Supporting Information

Molecular Dynamics Study on the Thermal Conductivity of the End-grafted Carbon Nanotubes Filled Polyamide-6.6 Nanocomposites

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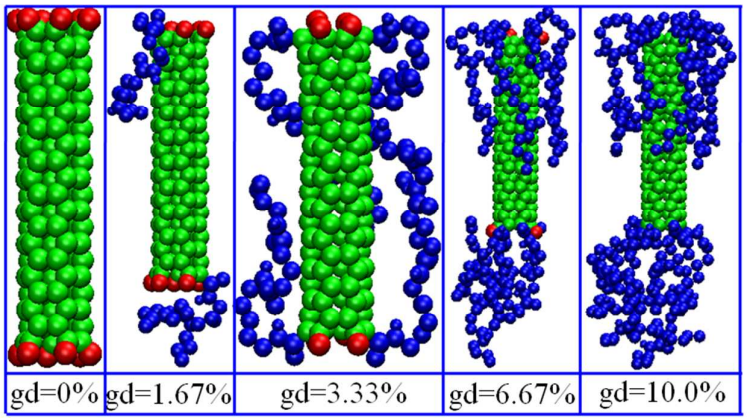

Fig. S1 Snapshots of polyamide (PA)-grafted carbon nanotubes (CNTs) (3,3) with different grafting densities (gd) (L(grafting length)=20). The green spheres denote the CNT atoms, blue spheres denote the grafted PA, and red spheres denote the hydrogen atoms.

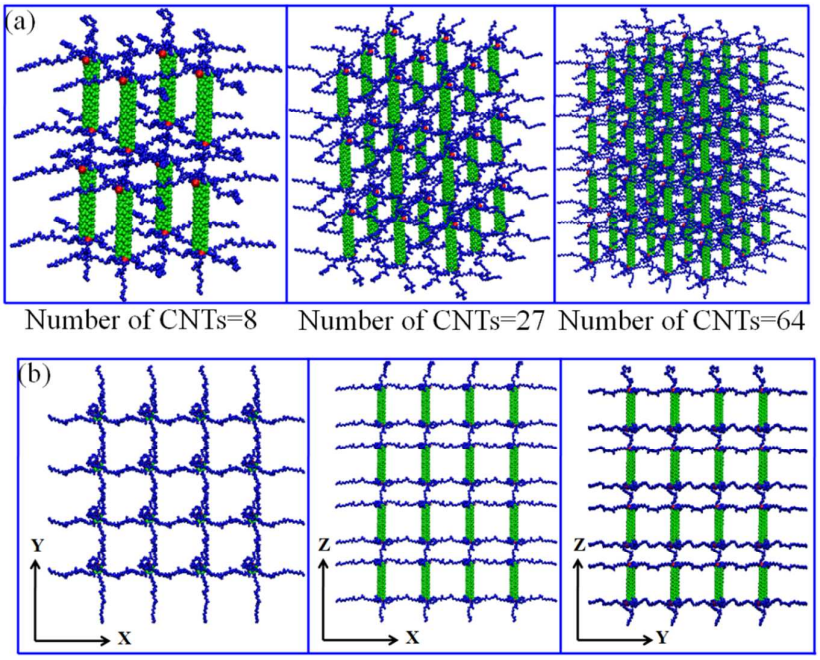

Fig. S2 Snapshots of (a) polyamide (PA)-linked carbon nanotubes (CNTs) with different total number of CNTs. To better describe the structure of PA-linked CNTs, the three projections (b) in different perspective directions are shown for number of CNTs=64. The green spheres denote the CNT atoms, blue spheres denote the grafted PA, and red spheres denote the hydrogen atoms.

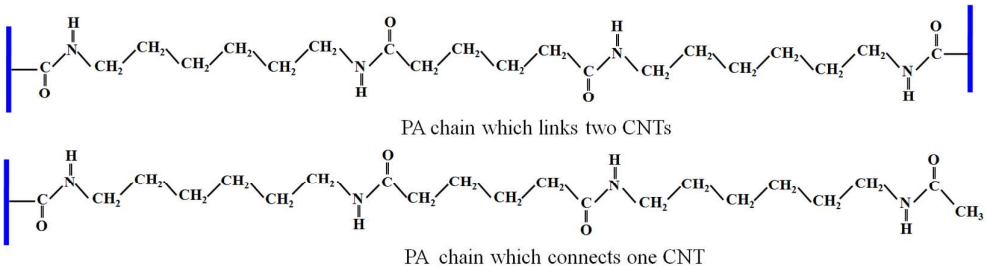

Fig. S3 Chemical details of polyamide (PA) chains which connect carbon nanotubes (CNTs) together to form network CNTs. There are two kinds of linking PA chains: (1) one PA chain which links two CNTs, (2) one PA chain which connects one CNT.

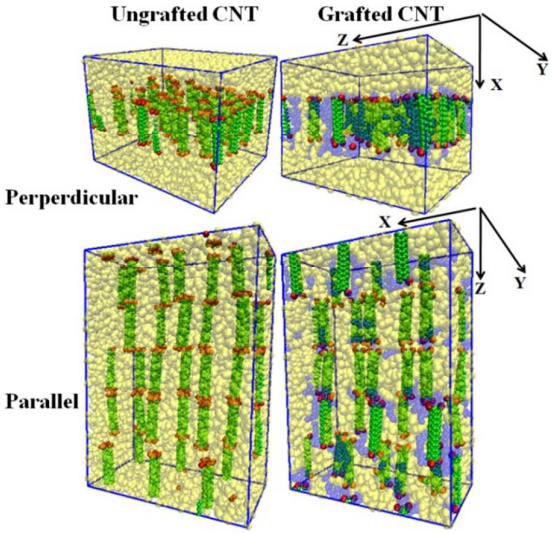

Fig. S4 Snapshots of the systems filled with ungrafted carbon nanotube (CNT) (left) and grafted CNT (right) (gd(grafting density)=6.67%, L(grafting length)=20) where the CNTs shows perpendicular (top) and parallel (bottom) orientation along the heat flux z. The green spheres denote the CNT atoms, red spheres denote the hydrogen atoms, dark blue spheres denote the grafted polyamide (PA), and the dark yellow spheres denote the free PA. (f(CNT volume fraction)=6.13%)

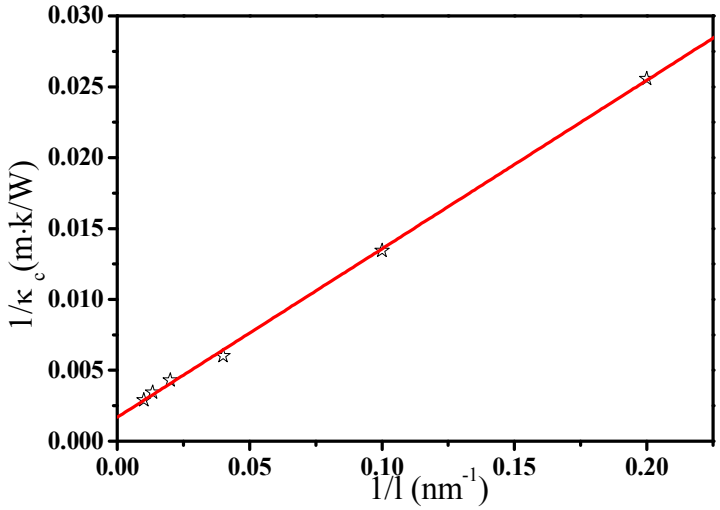

Fig. S5 Change of the inverse thermal conductivity with $(5,\ 5)$ carbon nanotube (CNT) ($1/\kappa_c$) respect to inverse CNT length ($1/l$).

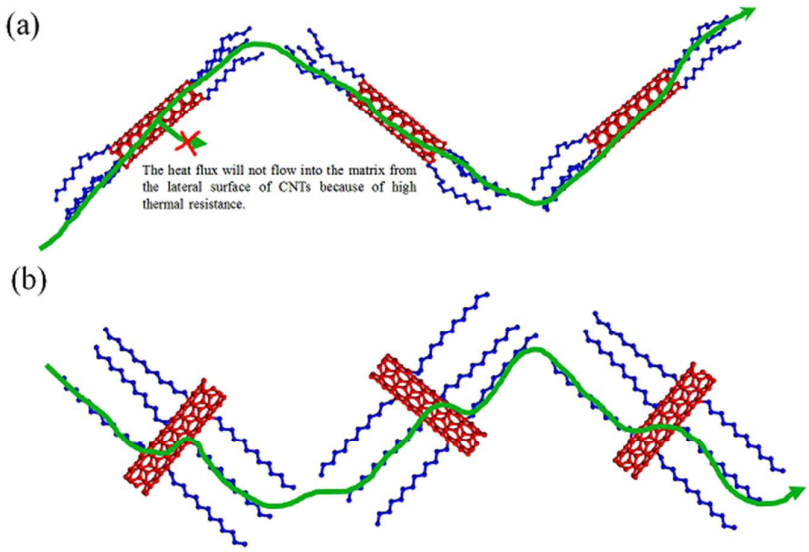

Fig. S6 Schematic diagram of the heat transfer process for (a) the end grafted carbon nanotubes (CNTs) and (b) the lateral grafted CNTs. The blue spheres denote grafted polyamide (PA). The red spheres denote the CNTs, and for clarity the free PA chains are not shown here. Green line stands for the direction of the heat flux;

Table S1. Details of the considered systems for different grafting densities at three carbon nanotube (CNT) volume fractions.

Systems	Number of free PA chains	Number of CNT	Grafting density (%)	Grafting length	Volume fraction of CNTs (%)
1	292	30	0.00	0	6.13
2	275	30	1.67	20	6.13
3	257	30	3.33	20	6.13
4	223	30	6.67	20	6.13
5	190	30	10.0	20	6.13
6	269	48	0.00	0	10.2
7	241	48	1.67	20	10.2
8	214	48	3.33	20	10.2
9	160	48	6.67	20	10.2
10	105	48	10.0	20	10.2
11	240	64	0.00	0	14.5
12	204	64	1.67	20	14.5
13	170	64	3.33	20	14.5
14	103	64	6.67	20	14.5
15	30	64	10.0	20	14.5

Table S2. Details of the considered systems for different grafting lengths for three carbon nanotube (CNT) volume fractions.

Systems	Number of free PA chains	Number of CNT	Grafting density (%)	Grafting length	Volume fraction of CNTs (%)
1	292	30	0.00	0	6.13
2	270	30	6.67	6	6.13
3	244	30	6.67	14	6.13
4	223	30	6.67	20	6.13
5	197	30	6.67	28	6.13
6	269	48	0.00	0	10.2
7	235	48	6.67	6	10.2
8	193	48	6.67	14	10.2
9	160	48	6.67	20	10.2
10	117	48	6.67	28	10.2
11	240	64	0.00	0	14.5
12	200	64	6.67	6	14.5
13	145	64	6.67	14	14.5
14	103	64	6.67	20	14.5
15	44	64	6.67	28	14.5

Table S3. Details of the considered systems filled with ungrafted carbon nanotube (CNT), grafted CNT and network CNTs.

Systems	Number of free PA chains	Number of CNT	Total number of grafted PA	Grafting length	Volume fraction of CNTs (%)

1	330	0	0	0	0.00
2	320	8	0	0	1.57
3	295	27	0	0	5.51
4	240	64	0	0	14.5
5	298	8	64	20	1.57
6	235	27	216	20	5.51
7	103	64	512	20	14.5
8	302	8	60	24	1.57
9	235	27	180	24	5.51
10	106	64	400	24	14.5

System 1 is pure polyamide (PA); systems 2-4 are ungrafted carbon nanotubes (CNTs) filled nanocomposites; systems 5-7 are grafted CNTs filled nanocomposites (gd(grafting density)=6.67%); and systems 8-10 are network CNTs filled nanocomposites.

Table S4. The details of systems filled with ungrafted carbon nanotube (CNT) and grafted CNT for different CNT volume fractions.

Systems	Number of free PA chains	Number of ungrafted CNT	Volume fraction of CNTs (%)
1	330	0	0.00
2	325	6	1.16
3	312	15	2.97
4	292	30	6.13
5	269	48	10.2
6	240	64	14.5
7	220	80	18.8
8	193	100	24.8
9	155	125	33.9

Systems	Number of free PA chains	Number of grafted CNT	Grafting densities (%)	Grafting length	Volume fraction of CNTs (%)
10	298	8	6.67	20	1.56
11	278	15	6.67	20	2.97
12	223	30	6.67	20	6.13
13	160	48	6.67	20	10.2
14	103	64	6.67	20	14.5
15	47	80	6.67	20	18.2
16	0	93	6.67	20	21.9

System 1 is pure polyamide (PA); systems 2-9 are ungrafted carbon nanotubes (CNTs) filled nanocomposites; systems 10-16 are end or lateral grafted CNTs filled nanocomposites; The distribution of grafted chains on the lateral surface of CNT is random.