

MAR08-2007-000466

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Application of Integral Equation Theory to Polymers in the Condensed State

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Large scale computer simulations involving many chains can be used to model the physical properties and structure of amorphous polymers, however, such simulations are computationally intensive. An alternative is to employ the approximate, but computationally less demanding, Polymer Reference Interaction Site Model or PRISM theory. PRISM theory is an extension to polymers of liquid state, integral equation theories originally developed for atomic and small molecule liquids. From a computational standpoint, PRISM theory can be viewed as a self-consistent formalism to map the statistical mechanics of the difficult many-chain system to a much simpler, single chain problem. Depending on the model, the statistics of the single chain can be solved analytically or through a single chain Monte Carlo simulation. Solution of PRISM theory yields the intermolecular and intramolecular radial distribution functions characterizing the packing of the polymer chains in the condensed liquid. These distribution functions can then be employed to compute the thermodynamic properties of the polymer system. Various applications of PRISM theory to polymer liquids, blends and copolymers will be discussed and comparisons will be made with exact MD simulations and scattering experiments. Finally, a more accurate approach will be discussed that involves mapping the many chain system to an equivalent two-chain problem.