Abstract Submitted
for the OSF05 Meeting of
The American Physical Society

Monte Carlo Simulation of Reversibly Associated Network SHIHU WANG, CHUN-CHUNG CHEN, ELENA E. DORMIDONTOVA, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OH 44106 — Using the Monte Carlo simulation (MC) of bond fluctuation model (BFM) we have studied the reversible association between linear end-functionalized oligomers and crosslinkers (analogous to metal-ligand complexation) leading to network formation. The crosslinkers were capable of binding up to three oligomer end groups with different energies of association with the first, second and third end-groups respectively. By varying oligomer concentration and crosslinker/oligomer ratio in our simulations, a three dimensional structure spanning the whole system was obtained, signifying gel formation. We further studied the gel properties in terms of the average molecular weight and gel fraction. An analytical model based on the equilibrium among different associating species and classical gelation theory, was developed. This model allows prediction of fractions (concentrations) of different crosslinkers, bonded to three, two, one or none oligomer end groups as well as the sol-gel transition, which favorably compares to the simulation results.

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Date submitted: 23 Sep 2005 Electronic form version 1.4