Using Mesoscopic Models to Design Strong and Tough Biomimetic Polymer

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We use the lattice spring model (LSM) to simulate the globules and the crosslinked network. We utilize our modified Hierarchical Bell model (MHBM) to simulate the rupture and reforming of $N$ parallel bonds. We demonstrate that the mechanical properties of the system are sensitive to the values of $N_{in}$ and $N_{out}$, the respective values of $N$ for the intra- and inter-molecular bonds. We find that the strength of the material is mainly controlled by the value of $N_{out}$, with the higher value of $N_{out}$ providing a stronger material. We also find that if $N_{in}$ is smaller than $N_{out}$, the globules can unfold under the tensile load before the sample fractures and thus, can increase the ductility of the sample.