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Molecular simulation study of random block copolymer films prepared through solvent evaporation DMITRY BEDROV, KEITH HAMBRECHT, GRANT SMITH, University of Utah — Molecular simulations have been used to study equilibrium and non-equilibrium morphologies of random block copolymer films prepared through solvent evaporation. The polymer chains are comprised of "A" and "B" beads connected by FENE springs. Chains comprised of six blocks (ten beads each) and representing all possible combinations of A and B blocks were used to form films with 50/50 A/B fraction. Bead-bead interactions were chosen such that one of the blocks had higher glass transition temperature than the other and that the A and B blocks were incompatible in absence of the solvent. Initially the polymer chains were dissolved in a monomeric solvent at 75/25 solvent/polymer ratio. Then, polymer films were formed through solvent evaporation at various processing parameters. The nanoscale structure and viscoelastic properties of the polymer were investigated as a function of solvent quality, segment incompatibility and rate of evaporation. It was found that when the temperature is below the glass transition temperature of one of homopolymers, the morphology and properties of the film are strongly dependent on evaporation rate.

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