CPP 24: Poster: Polymer Dynamics

Time: Tuesday 18:00–20:00 Location: P2

CPP 24.1 Tue 18:00 P2

Adsorption and external stimulation of single polymer chains — •Kirsten Dammertz, Alexander Gerstmayr, Masoud Amirkhani, and Othmar Marti — Department of Experimental Physics, Ulm University

In the presented work, we study the behavior of externally stimulated single polymer chains (exposed to different vapors or electric fields) interacting with substrates like mica or graphite. Conformational changes and reorientation of adsorbed polymers are visualized by means of an advanced, custom-made atomic force microscope (AFM).

To verify our data and analyze the underlying chemical and physical processes, we perform molecular dynamics (MD) simulations. Moreover, we use Monte Carlo (MC) and density functional theory (DFT) simulation techniques to improve our analysis and to compare the experimental result with prior assumptions [1,2].

[1] Gallyamov et al., Macromol. Rapid Commun. 2005, 26, 456-460
[2] Gallyamov et al., Macromol. Chem. Phys. 2007, 208, 164-174

CPP 24.2 Tue 18:00 P2

Monte Carlo Studies of Semiflexible Branched Polymers — •Ganna Berezovska, Maxim Dolgushev, and Alexander Blumen — Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

An important class of macromolecules are the branched polymers. Their properties depend both on their topology (in which the branching points play a fundamental role) and also on the degree of semiflexibility of their segments. While analytical investigations are possible under idealized conditions [1], numerical simulations are required under more realistic situations. Here we make use of the bond fluctuation model (BFM). While previous investigations used BFM ideas either for flexible branched structures or for semiflexible linear chains, our simulations allow to account both for branching and also for semiflexible behavior. Examplary, we apply the method to study polymers, whose topological structures correspond to the simplest pair of cospectral graphs. Such graphs are mathematically and chemically very important since they have the same Laplacian spectra although being topologically different. Hence, in a generalized Gaussian framework, flexible polymers whose structures are cospectral graphs are predicted to be indistinguishable under usual dynamical measurements. According to our new mathematical-analytical study [2], introducing semiflexibility allows to differentiate between such pairs of polymers. This is qualitatively confirmed by our simulation results [2].

[1] M. Dolgushev, A. Blumen, J. Chem. Phys. 131, 044905 (2009).
[2] M. Dolgushev, G. Berezovska, A. Blumen, J. Chem. Phys. 133, 154905 (2010).

CPP 24.3 Tue 18:00 P2

Segregation of Identical Flexible Chains in Solution — •Ron Dockhorn[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany

We study the segregation of two long chains from parallel but randomly twisted start conformations under good solvent conditions using Monte Carlo simulations. For investigation of the segregation process we focus on the center of mass separation between the two chains and the average square distance between the monomers which were connected before segregation starts. We argue that segregation is dominated by free diffusion of the chains assuming that untwisting can be achieved by Rouse-like fluctuations on the length scale of the twisted loop. The free diffusion hypothesis is confirmed in the scaling analysis of individual chain dynamics, and segregation measures follow this scaling nearly. Long chains, however, show retardation effects which can be described by a new dynamical exponent which is slightly larger than the dynamical exponent for Rouse-like diffusion. Our results indicate that nearly free diffusion of chains during a time scale of a few Rouse-times can lead to segregation of chains. These results are applicable for DNA in eukaryotic cells and their chromatin segregation after replication.

CPP 24.4 Tue 18:00 P2

Multiple-quantum NMR observations of constraint release and contour-length fluctuation — •Marie-Luise Lehnich and Kay Saalwächter — Institut für Physik-NMR, Universität Halle, Betty-Heimann-Str. 7, 06120 Halle

The behaviour of entangled melts is still not fully understood. The predictions of de Gennes' famous reptation concept can be observed directly with ^{1}H multiple-quantum NMR. We monitor the dynamics of long-chain polymer melts over 5 decades in time. The regimes II-IV of the tube model are covered with this technique. The fixed-tube model, which is a combination of Rouse theory for unentangled melts and the reptation model, describes the mechanical data insufficiently. This causes ongoing discussions on also including the dynamics of the tube itself. Contour-length fluctuations (CLF) and constrained release (CR) could be the reason for the motion of the tube.

In extending previous work [1], we diluted protonated chains in matrices of deuterated chains, which are invisible in ^{1}H NMR. With this method, the influence of the "tube" can be analysed in an isolated fashion. The effects of CR and CLF can be separately studied.

[1] F. Vaca Cháves and K. Saalwächter. NMR Observation of Entangled Polymer Dynamics: Tube Model Predictions and Constrained Release, Phys. Rev. Lett., 104, 198305 (2010)

CPP 24.5 Tue 18:00 P2

Zipping dynamics of semiflexible polymers — Fabian Heisterkamp and •Jan Kierfeld — Technische Universität Dortmund, Fakultät Physik, Otto-Hahn-Str. 4, 44227 Dortmund, Germany

The adhesion or zipping of two polymers plays an important role in many biological processes, for example the formation of filament bundles in the cytoskeleton. We investigate the dynamics of a zipping process with polymer ends attached to two large beads using Brownian dynamics simulations and analytical arguments. In the limit of large adhesion we find circular trajectories of the end beads. Simulations for realistic parameter values exhibit deviations due to bending forces and buckling.

CPP 24.6 Tue 18:00 P2

Rotational and translational diffusion in hyperbranched polyglycerols — •Tilman Schubert, Joshua Rume Sangoro, Ciprian Iacob, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Molecular dynamics of hyperbranched polyglycerols of different molecular weights is studied by Broadband Dielectric Spectroscopy (BDS). The results for the characteristic quantities (structural alpha-relaxation rate and diffusion rate) are combined with the findings of PFG-NMR, rheology and calorimetry. Three different dielectric relaxation processes are observed. Upon application of Maxwell's relation to the rheology data structural relaxation rates are obtained corresponding to the slowest dipolar relaxation from BDS measurements. Extrapolated to lower temperatures, agreement is found with the glass transition temperatures measured by DS calorimetry. The results are discussed within the framework of recent theories of the dynamic glass transition.

CPP 24.7 Tue 18:00 P2

Patterned Polymer Carpets — •Ihsan Amin[1], André Beyer[2], Marin Steenackers[3], Rene Schubel[1], Ning Zhang[3], Armin Gölzhäuser[2], and Rainer Jordan[1] — [1]Professur für Makromolekulare Chemie, Department Chemie, TU Dresden, Zellescher Weg 19, 01069 Dresden, Germany — [2]Physik supramolekularer Systeme, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany — [3]Wacker-Lehrstuhl für Makromolekulare Chemie, TU München, Lichtenbergstrasse 4, 85747 Garching, Germany

We report on the first example for the fabrication of patterned polymer carpets. Polymer brushes of styrene and 4-vinyl pyridine were grafted by self-initiated surface photopolymerization and photografting (SIPGP) on a 2D framework of fully crosslinked and chemically patterned nanosheets. The grafted polymer brushes were observed over the entire nanosheets with a preferred grafting on the functionalized nanosheet areas. This results in continuous polymer carpets with an intact nanosheet framework but with amplification of the chemical patterning into a 3D topography of the grafted polymer brush. In the case of negative patterned nanosheet, the patterned carpet could be prepared as freestanding ultrathin membranes. Furthermore, swelling experiments with poly(4-vinyl pyridine) carpets showed that the direction of the resulting buckling of the flexible carpet is correlated to the

patterning. This may open the possibility of the development of micro- or nanoactuator devices with anisotropic responds upon environmental changes.