CPP 32 Polymer dynamics

Zeit: Mittwoch 11:15–12:30 Raum: TU C130

CPP 32.1 Mi 11:15 TU C130

Time resolved FTIR-Spectroscopy on Segmental Reorientation of Nematic Elastomers Under External Mechanical Fields — •Michael Tammer[1], Jianjun Li[1], Ansgar Komp[2], Heino Finkelmann[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig — [2]Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie, Stefan Meier-Str. 31, 79104 Freiburg

Time dependent polarized Fourier Transform Infrared (FTIR) spectroscopy is employed to study the segmental orientation and mobility of liquid crystalline elastomers (LCEs) with monodomain structure in response to external mechanical fields parallel and perpendicular to the nematic director. The reorientation and order parameter of the molecular moieties referring to the backbone, the spacer molecules and the mesogens are analyzed in detail. For parallel stretching, nearly no angular excursion is observed while the order parameter as measured by the IR dichroism of the different molecular segments is changed. For strain applied perpendicular to the mesogen orientation, a threshold is found in the reorientation process which varies strongly with the network density. Under sufficient high strain the network is no longer stable, i.e. a continuous reorientation is found while the order parameter dramatically decreases.

CPP 32.2 Mi 11:30 TU C130

Long-range correlations in polymer melts — •Hendrik Meyer, Joachim Wittmer, and Jörg Baschnagel — CNRS Institut Charles Sadron, 67083 Strasbourg, France

It is commonly accepted that in concentrated solutions or melts high-molecular weight polymers display random-walk conformational properties without long range memory between subsequent bonds. This has been anticipated already in the 1950s by Flory in his famous "ideality hypothesis". The absence of memory means that the correlation function, $C(n)$, of two bonds separated by n monomers along the chain should exponentially decay with n. This is the standard basis for defining an important experimental measure of chain stiffness, the persistence length.

We present numerical results and theoretical arguments, demonstrating a non-exponential, long ranged decay of $C(n)$ suggesting a profound analogy with the well-known long range velocity correlations in liquids and granular materials we find $C(n)$ to decay algebraically as $n^{-3/2}$.

J. Wittmer, H. Meyer, J. Baschnagel, A. Johner, S. Obukhov, L. Mattioni, M. Müller, and A.N. Semenov; Phys. Rev. Lett. **93** (2004), 147801.

CPP 32.3 Mi 11:45 TU C130

Molecular Dynamics simulation of active particles and polymers with full hydrodynamics — •Thomas Ihle[1], Erkan Tuzel[2], Vasanthi Iyengar[3], and Daniel Kroll[1] — [1]Department of Physics, North Dakota State University, Fargo, ND 58105, USA. — [2]School of Physics and Astronomy, 116 Church Streeet SE, University of Minnesota, Minneapolis, MN 55414, USA — [3]Institute for Computational Physics, Stuttgart University, 70565 Stuttgart

A recently introduced particle-based model for fluid flow, called Stochastic Rotation Dynamics, is a promising tool for the coarse-grained modeling of a fluctuating fluid, particularly for colloidal and polymer suspensions. SRD acts as a "hydrodynamic heat bath", the details of which are not fully resolved, but provides the correct hydrodynamic interactions between embedded objects. We explain the coupling between the fluid algorithm and the polymers which are treated by conventional Molecular Dynamics. The polymers can grow and shrink at both ends and can be connected by a class of proteins called molecular motors. Preliminary results for the observed patterns, orientational ordering, length distributions and drift of the chains will be presented.

CPP 32.4 Mi 12:00 TU C130

Molecular dynamics in semifluorinated side-chain Polyesters as studied by Broadband Dielectric Spectroscopy — •Julius Tsuwi[1], Lutz Hartmann[1], Liane Häussler[2], Dieter Jehnichen[2], Doris Pospiech[2], and Friedrich Kremer[1] — [1]Institute for Experimental Physics I, University of Leipzig,Linné Straße 5, 04103 Leipzig, Germany — [2]Leibniz-Institute of Polymer Research Dresden, Hohe Straße 6, 01069 Dresden, Germany

The molecular dynamics in fluorinated side-chain (SC) polyesters was studied using Broadband Dielectric Spectroscopy (0.1Hz to 10MHz) at temperatures from 120 K to 500 K. It is observed that the fluorinated SC exhibits γ and δ-like relaxations. The γ process is assigned to librational fluctuations at the terminal position of the SC while the δ-like process reflects a cooperative motion of the SC as a whole. Two more processes, which are associated with main chain motion, are observed: A β process assigned to fluctuations of the carbonyl groups together with the phenyl ring and an α relaxation being the glass transition process. With respect to the flexibility of the main chain based on the analysis of the activation plot, it is concluded that a flexible main chain exhibits faster mobility in direct contrast to its side chain motion. On the other hand, the less flexible backbone show the reverse trend. The dielectric results are supported by DSC and temperature dependent SAXS. References [1] Gottwald A, et.al (2002) Macromol.Chem.Phys.203: 854[2] Tsuwi J, et.al(2004); Macromolecules 37:6050 [3]Tsuwi J, et.al;Coll.Poly.Sci.(subm.)[4] Tsuwi J,et.al;J.Poly.Sci.B (in prep.)

CPP 32.5 Mi 12:15 TU C130

Intra-molekulare Reaktionen in linearen und nichtlinearen Polymerisationen — •Michael Lang, Dietmar Göritz und Stefan Kreitmeier — Fakultät für Physik, AG Polymerphysik, Universität Regensburg, 93040 Regensburg

In diesem Beitrag wird ein allgemeiner Ansatz zur vereinfachten Beschreibung von intra-molekularen Reaktionen für lineare und nichtlineare Polymerisationsreaktionen vorgestellt und mit geeigneten Computer-Simulationen überprüft. Mit den Ergebnissen kann der Einfluss intramolekularer Reaktionen auf die Verschiebung des Sol-Gel Überganges beschrieben werden. Außerdem ist es möglich, den Einfluss auf die Molekulargewichtsverteilungen oder den Volumenanteil des aktiven Materials im Netzwerk zu berechnen. Die Analogie zu linearen Reaktionen in der vorgestellten Theorie erlaubt zudem, Polymerisationen von linearen Vergleichssystemen zur Bestimmung von intra-molekularen Reaktionen in verzweigenden Systemen zu verwenden.