

597b Coarse-Grained Modeling of Sol-Gel Materials

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We present a simple coarse-grained model of silica sol-gel materials which is applied to investigate the structural and mechanical properties of these systems. Our model, unlike many previous developments, is fully flexible and can account for bond breaking and creation upon motion of the gel structure. Simulations of gel formation, syneresis, compression, extension, and shear are performed and microscopically analyzed in order to correlate macroscale behavior with local gel structure and its evolution.