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Polymer Statics and Dynamics Under Box Confinement 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. We are concerned with whether or not there is a critical length scale for a confined polymer system. 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 confined to a box by measuring dynamical quantities such as the end-to-end vector and single monomer positions (JACS 124, 20 (2004)). A primary question is how spatial correlations between monomers, 'blob's, influence the dynamics. 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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