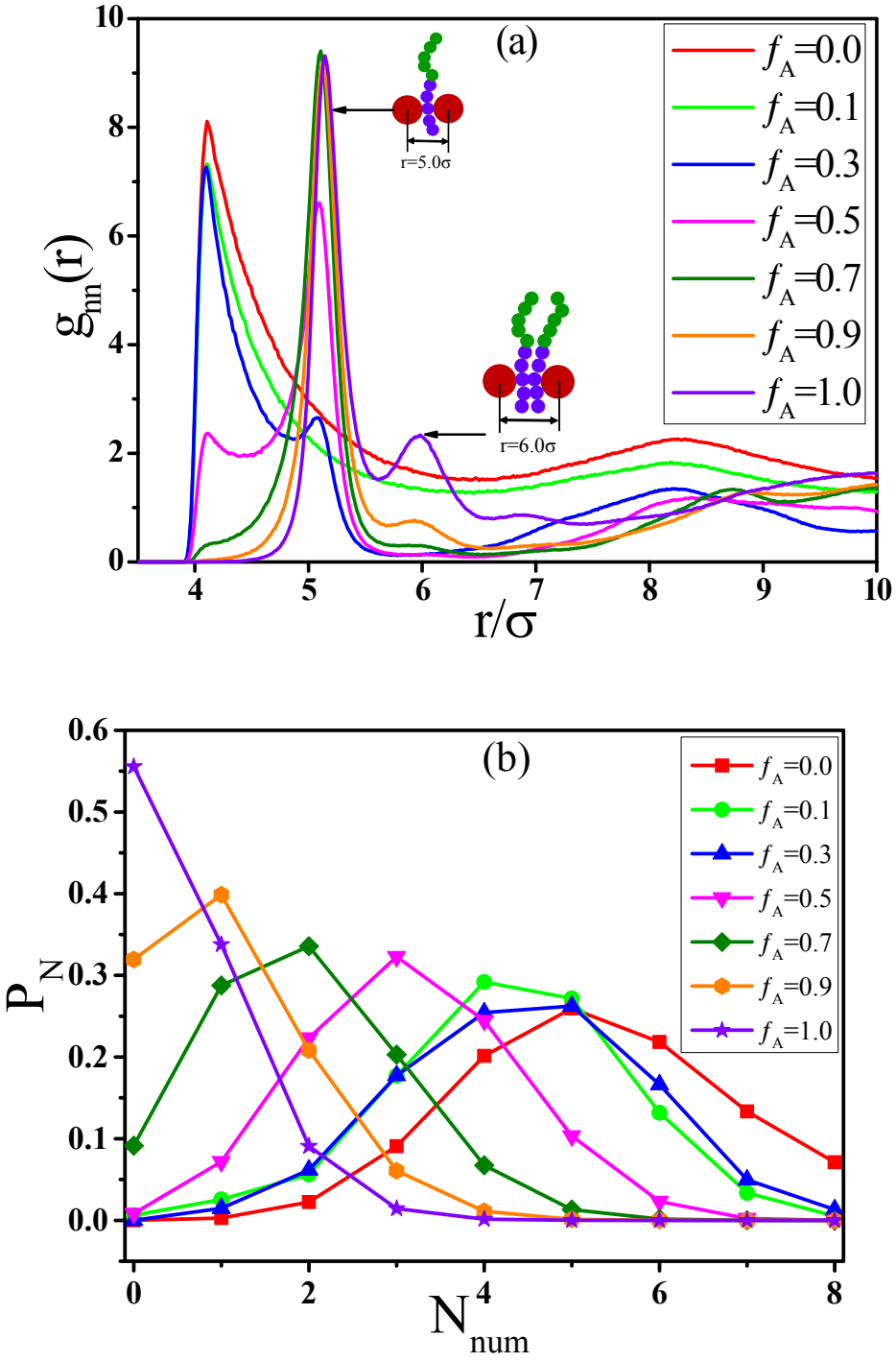
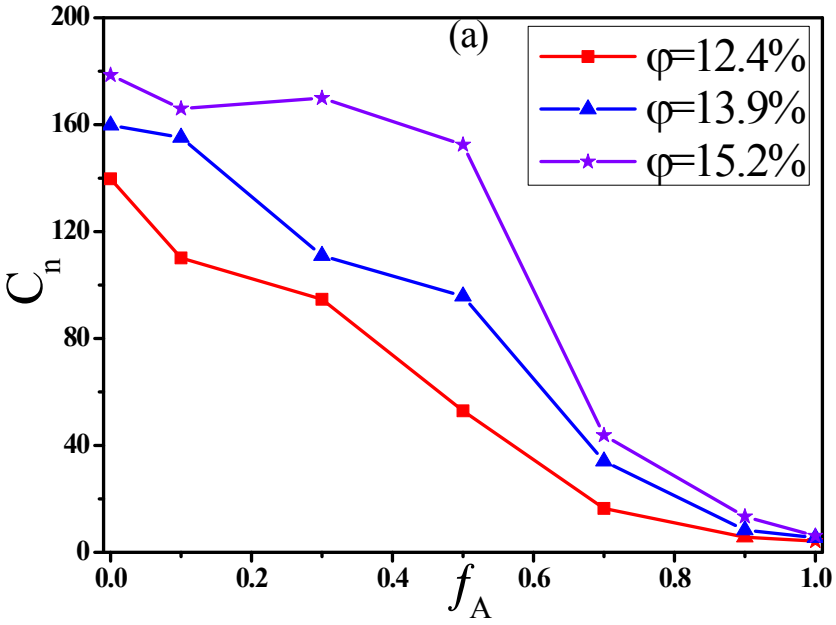
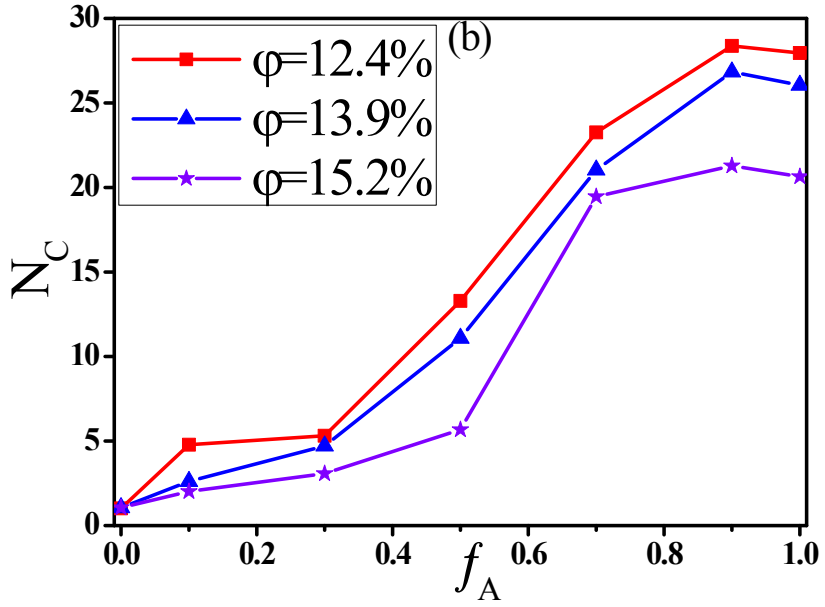


Fig. S4(a) RDF and (b) the probability distribution (P_N) of the nearest neighbor nanoparticles (NPs) surrounding one NP at a separation closer than 5.0σ (N_{num}) with respect to the fraction of A block (f_A) where the polymer chains are neglected for clarity at φ =15.2%. (T^* =1.0)


(a)
φ=12.4%
φ=13.9%
φ=15.2%
C_n
f_A
0
40
80
120
160
200
0.0
0.2
0.4
0.6
0.8
1.0


(b)
φ=12.4%
φ=13.9%
φ=15.2%
N_C
f_A
0
5
10
15
20
25
30
0.0
0.2
0.4
0.6
0.8
1.0

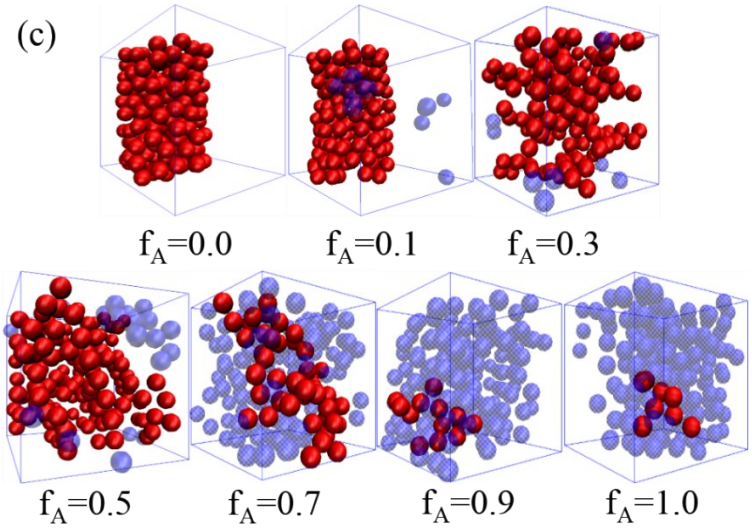

(c)
f_A=0.0
f_A=0.1
f_A=0.3
f_A=0.5
f_A=0.7
f_A=0.9
f_A=1.0

Fig. S5 Change of (a) the main cluster size C_n and (b) the total number of clusters N_c as a function of the fraction of A block (f_A) for three NP volume fractions (φ). (c) Some snapshots of the NPs with different f_A where the polymer chains are neglected for clarity at φ =15.2%. The red spheres denote the NPs within the main cluster. The blue spheres are the other NPs. (T^* =1.0)

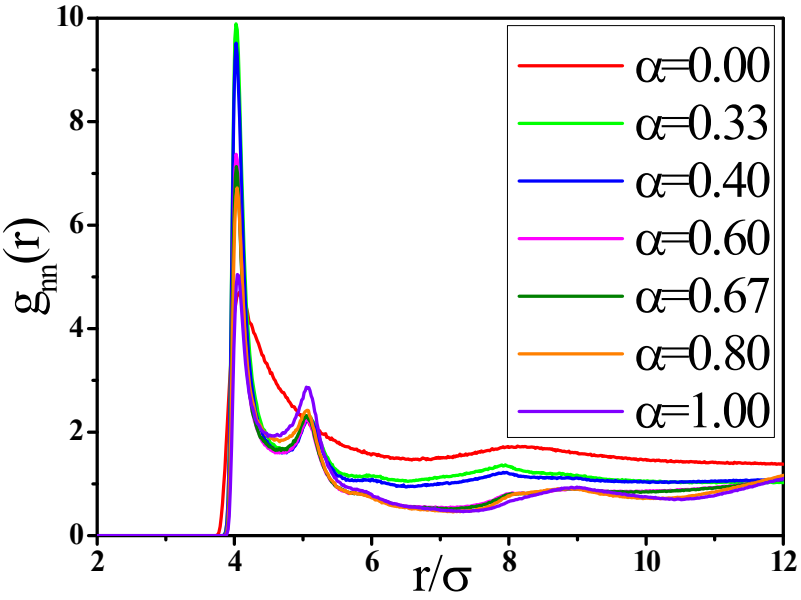


Fig. S6 RDF of nanoparticles as a function of the ratio (α) of the number of beads of BCPs to that of all the chains at φ =15.2%. (T^* =1.0, $\dot{\gamma}$ =0.1)

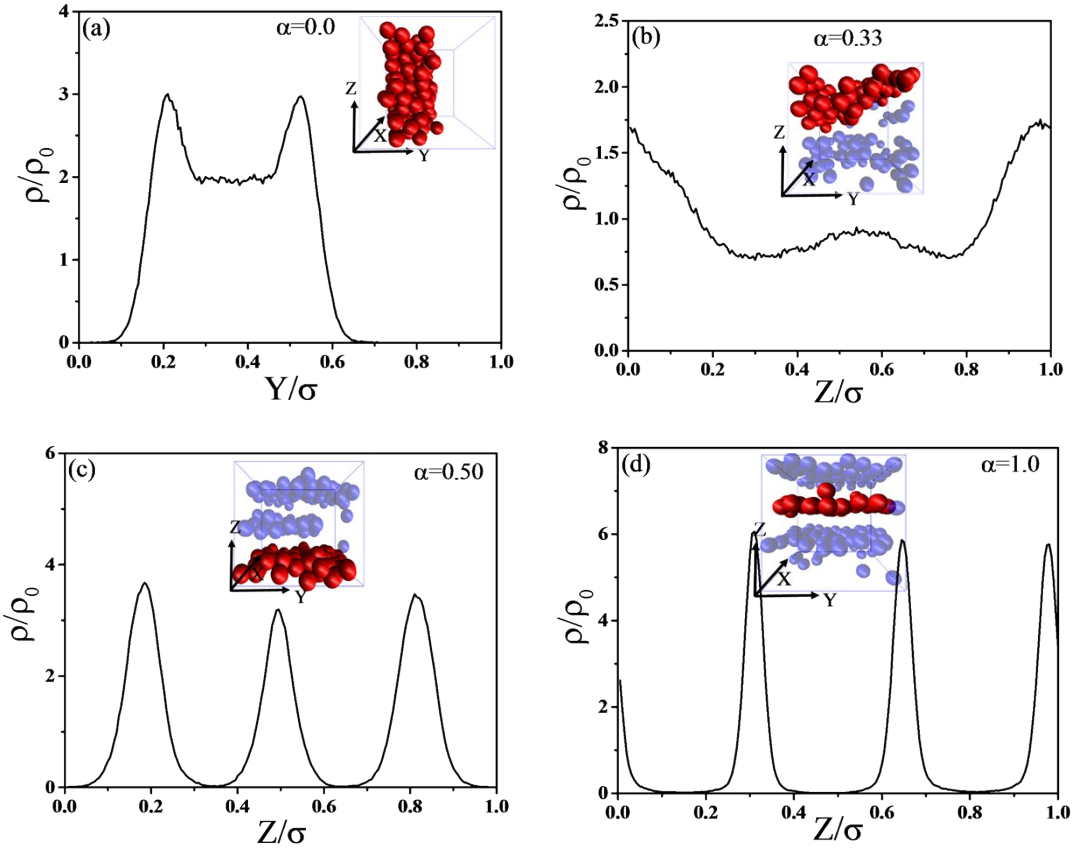


Fig. S7 Local density profiles of the nanoparticles along the Y-axis or Z-axis direction with different ratio (α) of the number of beads of BCPs to that of all the chains at φ=15.2%. (T^*=1.0, $\dot{\gamma}$=0.1)

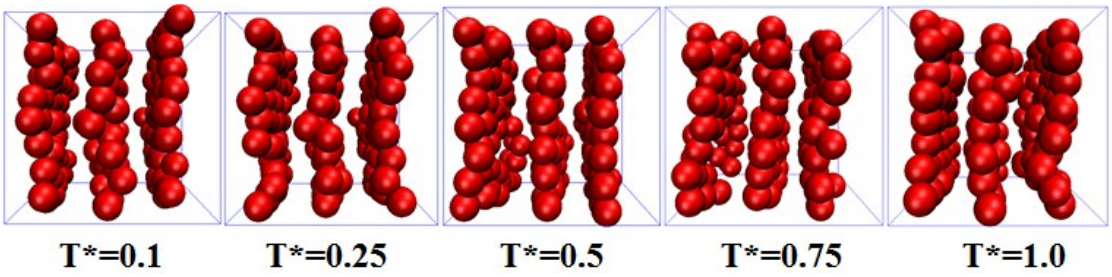


Fig. S8 Snapshots of the sandwich-like structures for different temperature T^*.

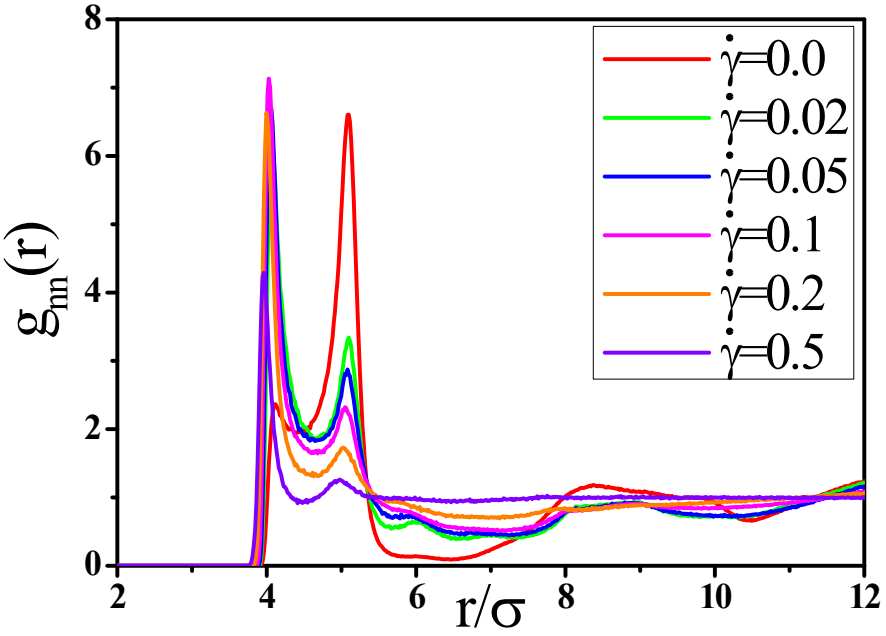
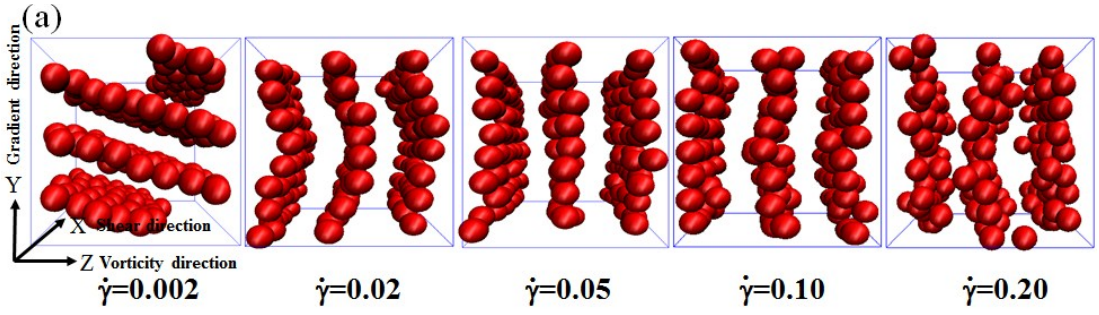


Fig. S9 RDF of nanoparticles as a function of the shear rate ($\dot{\gamma}$) at φ=15.2%. (T^*=1.0, α=0.67)



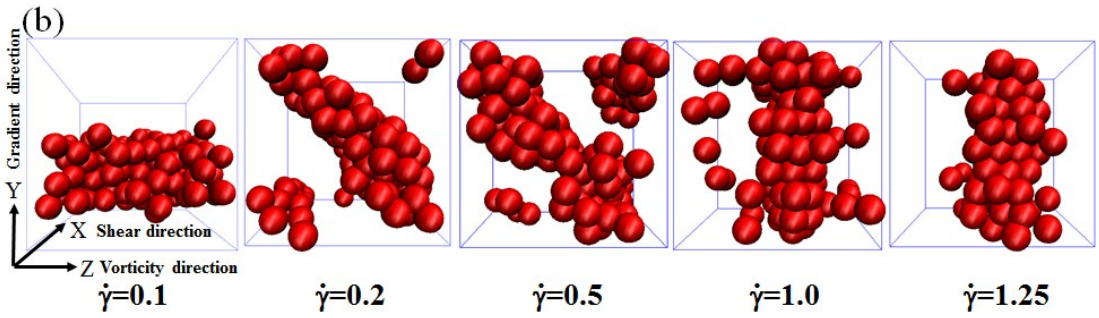
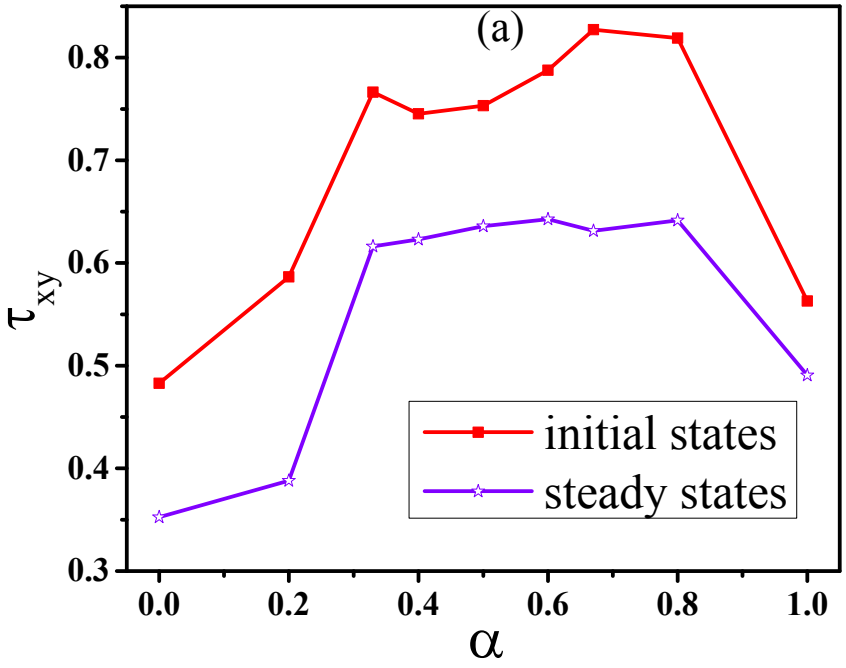


Fig. S10 Some snapshots of the nanoparticles (NPs) for (a) the ratio $\alpha = 0.67$ and (b) $\alpha = 0.00$ with different shear rate ($\dot{\gamma}$) where the polymer chains are neglected for clarity at φ=15.2%. The red spheres denote the NPs. (T^*=1.0)



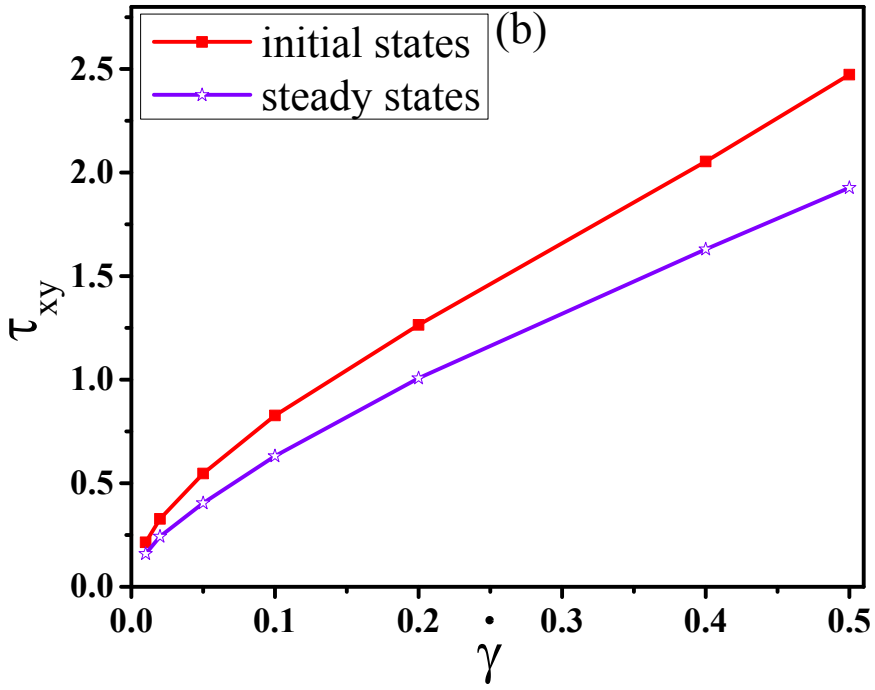


Fig. S11 Comparison of the shear stress τ_{xy} of the initial states and steady states for different α and shear rate ($\dot{\gamma}$) at φ=15.2%. (T^*=1.0)

Table SI. Beads parameters

Atom Type	Representation	Bead diameter (σ)	Bead mass (m)
1	Nanoparticle	4	64
2	A-block of BCP	1	1
3	B-block of BCP	1	1
4	Matrix chains	1	1

BCP is the diblock copolymers.

Table SII. Parameters of each simulated system

System	φ (%)	N_{BCP}/N_m	α	ε_{AN}	f_A
1	12.4	0/800	0.00	3.0	0.5
2	12.4	480/640	0.20	3.0	0.5
3	12.4	792/536	0.33	3.0	0.5

4	**12.4**	**960/480**	**0.40**	**3.0**	**0.5**
5	**12.4**	**1200/400**	**0.50**	**3.0**	**0.5**
6	**12.4**	**1440/320**	**0.60**	**3.0**	**0.5**
7	**12.4**	**1608/264**	**0.67**	**3.0**	**0.5**
8	**12.4**	**1920/160**	**0.80**	**3.0**	**0.5**
9	**12.4**	**2400/0**	**1.00**	**3.0**	**0.5**
10	**13.9**	**0/800**	**0.00**	**3.0**	**0.5**
11	**13.9**	**480/640**	**0.20**	**3.0**	**0.5**
12	**13.9**	**792/536**	**0.33**	**3.0**	**0.5**
13	**13.9**	**960/480**	**0.40**	**3.0**	**0.5**
14	**13.9**	**1200/400**	**0.50**	**3.0**	**0.5**
15	**13.9**	**1440/320**	**0.60**	**3.0**	**0.5**
16	**13.9**	**1608/264**	**0.67**	**3.0**	**0.5**
17	**13.9**	**1920/160**	**0.80**	**3.0**	**0.5**
18	**13.9**	**2400/0**	**1.00**	**3.0**	**0.5**
19	**15.2**	**0/800**	**0.00**	**3.0**	**0.5**
20	**15.2**	**480/640**	**0.20**	**3.0**	**0.5**
21	**15.2**	**792/536**	**0.33**	**3.0**	**0.5**
22	**15.2**	**960/480**	**0.40**	**3.0**	**0.5**
23	**15.2**	**1200/400**	**0.50**	**3.0**	**0.5**
24	**15.2**	**1440/320**	**0.60**	**3.0**	**0.5**
25	**15.2**	**1608/264**	**0.67**	**3.0**	**0.5**
26	**15.2**	**1920/160**	**0.80**	**3.0**	**0.5**
27	**15.2**	**2400/0**	**1.00**	**3.0**	**0.5**
28	**12.4**	**1608/264**	**0.67**	**1.0**	**0.5**
29	**12.4**	**1608/264**	**0.67**	**1.5**	**0.5**
30	**12.4**	**1608/264**	**0.67**	**2.0**	**0.5**

31	**12.4**	**1608/264**	**0.67**	**2.5**	**0.5**
32	**12.4**	**1608/264**	**0.67**	**3.0**	**0.5**
33	**12.4**	**1608/264**	**0.67**	**4.0**	**0.5**
34	**12.4**	**1608/264**	**0.67**	**5.0**	**0.5**
35	**12.4**	**1608/264**	**0.67**	**8.0**	**0.5**
36	**13.9**	**1608/264**	**0.67**	**1.0**	**0.5**
37	**13.9**	**1608/264**	**0.67**	**1.5**	**0.5**
38	**13.9**	**1608/264**	**0.67**	**2.0**	**0.5**
39	**13.9**	**1608/264**	**0.67**	**2.5**	**0.5**
40	**13.9**	**1608/264**	**0.67**	**3.0**	**0.5**
41	**13.9**	**1608/264**	**0.67**	**4.0**	**0.5**
42	**13.9**	**1608/264**	**0.67**	**5.0**	**0.5**
43	**13.9**	**1608/264**	**0.67**	**8.0**	**0.5**
44	**15.2**	**1608/264**	**0.67**	**1.0**	**0.5**
45	**15.2**	**1608/264**	**0.67**	**1.5**	**0.5**
46	**15.2**	**1608/264**	**0.67**	**2.0**	**0.5**
47	**15.2**	**1608/264**	**0.67**	**2.5**	**0.5**
48	**15.2**	**1608/264**	**0.67**	**3.0**	**0.5**
49	**15.2**	**1608/264**	**0.67**	**4.0**	**0.5**
50	**15.2**	**1608/264**	**0.67**	**5.0**	**0.5**
51	**15.2**	**1608/264**	**0.67**	**8.0**	**0.5**
52	**12.4**	**1608/264**	**0.67**	**3.0**	**0.0**
53	**12.4**	**1608/264**	**0.67**	**3.0**	**0.1**
54	**12.4**	**1608/264**	**0.67**	**3.0**	**0.3**
55	**12.4**	**1608/264**	**0.67**	**3.0**	**0.5**
56	**12.4**	**1608/264**	**0.67**	**3.0**	**0.7**
57	**12.4**	**1608/264**	**0.67**	**3.0**	**0.9**

58	**12.4**	**1608/264**	**0.67**	**3.0**	**1.0**
59	**13.9**	**1608/264**	**0.67**	**3.0**	**0.0**
60	**13.9**	**1608/264**	**0.67**	**3.0**	**0.1**
61	**13.9**	**1608/264**	**0.67**	**3.0**	**0.3**
62	**13.9**	**1608/264**	**0.67**	**3.0**	**0.5**
63	**13.9**	**1608/264**	**0.67**	**3.0**	**0.7**
64	**13.9**	**1608/264**	**0.67**	**3.0**	**0.9**
65	**13.9**	**1608/264**	**0.67**	**3.0**	**1.0**
66	**15.2**	**1608/264**	**0.67**	**3.0**	**0.0**
67	**15.2**	**1608/264**	**0.67**	**3.0**	**0.1**
68	**15.2**	**1608/264**	**0.67**	**3.0**	**0.3**
69	**15.2**	**1608/264**	**0.67**	**3.0**	**0.5**
70	**15.2**	**1608/264**	**0.67**	**3.0**	**0.7**
71	**15.2**	**1608/264**	**0.67**	**3.0**	**0.9**
72	**15.2**	**1608/264**	**0.67**	**3.0**	**1.0**

The volume fraction of nanoparticles (NPs) φ, the number of the diblock copolymers (BCP) N_{BCP}, the number of matrix chains N_{m}, the ratio of the number of beads of BCPs to that of all the chains α, the A-Block-NP interaction ε_{AN}, the fraction of A block f_A.

Table SIII Nonbonded interaction parameters used in this work.

Interaction types	$\varepsilon_{ij}^{\ a}(\varepsilon)$	$\Delta^b(\sigma)$	$r_{cutoff}^{\ b}(\sigma)$
NP-NP	**1.0**	**3.0**	**2.5**
NP-A-block	**1.0-8.0**	**1.5**	**2.5**
NP-B-block	**1.0**	**1.5**	**1.12**
NP-matrix	**1.0**	**1.5**	**2.5**
A-block-A-block	**1.0**	**0.0**	**2.5**
A-block-B-block	**1.0**	**0.0**	**1.12**
B-block-B-block	**1.0**	**0.0**	**2.5**
A-block-matrix	**1.0**	**0.0**	**1.12**
B-block-matrix	**1.0**	**0.0**	**2.5**

matrix-matrix	**1.0**	**0.0**	**2.5**

NP is the nanoparticles.