CPP 34: Poster: Elastomers and Gels

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 34.1 Wed 17:30 Poster C

4-arm Star Polymer Networks — •Konrad Schwenke[1,2], Michael Lang[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany

We simulate solutions of 4-arm star polymers with stars of two different types A and B with the help of the Bond Fluctuation Model. We use these solutions to construct networks out of the stars where only types A and B are allowed to react with each other. It is investigated how the properties of the star polymer networks depend on the initial polymer concentration and on the size of the stars. One property that we focus on is the ratio of defects in the network, where we see a strong concentration dependence. This system also serves as a model for networks obtained from non-linear precursors. Our work is motivated by experimental results of Sakai et al [1] who synthesized this novel kind of network which resulted in particular homogeneous model-like network structures.

[1] Sakai et al, Macromolecules 2008 41 (14), 5379-5384

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Stress relaxation and viscoelasticity of physically crosslinked networks — •Stephan Baeurle[1], Atsushi Hotta[2], and Andrei Gusev[3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Universitätstr. 31, 93053 Regensburg, Germany — [2]Department of Mechanical Engineering, Keio University, 3-14-1 Hiyoshi Kohoku-ku, Yokohama 223-8522, Japan — [3]Department of Materials, Institute of Polymers, ETH, CH-8093 Zurich, Switzerland

In this presentation we report on a new semi-phenomenological theory, to describe and explain the long-time stress relaxation behavior as well as viscoelasticity of thermoplastic elastomers composed of styrenic-block copolymers. The investigated materials form networks of glassy polystyrene crosslinks, which are physically linked by soft rubbery chain segments made of either polybutadiene or polyisoprene. We demonstrate that the model correctly reproduces the crossover from power-law to stretched-exponential behavior of the stress relaxation at a characteristic crossover temperature, found in recent tensile experiments, and that it provides new insights about the nature of the glassy state in the polystyrene crosslinks.

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Predicting water sorption and volume swelling in dense polymer systems via computer simulation — •Henning Hörstermann[1], Reinhard Hentschke[1], Marc Amkreutz[2], Michael Hoffmann[2], and Martin Wirts-Rütters[2] — [1]Bergische Universität Wuppertal, Germany — [2]Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung, Bremen, Germany

Atomistic model structures of amorphous polyamide 6 (PA-6) and of an adhesive system consisting of the diglycidyl ether of bisphenol A (DGEBA) as epoxy resin and isophorone diamine (IPD) as curing agent are generated. In the case of the adhesive, we use a new approach for the generation of the cross-linked polymer networks. This takes into account the chemical reaction kinetics of the curing reaction and thus, results in more realistic network structures. Based on these, the equilibrium water content and the swelling ratio of the DGEBA + IPD networks and the amorphous PA-6 are calculated via computer simulation for different thermodynamic conditions. Therefore, we use a hybrid method combining the molecular dynamics technique with an accelerated test particle insertion method. Our results are in reasonable agreement with experiments and, in the case of the PA-6 system, with results from other computer simulation methods.

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Simulating coarse grained filled rubber networks under shear stress — •Fan Zhang, Nils Hojdis, and Reinhard Hentschke — Fachbereich Mathematik und Naturwissenschaften, Bergische Universität, Gauss-Str. 20, 42097 Wuppertal

A simple model for filled rubber networks is studied via stochastic dynamics simulation. The model consists of different types of masses joined via simple short-ranged potentials. One type of mass represents filler particles, whereas a second type represents equivalent rubber volume elements. The filler-filler, rubber-rubber, and filler-rubber interaction potentials may be designed according to the (statistical) mechanical properties of the different interfaces. In this exploratory study the potentials simply are harmonic and merely distinguished by different force constants. A harmonic shear stress is imposed via boundary conditions due to Lees and Edwards. Our results include $\tan\delta$ vs. temperature for different force constant combinations, shear frequencies, and amplitudes. The mapping of the model onto real materials is discussed.

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Electromechanical properties and structural changes of smectic C* liquid crystal elastomers under shear — •Periklis Papadopoulos[1], Patrick Heinze[2], Wilhelm Kossack[1], Friedrich Kremer[1], and Heino Finkelmann[2] — [1]Universität Leipzig, Institut für Experimentelle Physik I — [2]Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie

Liquid crystal elastomers combine the electrical and optical properties of liquid crystals with the mechanical ones of polymer networks. In smectic C systems, doping with chiral mesogen induces the formation of domains with permanent electric dipole moment, which exhibit piezoelectric properties. During the simultaneous crosslinking and orientation of the mesogen in a magnetic field a polydomain morphology is obtained, where the piezoelectric effects are averaged out on a macroscopic length scale. The application of shear breaks the symmetry and induces the formation of monodomain structure. In this study the structural changes during stepwise shear are compared with the measurements of the direct piezoelectric effect. It is shown that the piezoelectric coefficient reaches its maximum at a certain shear angle that corresponds to the completion of polydomain to monodomain transformation. The complex coefficient shows a strong dependence on temperature, especially near the smectic to isotropic transition, but also on the static mechanical stress and frequency. The effects are discussed with respect to system non-linearity.