Supporting Information

Self-Assembly and Structural Manipulation of Diblock-Copolymer Grafted Nanoparticles in Homopolymer Matrix

Sai Li[1], Zhiyu Zhang[1], Guanyi Hou[1], Jun Liu[1,2,3,4*], Yangyang Gao[1,2,3,4*], Phil Coates[6*] Liqun Zhang[1,2,3,4,5*]

[1]Key Laboratory of Beijing City on Preparation and Processing of Novel Polymer Materials, Beijing University of Chemical Technology, People's Republic of China

[2]Beijing Engineering Research Center of Advanced Elastomers, Beijing University of Chemical Technology, People's Republic of China

[3]Engineering Research Center of Elastomer Materials on Energy Conservation and Resources, Beijing University of Chemical Technology, People's Republic of China

[4]Beijing Advanced Innovation Center for Soft Matter Science and Engineering, Beijing University of Chemical Technology, 100029 Beijing, People's Republic of China

[5]State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, 100029 Beijing, People's Republic of China

[6]Joint-International Laboratory for Soft Matter Technologies Bradford-BUCT

Figure S1. The radial distribution function of NPs with grafted beads, diblock copolymer chains and matrix chains in the system with $L_g = 10$, $N_g = 90$ and $\alpha = 0.5$.

Figure S2. (a)-(b) display the tensile stress with different grafting density (from $N_g = 30$ to $N_g = 90$). The blue, green and red lines represent the stress contributed by different components during the stretching process. The yellow line represents the total tensile stress.

*Corresponding author: liujun@mail.buct.edu.cn or zhanglq@mail.buct.edu.cn

(1) The distribution of diblock copolymer chains on NP surface illustrated by the radial distribution function

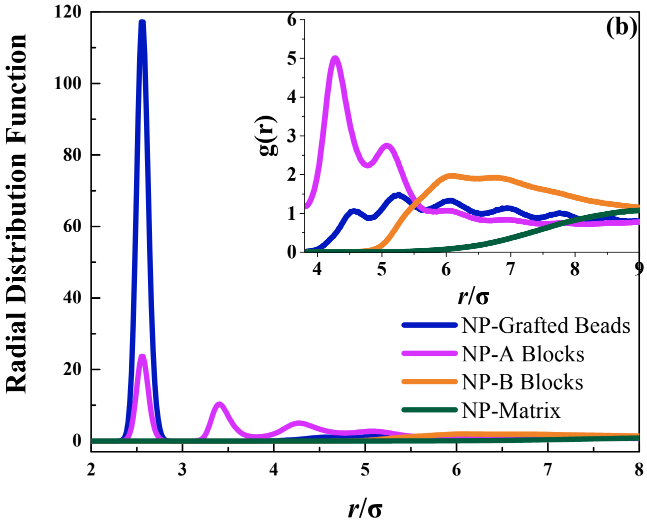
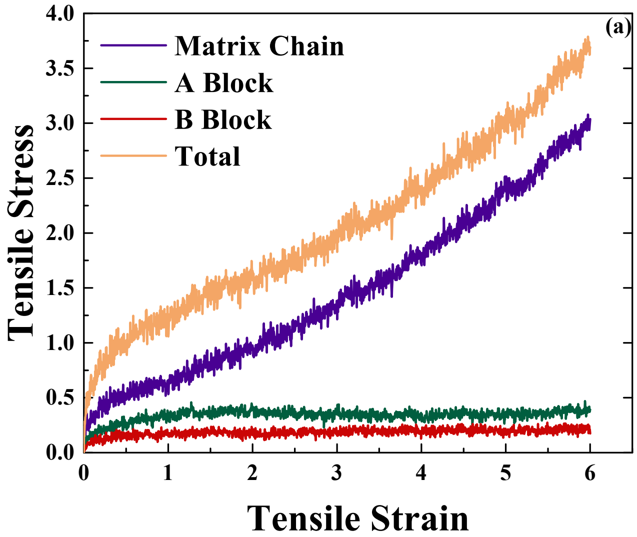


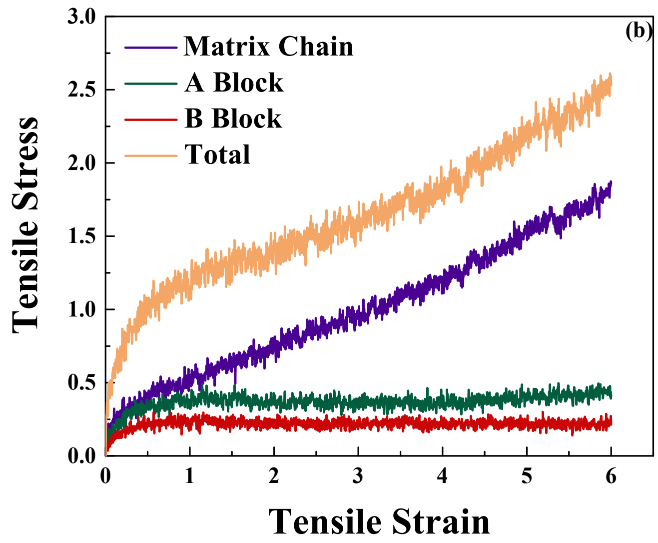
Figure S1. The radial distribution of NPs with grafted beads, diblock copolymer chains and matrix chains in the system with $L_g = 10$, $N_g = 90$ and $\alpha = 0.5$.

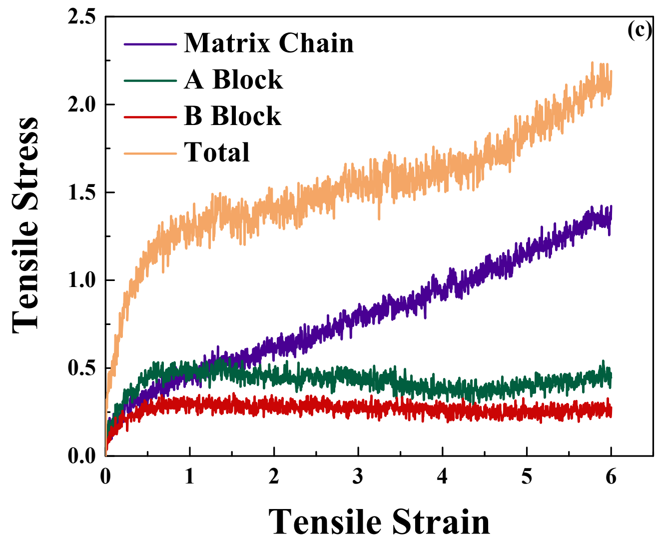
Figure S1 displays the radial distribution function of NPs with grafted beads, diblock copolymer chains and matrix chains in the system with $L_g = 10$, $N_g = 90$, and $\alpha = 0.5$. The first two peaks are located at $r = 2.5\sigma$ with the intensity of 118 and 22 separately, corresponding to the grafting point beads and A blocks beads, separately. The A blocks of diblock copolymer chains are distributed at $2.5 - 5.5\sigma$ from the mass center of the NPs, while the B blocks are distributed on the outside of the A blocks with a wide peak at about $6.0 - 7.0\sigma$. Besides, the matrix chains are interspersed with the B blocks, or are distributed outside of the B blocks because of the compatibility with B blocks.

(2) Plateau appearing in stress-strain curves

To provide a further understanding on the stress-strain behavior, we quantitatively calculate the distribution of different components on the total tensile stress as shown in Figure S2. The yellow curve represents the total tensile stress. The blue, green and red curves represent the stress component of the polymer matrix, A blocks and B blocks respectively. The total stress is mainly composed of two parts-the stretching of the matrix chain and the non-bond interactions between components. By analyzing Figure S2, we believe that the emergence of the plateau in the stress-strain curves is due to two reasons. The first reason is that the volume fraction of the matrix chain gradually decreases as the grafting density increases. In our work, we fix the total number of the matrix chain at 100. Therefore, as the grafting density increases, the stress provided by the matrix chain at the initial stage of the strain is decreasing. From the blue curve in Figure S2 we can see that the stress contributed by the polymer matrix is becoming much lower. The second reason is attributed to the non-bonded interaction between components. In our work, we define the non-bonded interaction of the same components that are attractive. Meanwhile, the B block is compatible with the matrix chain. Because the non-bonded interactions work within a certain distance and the grafted chain length is short, the stress component carried by the grafted polymer chains have a long plateau and a relatively low maximum stress value.




3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
1
2
3
4
5
6
Tensile Stress
Tensile Strain
Matrix Chain
A Block
B Block
Total
(b)


2.5
2.0
1.5
1.0
0.5
0.0
0
1
2
3
4
5
6
Tensile Stress
Tensile Strain
Matrix Chain
A Block
B Block
Total
(c)

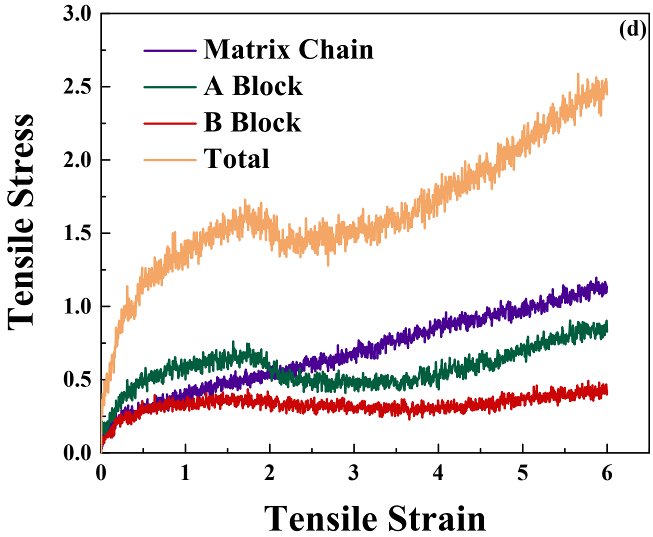


Figure S2 (a)-(d) display the tensile stress with different grafting density (from $N_g = 30$ to $N_g = 90$). The blue, green and red lines represent the stress assumed by different components during the stretching process. The yellow line represents the total tensile stress. The systems are grafted flexible diblock copolymer chains with $L_g = 10$ and $\alpha = 0.5$.