Polymer Statics and Dynamics in Confined Geometries JOSHUA KALB, BULBUL CHAKRABORTY, Brandeis University — Current work on biological systems and glass forming polymers (JCP 106, 6176 (1997)) has led to an interest in the study of single polymer systems. The main questions concern relaxation phenomena and the shape adopted by single polymers under hard and soft boundaries. Little is known about the possibility of inducing a glass transition through pure dimensional confinement. We are concerned with whether or not there is a critical value of the confining length scale. Both structure and relaxation can be described using scaling arguments and tested with Monte Carlo simulations using the bond-fluctuation algorithm (Macromolecules 21,2819 (1988)), which uses a lattice representation of the polymer chain with excluded volume effects. We look at the effects of confinement on a single polymer chain by measuring quantities such as the magnitude end-to-end vector, the radius of gyration, and single monomer motion (JACS 124, 20 (2004)). A primary question is whether the self-avoidance constraint manifests itself in a manner similar to kinetically constrained models of the glass transition. Understanding how these quantities change with various confining geometries will lead to a deeper understanding of biological structures and glass formation. Work supported by NSF-DMR 0403997.

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