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Dynamics of melts consisting of circular and linear polymers MICHAEL LANG, MICHAEL RUBINSTEIN, Department of Chemistry, Venable Hall, University of North Carolina, N.C. 27599 — Recent experimental results indicate that small contaminations of linear polymers with 0.1% volume fraction or less in ring polymer melts lead to dramatic changes in the rheology of the melt. These volume fractions are clearly below overlap concentration of the linear species. Thus, the experimental observations cannot be explained by a simple picture based on a percolating cluster of linear chains penetrating rings. The goal of our computer simulation studies of comparable systems is to solve this puzzle. We use the bond fluctuation method on a lattice as introduced by Carmesin and Kremer (Macromolecules 21, 2819-2823 (1988)) to model homopolymer melts ranging from 32 to 1024 monomers per chain. The volume fraction of linear polymer is varied from 1/16 to zero. We simulate small melts of 16384 monomers in order to have access to the long-time behavior of the samples. We will present and discuss simulation data on diffusion, ring and linear polymer conformations, mobility and contact statistics of different samples with varying volume fraction of linear polymer.

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