Multiple Time Scales in Polymer Dynamics: Models & Simulations

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Multiple Time Scales in Polymer Dynamics: Models & Simulations

A. Stochastic Model for Dense Polymerization

- RH & Somer, JPCB 103, 1064 & 1070 (1999)
- RH, JCP 111, 7701 (1999)
- Vogt & RH, JCP 123, 144109 (2005)

1. Stochastic Model (iGLE)
2. Polymer Model
3. Qualitative Behavior: Time-Dependence!

B. Lattice Model for Dense Polymerization

- Vogt & RH, JCP 115, 1575 (2001)

1. Monte Carlo Hamiltonian in 2D
2. Monte Carlo Hamiltonian in 3D

Nonequilibrium Chemistry & Materials

- **Diffusion in Swelling/Contracting/Rotating Colloids**

- **Control and Simulation of Transport on Surfaces**

- **A Geometric Perspective on TST in Dissipative Systems**

- **MD simulations of Cybotactic Region in GXLs**

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Nonequilibrium Chemistry & Materials

• A Stochastic Model for Polymerization

• A Lattice Model for Polymerization

• Biophysics & Bioinformatics

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