Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Influence of the solvent size on the behavior in polymer solution[1]

LIJIA AN, YUNQI LI, TONGFEI SHI, Changchun Inst. of Applied Chemistry, Chinese Academy of Sciences — The effects of solvent size on properties of homopolymer solution have been investigated by Monte Carlo Simulation. Increasing the solvent molecular size leads to shrinkage of the polymer chains and increase of the critical overlap concentrations. The root-mean-square radius of gyration of polymer chains (R_g) is less sensitive to the variation of polymer concentration in solutions of larger solvent molecules. In addition, the dependency of R_g on polymer concentration under normal solvent conditions and solvent molecular size is in good agreement with scaling laws. When the solvent molecular size approaches the ideal end-to-end distance of the polymer chain, an extra aggregation of polymer chains occurs, and the solvent becomes the so-called medium-sized solvent. When the size of solvent molecules is smaller than the medium size, the polymer chains are swollen or partially swollen. However, when the size of solvent molecules is larger than the medium size, the polymer coils shrink and segregate, enwrapped by the large solvent molecules.

[1]This work is supported by the NSFC (20334010, 50503022) Programs and CAS(KJCX2-SW-H07), and Special Funds for National Basic Research Program of China(2003CB615600).

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Date submitted: 27 Oct 2006 Electronic form version 1.4