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Plastic deformation of triblock elastomers by molecular simulation AMANDA PARKER, University of British Columnbia, JÖRG ROTTLER, The University of British Columnbia — The mechanical properties of thermoplastic elastomers (TPE) can be greatly enhanced by exploiting the complex morphology of triblock copolymers. A common strategy consists of confining chain ends into hard glassy regions that effectively crosslink a soft rubbery phase. We present molecular dynamics simulations that provide insight into key microscopic behaviour of the copolymer chains during deformation. First, a coarse-grained polymer model with an ABA type configuration and soft interactions is employed to achieve equilibrated spherical morphologies. Our model TPEs contain at least 30 spheres in order to ensure configurational averaging. Elastoplastic deformation with uniaxial extension or volume conserving shear is then studied after hard excluded volume interactions have been reintroduced. We consider trends of stress-strain curves for different chain lengths, and compare to equivalent homopolymeric systems. During deformation we simultaneously track the evolution of the number and shape of the minority spheres, the proportion of chains bridging from one sphere to another, as well as local plastic deformation. The simulations reveal strong differences between deformation modes, the evolution of sphere morphology and chain anisotropy.

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