Simulation of polymer network formation: Phase behavior of aggregating chains

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Filamentous biological materials display highly nonstandard mechanical response, among which a strong tendency to stiffen with increasing strain. This behavior is, in large part, determined by the stiffness of the constituent fibers and the degree of crosslinking among them. To replicate some of the properties of biological materials in a synthetic, self assembling system we study, experimentally and theoretically, the phase behavior of long, repeating copolymer motifs which alternate strongly hydrophobic bis-urea core blocks with long PEG spacers whose length may be varied. By tuning the relative importance of spacer entropy and core attractive energy, these molecules may either collapse, behave as random coils, or form an intermediate, network-like aggregate which shares important morphological characteristics with filamentous bionetworks. We present results from molecular dynamics studies of the phase behavior, and compare to the experimental findings.