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Structure and dynamics of random block copolymers in the bulk and thin films MARCUS MÜLLER, BIRGER STEINMÜLLER, Georg-August University, Göttingen, Germany, KEITH H. HAMBRECHT, GRANT D. SMITH, DMTIRY BEDROV, University of Utah, Salt Lake City — Using a soft, coarse-grained model and a Lennard-Jones bead-spring model, we study the morphology of random block copolymers in the bulk and in contact with a hard wall that preferentially attracts one component. We show that both coarse-grained models yield similar equilibrium morphologies at intermediate and long length scales, and identify a mapping between the parameters of the two models. For most parameters we observe a disordered, microemulsion-like morphology. We study the single-chain dynamics in the bulk and in contact with a preferential surface. The relaxation times of the soft, coarse-grained model is about two orders of magnitude faster than the Lennard-Jones bead-spring model. In both models the relaxation time increases with segregation but the Lennard-Jones bead-spring model is additionally slowed down by the densification of the local packing at low temperatures. We employ the soft, coarse-grained model to generate starting configurations for the bead-spring model. Then, the bead-spring model is quenched below its glass transition temperature, and we investigate the local mechanical properties of the disordered, yet structured morphology.

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