254g Brownian Dynamics Simulations of Polymer Blend Droplets

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We present the results of a multiscale simulation approach which combines Brownian dynamics simulations with polymer self-consistent field theory and continuum mechanics to study the deformation characteristics of polymer droplets. We use this approach to study the influence of the bulk rheological properties, such as viscosity and elasticity ratios, upon droplet deformation. Despite the comparatively small size of our droplets and the 2-D nature of our simulations, our results agree semi-quantitatively with the asymptotic predictions for the droplet deformations. In addition, we are able to examine the effects of the droplet and the matrix Weissenberg numbers and their effects upon the droplet deformations. We also present results elucidating the influence of block compatiblizers upon the droplet deformations. Our results suggest that even trace fractions of compatiblizers can lead to significant changes in the flow fields around the droplets and their deformation characteristics. We study the influences of the molecular weight of the block copolymer, the coverage of block copolymers upon the dynamical properties of polymer blend interfaces.