Phantom chain simulations for the rupture of star-polymer networks

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Despite many attempts, the structure-property relationship of network polymers is yet to be clarified. For instance, the effect of network node functionality on the network fracture has yet to be understood. This study [1,2] conducted coarse-grained simulations for polymer networks with various node functionalities and conversion rates. Figure 1 represents a schematic of the model and the simulation scheme employed. Sols of bead-spring chains without excluded volume were equilibrated and gelated via the Brownian dynamics scheme, and the resultant networks were validated regarding cycle rank, which was fully consistent with the mean-field theory. The networks were stretched until the break via the energy-minimization scheme, and the fracture behavior was characterized by strain and stress at the break and work for fracture. For the networks with monodisperse strand length but various node functionalities and conversion rates, the fracture characteristics as functions of cycle rank lie on master curves when the values are normalized according to the branch point density. The same master curves have been confirmed for networks created from mixtures of prepolymers with different node functionalities [3]. Further, the data draw the same curves for mixtures of linear prepolymers and multi-functional linkers, even though primary loops are included [4]. These results imply that the fracture behavior of polymer networks is dominated by cycle rank.

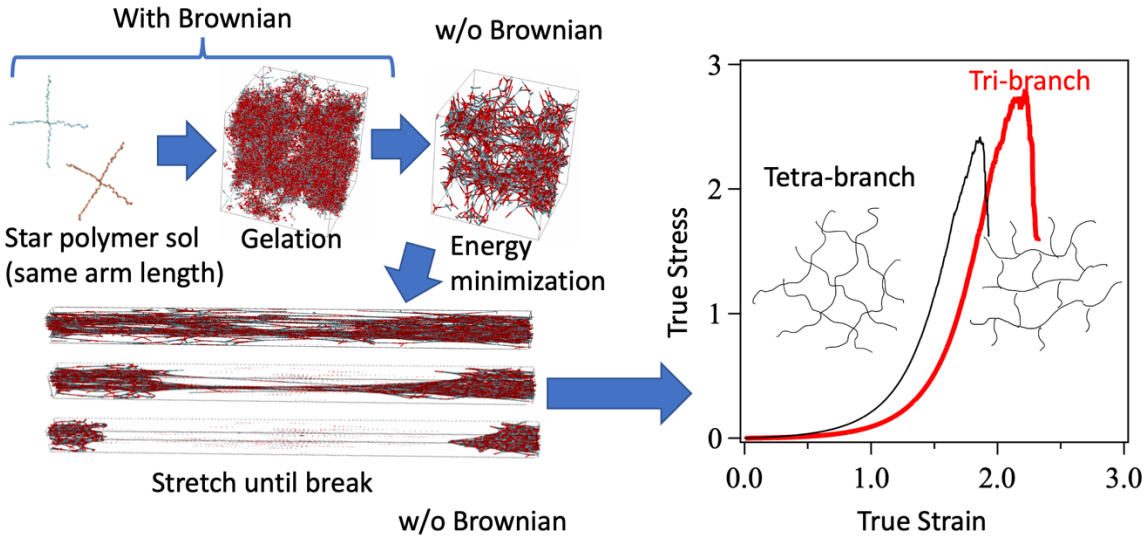

Figure 1 Schematic of the model and the simulation

References

[1] Y. Masubuchi, *et al.*, *Macromolecules*, **56**, 2217 (2023).
[2] Y. Masubuchi, *et al.*, *Macromolecules*, **56**, 9359 (2023).
[3] Y. Masubuchi, *Polymer J*, **56**, 163 (2024).
[4] Y. Masubuchi, *Polymer*, **297**, 126880 (2024).

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