

Supporting Information

Optimizing Heterogeneous Network Structure to Achieve Polymer and its Nanocomposites with Excellent Mechanical Properties

Tongkui Yue¹, Sai Li¹, Zhiyu Zhang¹, Yulong Chen^{4*}, Liquan Zhang^{1,2,3}, Jun
Liu^{1,2,3*}

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

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

³State Key Laboratory of Organic-Inorganic Composites, Beijing University of
Chemical Technology, People's Republic of China

⁴College of Materials Science and Engineering, Zhejiang University of
Technology, People's Republic of China

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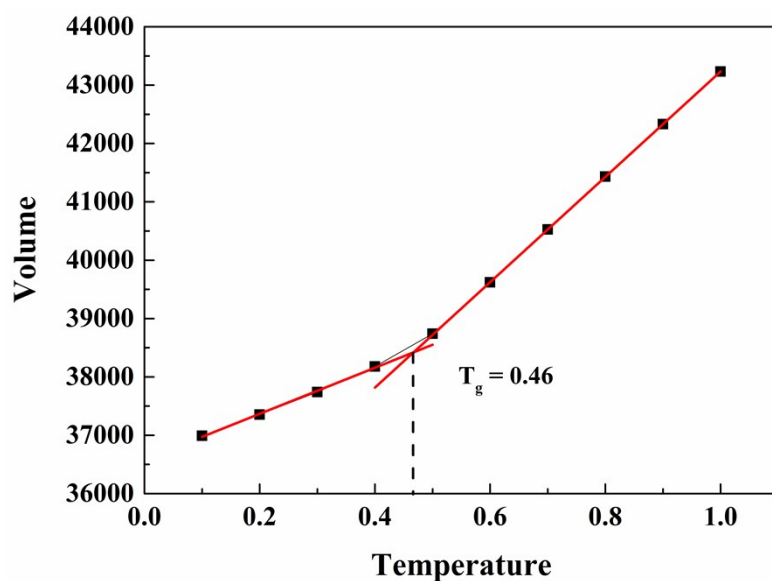


Fig. S1 The glass transition temperature (T_g) calculated by fitting the volume-temperature curve.

Glass transition temperature (T_g) was checked as a preliminary measure since our system should be in rubbery state, and from Fig. S1, it can be seen that the T_g was 0.46. Noting that the system used here is system 5 in table 3. NPT ensemble was used to cool the system from 1.0 to 0.1, and the equilibrium time at each temperature is fixed to 3ns.

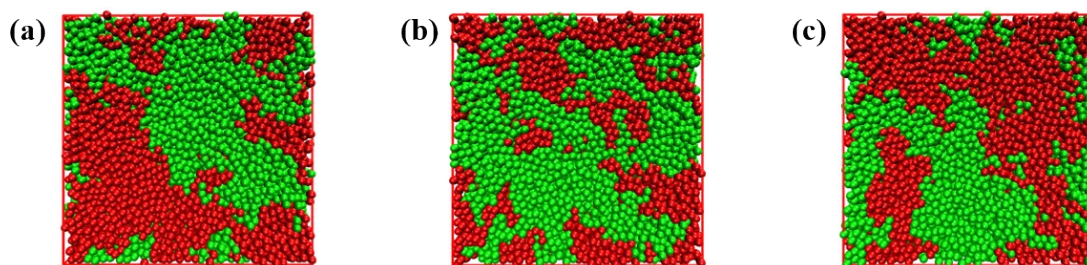


Fig. S2 Snapshots of the equilibrium state of different network structures: (a) aggregation distribution system, (b) random distribution system and (c) uniform distribution system.

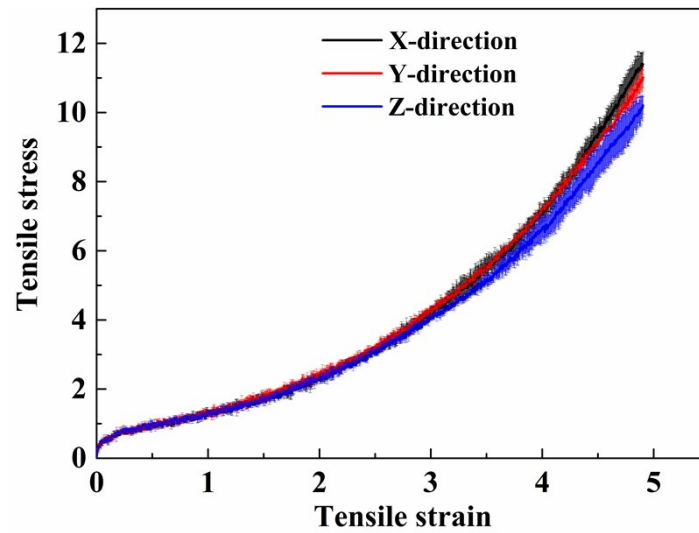


Fig. S3 Stress-strain curve obtained by stretching in different directions. The black line, red line and blue line represent stretching the system along the X, Y and Z directions, respectively.

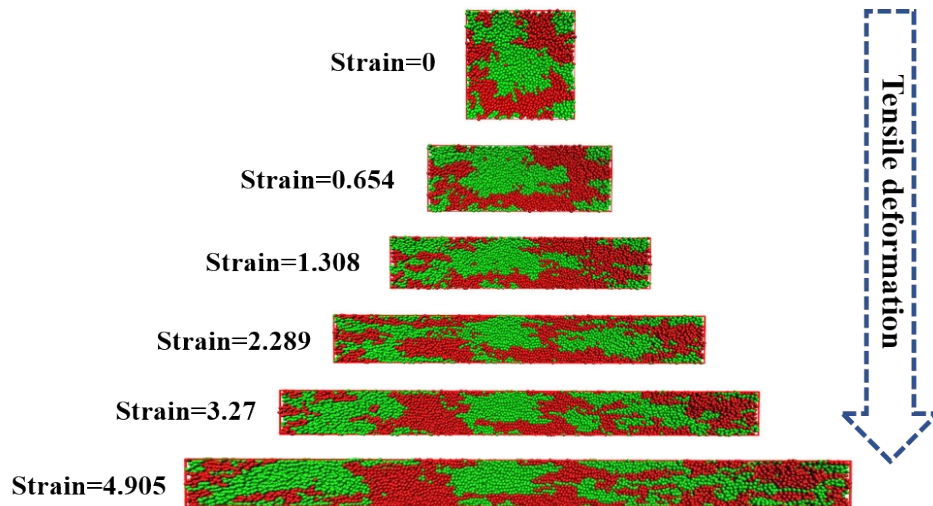


Fig. S4 The deformation of the simulation system ($\rho = 0.07$) during uniaxial stretching.

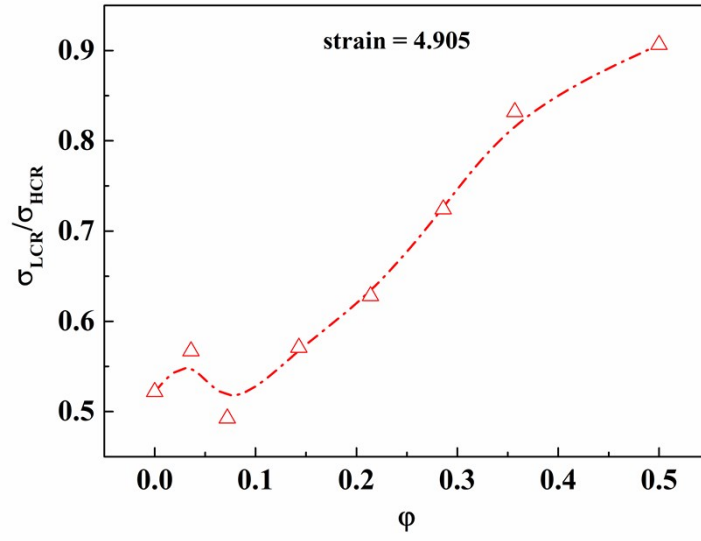
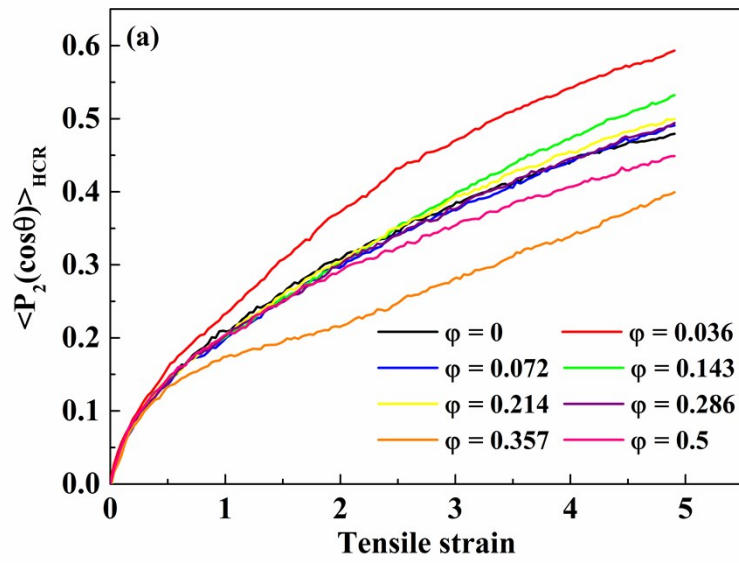


Fig. S5 Ratio of stress component of LCR to that of HCR at maximum strain.



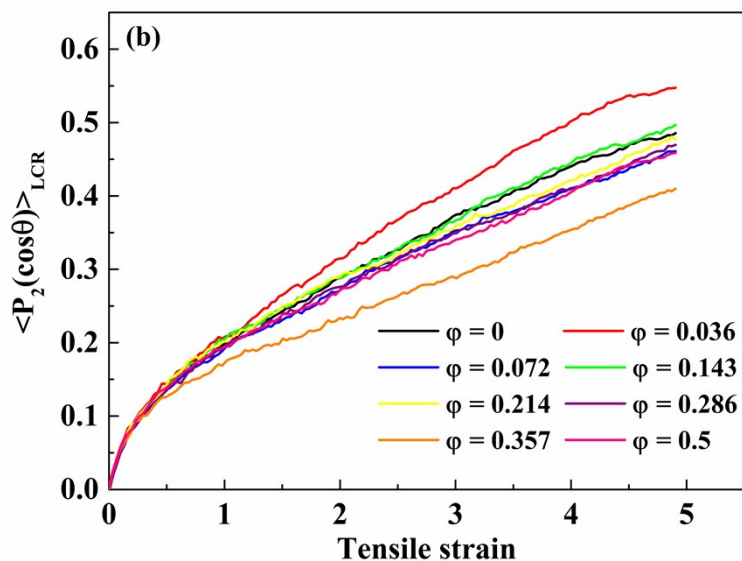


Fig. S6 The bond-orientation behavior of (a) HCR and (b) LCR in the system with different cross-linking density ratio during the stretching process.

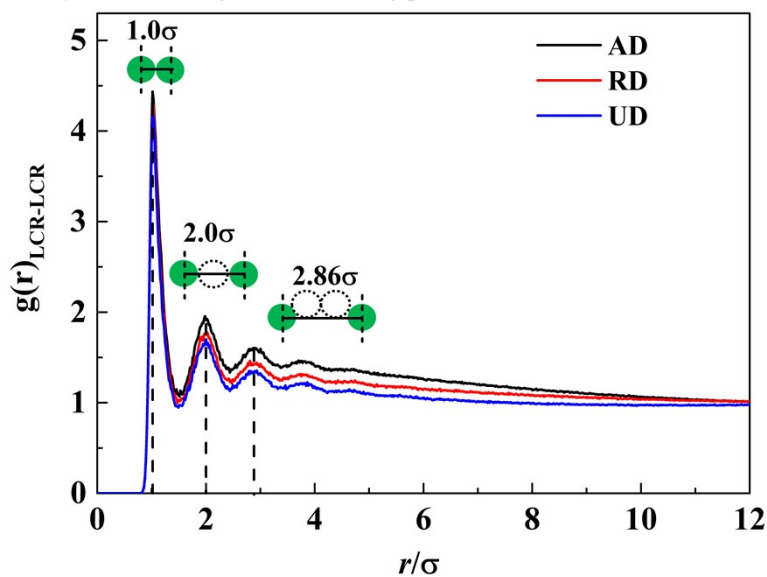


Fig. S7 The radial distribution function of the LCR in the simulated systems with different distribution states. The, black, red, and blue curves represent the aggregation distribution system (AD), random distribution system (RD) and uniform distribution system (UD), respectively.

The larger the peak, the more obvious the aggregation of LCR itself, which means that the separation degree of HCR and LCR is greater, and the distribution tends to be more aggregated.

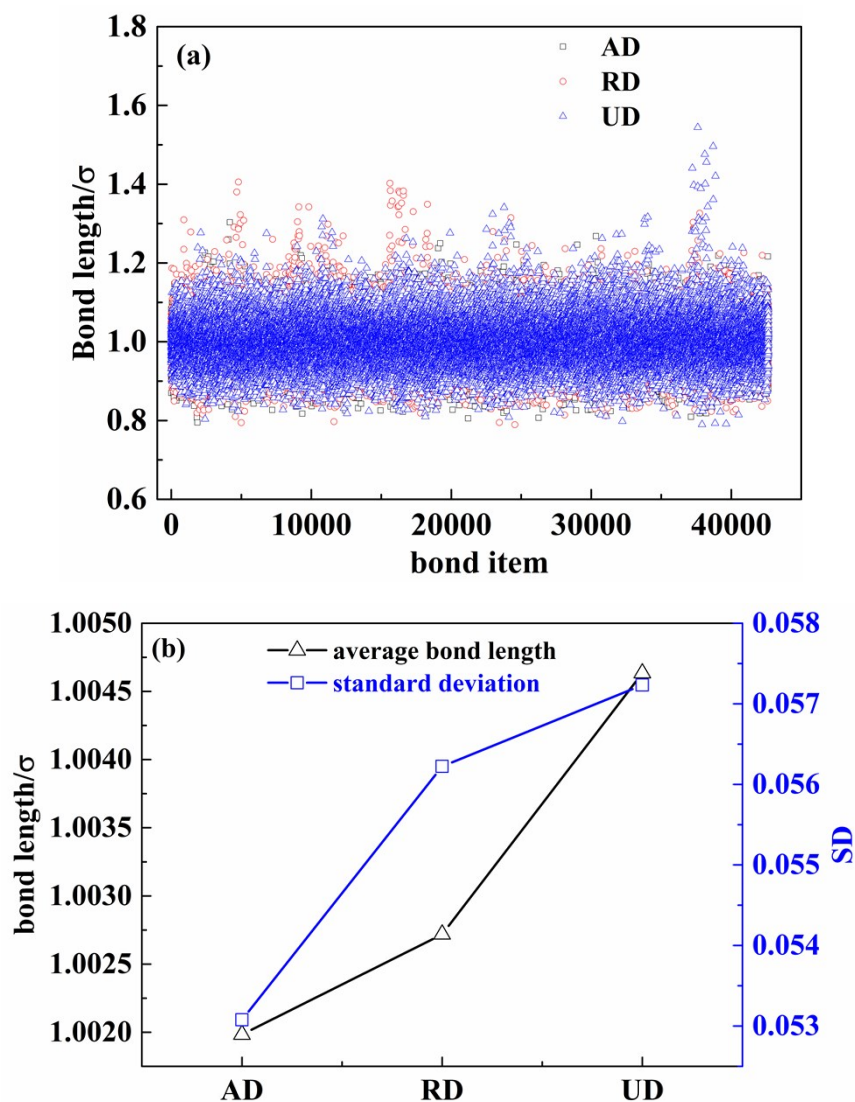


Fig. S8 (a) Bond length distribution in the last frame of stretching process. (b) Average bond length and standard deviation (SD) of different systems.

For the stretching process, if some bonds are stretched too long, other molecular chains may slip through them, which will make the model lose its authenticity. By calculating the bond length distribution, it can be found from Figure S6(a) that the maximum bond length does not exceed 1.6σ , and the length of 0.6σ except the occupied volume of the bead itself is not enough to pass through another molecular chain, indicating that our model is credible.