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Coarse-Grained Modeling of the Mechanical Properties of Entangled Polymer Systems BRIAN PASQUINI, FERNANDO ESCOBEDO, YONG L. JOO, Cornell University — The complexity of entangled polymer interactions is a promising area for simulation studies to build upon polymer physics theories; however, it is necessary to use a coarse-grained approach to simulate the dynamic response of large polymer systems. Such studies have been done by treating the entanglement interactions as a set of entanglement points, which serve as the ends for the coarse-grained simulation unit. One method from literature (Smith and Termonia) formulates the free energy of an entanglement network based exclusively on neighboring entanglement points and uses temporary bonds which break as the simulation progresses. Another method (Terzis, Theodorou and Stroeks) treats the coarse-grained units as delocalized polymer density clouds, and formulates an expression for the free energy based on local polymer density. The first method has been extended to three dimensions for direct comparison to the second in tensile strain experiments. These models also show promise to understanding microstructure effects on mechanical properties in materials such as spider silk.

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