

Multiscale Simulation of the Shape Deformation of a Glassy Polymersome

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Vesicles composed of diblock copolymers, or polymersomes, have proven to possess numerous applications ranging from drug delivery to catalytically driven nano-motors. The shape of a polymersome can be responsive to external stimuli, such as light or solvent. Molecular dynamics simulations reveal that the shape change upon the contraction of the inner volume of a glassy polymersome vesicles occurs in two separate regimes—a stretching regime and a bending regime. The barrier is shown to be dependent on the solvent environment. These results suggest that tailoring the bending modulus of polymer membranes can be used as a design methodology to engineer new stimuli-responsive vesicles.