

CPP 5: Polymer Physics II

Time: Monday 14:30–15:45

Location: H40

CPP 5.1 Mon 14:30 H40

Characterizing knots in polymer coil and globule phases— ●PETER VIRNAU¹, MEHRAN KARDAR², and YACOV KANTOR³ —
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We examine the statistics of knots with numerical simulations of a model polymer, spanning high temperature (coil) and low temperature (globule) phases. All monomers in the model interact via a Lennard-Jones potential, while adjacent beads are connected by flexible springs. Although relatively simple, this model provides a realistic description of polyethylene, thus relating the simulation results to specific polymers. We find that knots are common in the globule phase and under confinement, but rare in coils. We also associate a typical size with the knots, and find knots to be small (tight) in the swollen phase, and large (loose) in the dense phase.

CPP 5.2 Mon 14:45 H40

Dynamics of melts consisting of circular and linear polymers

— ●MICHAEL LANG and MICHAEL RUBINSTEIN — Department of Chemistry, University of North Carolina at Chapel Hill, Venable Hall, 27599 Chapel Hill, N.C., United States of America

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.

CPP 5.3 Mon 15:00 H40

On the influence of excluded volume in polymer melts

— ●HENDRIK MEYER, JOACHIM WITTMER, and JÖRG BASCHNAGEL — Institut Charles Sadron, CNRS, 67083 Strasbourg, France

Flory's ideality hypothesis states that polymer chains in the melt have random walk like conformations as if there would be no excluded volume. However, it was shown recently that the excluded volume interaction induces corrections to scaling which are long range and which give rise to a power law decay of bond-bond correlation function [1] as well as to corrections to the Kratky plateau of the form factor [2]. In this presentation, we extend the study to dynamic quantities: The excluded volume potential is switched on gradually to study the crossover from phantom chains (representing perfect random walks described by the Rouse model) to real polymer melts. This gives evidence that subdiffusive behaviour found in contradiction to the Rouse model [3] is also caused by the excluded volume interaction.

[1] J. Wittmer, H. Meyer, J. Baschnagel et. al. Phys. Rev. Lett.

93 (2004) 147801.

[2] J. Wittmer et. al. cond-mat/0610359, cond-mat/0611322

[3] W. Paul, Chem. Phys. 284 (2002) 59.

CPP 5.4 Mon 15:15 H40

Untangling polymer systems: Structure prediction in polymer networks with quenched disorder— ●ABIGAIL KLOPPER¹, RALF EVERAERS², and CARSTEN SVANEBOG³ — ¹Max-Planck-Institut fuer Physik komplexer Systeme, Dresden — ²Laboratoire de Physique, Ecole Normale Supérieure Lyon, France — ³Department of Chemistry, University of Aarhus, Denmark

Highly concentrated liquids comprising long polymeric chains can undergo processes of cross-linking and entanglement, giving rise to intriguing macroscopic properties. The key ingredient is connective quenched disorder, which freezes the topology of the liquid in the form of a polymer network. The translational invariance in the system is spontaneously broken and the phase space is divided into disjoint ergodic regions.

Such behaviour is well-known from a large class of systems exhibiting the so-called glassy phase, characterised by randomness and slow dynamics. This opens the door to an extensive analytic formalism for structure prediction in cross-linked polymer systems. By constructing a theoretical framework which makes use of simulation data, one can draw from these techniques without resorting to microscopic detail and otherwise unphysical assumptions. In the study presented, the spin-glass replica formalism is applied to data from molecular dynamics simulations of ideal non-interacting cross-linked polymer systems in order to describe neutron scattering measurements in interacting systems.

CPP 5.5 Mon 15:30 H40

The scattering of polymer gels and networks: Origin and relation to network structure— ●MICHAEL LANG¹ and JENS-UWE SOMMER² — ¹University of North Carolina, Department of Chemistry, Venable Hall, 27599 Chapel Hill, N.C., United States of America — ²Leibniz Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden

We utilize computer simulations to directly relate connective and topological structure, density, and particle fluctuations with the scattering of polymer gels. We observe density fluctuations on three different length scales upon swelling independent of whether the original sample was homogeneous or heterogeneous in the dry state. The observed density fluctuations and length scales are a) dynamic fluctuations on the length scale of single monomers or substrands of the polymer chains due to thermal fluctuations, b) static density fluctuations on the length scale comparable to the size of prime network rings which result from network connectivity, and c) static density fluctuations on length scales larger than the size of network rings due to frozen in density fluctuations of the elastically active material, whereby origin, length scale, and amplitude of these longest fluctuations depend mostly on the preparation conditions of the sample. Connective and topological analysis, scattering curves, dynamic as well as static spatial density profiles, and the pair correlations of cross-links and polymers are compared and discussed with the results obtained from polymer solutions at the same concentrations.