CPP 3: Polymer Networks and Elastomers

Time: Monday 9:30–12:15 Location: H40

Invited Talk CPP 3.1 Mon 9:30 H40

Orientation effects in polymer networks — •Vladimir Toshchevikov — Leibniz-Institut für Polymerforschung Dresden e.V.

Crosslinked polymer networks remain a subject of extensive investigations due to their importance for technical applications and everyday life. Mechanical properties of these materials are determined by the change of conformations of network strands and by reorientation of chain segments under external stimuli. Incorporation of functional moieties, which can form the orientation order under external stimuli, into polymer networks opens up fascinating possibilities for creation of novel stimuli-sensitive smart materials. The present overview deals with recent theoretical developments to describe the influence of the orientation order on the mechanical properties of polymer networks. In particular, effects of the orientation order, which appears in liquid-crystalline networks [1] and in functional crosslinked polymers under mechanical [2] or electromagnetic fields [3], on the shape and on the static and dynamic moduli are discussed. The Gaussian approach for describing the statistics and mechanical properties of polymer networks is verified. [1] V. Toshchevikov et al. Macromolecules 42 (2009), 3417. [2] V. Toshchevikov et al. Macromol. Theory Simul. 19 (2010), 195. [3] V. Toshchevikov et al. J. Phys. Chem. B 116 (2012), 913; 118 (2014) 12297.

CPP 3.2 Mon 10:00 H40

Development of a new micro-structure based model for the stress-strain response of filler reinforced elastomers including temperature and rate-dependence — •Jan Plagge and Manfred Klüppel — DIK e.V., Hannover, Germany

A newly developed physical material model is presented, which was built on the main assumptions of the Dynamic Flocculation Model (DFM), but includes the stress-softening via the breakdown of highly stressed polymer-filler domains under load. The polymer-response is modeled with the non-affine tube model. Key parameters can be identified with exponents derived from percolation theory describing the cluster size distribution of fillers. Set stress and hysteresis are introduced via a continuous reaggregation mechanism, completely characterized by a critical stress parameter. This is implemented with a convolution-like memory kernel. Modeled stress-strain response is in perfect agreement with experiments. The critical stress parameter was predicted to be dependent of temperature and deformation rate by means of Kramers escape rate. This is confirmed for a wide range of temperatures and speeds by a fit to multihysteresis measurements carried out in a heat chamber. Fitting parameters reveal that the mechanism responsible for hysteresis and set stress takes place on the nanometer scale with energies of roughly 100 kJ/mol, possibly rearrangement of primary filler particles. To conclude, the newly developed model reproduces all major rubber characteristics with a small set of physically motivated parameters, making it a promising option to further understand the complex polymer-filler interplay.

CPP 3.3 Mon 10:15 H40

Morphology and Mechanical Properties of reinforced and crosslinked Polymer Blends containing EPDM — •Christoph Gögelein[1], John Beelen[2], Martin van Duin[2], Dina Gabriel[3], Alexander Karbach[3], and Brigitte Mosbach-Wetzka[4] — [1]Lanxess Deutschland GmbH — [2]Lanxess Elastomers B.V. — [3]Currenta GmbH & Co. OHG — [4]Bayer Technology Services GmbH

Due to stepwise improvements in polymer processing and recent catalyst developments, new Ethylene-Propylene-Diene-Monomer (EPDM) polymers of very high molar mass have recently been synthesized. These terpolymers exhibit up to date unseen strong mechanical properties, especially at elevated temperatures. In the present study, we investigate the dynamic-mechanical properties of certain crosslinked polymer blends containing EPDM reinforced with carbon black with respect to a significant increase of crack growth resistance and the fatigue lifetime without deteriorating the excellent heat stability of EPDM-based elastomers. Applications such as engine mounts, vibration isolation applications, exhaust mounts, and suspension bushings can benefit from the advantage of the saturated polymer backbone of EPDM, the strength and resilience of high molar mass EPDM, and the compounding techniques shown in this paper.

CPP 3.4 Mon 10:30 H40

Shape-memory polymer networks on the basis of high-density polyethylene — •Oleksandr Dolynchuk[1], Igor Kolesov[2,3], Hans-Joachim Radusch[2,3], and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden, Germany — [2]Martin Luther University Halle-Wittenberg, Center of Engineering Sciences, D-06099 Hale (Saale), Germany — [3]Polymer Service GmbH Merseburg, D-06217 Merseburg, Germany

Shape-memory (SM) polymers lead to many applications, in particular, as stimuli-responsive sensors and actuators. Polyethylene is considered as a promising SM material due to suitable thermal and mechanical properties, low costs and highly developed production. A theory of two-way invertible SME was developed and allowed calculation of the free energy change of high-density polyethylene (HDPE) drawn under constant load σ and cooled down below crystallization temperature. The free energy ΔF was assumed to consist of three terms: ΔF of transferring links from the amorphous to crystalline region, surface free energies, and the entropy change in the amorphous subchains. The analysis of ΔF predicted the possible morphology and orientation of crystallites generated at cooling. Experimentally determined crystallinity, size and orientation of the crystals formed in HDPE under different σ were compared with theoretical predictions got by modeling the two-way SME in HDPE. All qualitative and quantitative characteristics of the two-way SME, the experimental curves of temperature dependent strain as well as the features of generated crystalline structures are in good accordance with the results of our theoretical analysis.

15 min. break

CPP 3.5 Mon 11:00 H40

Characterization of damage mechanisms in elastomers under constraint load by x-ray investigations — •Konrad Schneider — Leibniz-Institut für Polymerforschung Dresden, Deutschland

Under conditions of use very different loading situations are applied to elastomers, mainly multiaxial loading with superimposed hydrostatic tension. The load can be applied steadily as well as cyclically. Equally diverse is the damage behaviour. First steps of damage under different conditions were investigated by x-ray scattering as well as computer tomography and discussed with respect to the damage criterion.

CPP 3.6 Mon 11:15 H40

Electric- and magnetic field responsive soft materials — •Miklos Zrinyi — Semmelweis University, Budapest, Hungary

Electric-, and magnetic field sensitive polymer gels and elastomers are soft smart materials whose elastic- and thermodynamic properties are strong function of the field strength imposed upon them. Colloidal (nano-) particles with special electric and magnetic properties are built into flexible polymer matrix. The particles couple the shape of the gel (or elastomer) to the external fields. Shape distortion occurs instantaneously and disappears abruptly when electric- or magnetic field is applied or removed, respectively. Giant deformation effect, field controlled elastic modulus, non-homogeneous deformation and quick response to magnetic- and electric field open new opportunities for using such materials for various applications. The development of smart polymer composites that show spinning in static uniform field will also be presented. The rotating disk acts like micro sized motors with tuneable angular frequency.

CPP 3.7 Mon 11:30 H40

Dynamic moduli of anisotropic magneto-sensitive elastomers — •Dmytro Ivaneyko, Vladimir Toshchevikov, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

The dynamic mechanical behavior of anisotropic magneto-sensitive elastomers (MSEs) with chain-like or plane-like distributions of magnetic particles is investigated in a low-frequency regime under a uniform external magnetic field. By this study we continue our previous work [1], in which a coarse-grained network model was proposed for description of dynamic mechanical behavior of isotropic MSEs. The average positions of magnetic particles are distributed on the sites of tetragonal lattice. The lattice anisotropy is defined by the ratio α of average distances between neighboring particles along and perpendicular to the symmetry axis: $\alpha = \langle r_{\parallel} \rangle / \langle r_{\perp} \rangle$. Equations of motion for

magnetic particles take into account the influence of the elastic network and magnetic interactions between the particles under external magnetic field. It is shown that the relaxation spectrum depends on the anisotropy parameter α. The shear dynamic moduli G' and G'' of anisotropic MSEs are calculated for different geometries of application of the oscillating shear strain with respect to the magnetic field H, applied along the symmetry axis of the MSE.

[1] Ivaneyko D. et al., Soft Matter, 2015, 11, 7627-7638.

CPP 3.8 Mon 11:45 H40

Microstructural Study of SiO2 Coated Spherical Polyelectrolyte Brushes and Hollow Silica Nanoparticles as Observed by Small-Angle X-Ray Scattering — •Haoya Han[1,2], Li Li[1], Xuhong Guo[1], and Regine v. Klitzing[2] — [1]East China University of Science and Technology, Shanghai, PR China — [2]Technical University of Berlin, Berlin, Germany

Organic-inorganic core-shell silica nanoparticles and silica hollow spheres with a porous morphology and tailored structure have received many attentions due to their versatile characteristics such as non-toxicity, biocompatibility and high mechanical strength. Here nano-sized spherical polyelectrolyte brushes were successfully used as templates to synthesize monodisperse silica-coated core-shell nanospheres and hollow silica nanospheres. In order to better understand the formation mechanism of silica layer onto the brush layer and the structural details, the formed particles were systematically characterized by SAXS in combination with DLS, TEM, etc. The electron density of the outer silica layer was found higher than the inner silica layer from the SAXS fitting model. Core-shell microgel nanoparticles with polystyrene cores and crosslinked shell were further used as templates. The net-shape structure of the crosslinked shell hindered the free silica nanoparticle from going inside the brush layer. These results could promote better designs of core-shell silica nanospheres and hollow silica nanospheres, which should be ideal candidates for promising applications in drug delivery, catalysis and functional materials.

CPP 3.9 Mon 12:00 H40

Probing Polyethylene Glycol Elasticity by Single Molecule Force Spectroscopy and Molecular Dynamic Simulation — •Susanne Liese[1], Manuel Gensler[2], Stefanie Krysiak[3], Andreas Achazi[4], Beate Paulus[4], Thorsten Hugel[5], Jürgen P. Rabe[2], and Roland R. Netz[1] — [1]Freie Universität Berlin, Fachbereich Physik — [2]Humboldt-Universität zu Berlin, Department of Physics — [3]Technische Universität München, Physik Department — [4]Freie Universität Berlin, Fachbereich Chemie — [5]Universität Freiburg, Institute of Physical Chemistry

Polyethylene glycol (PEG) is a water soluble, non-toxic and very flexible polymer, which is widely used in medical and chemical applications. We investigate the elastic properties of PEG in a multi-scale approach based on a combination of ab-initio calculations, molecular dynamic simulations and single molecule force spectroscopy. A detailed analysis of the force-extension relation shows, that the entropy remains almost constant, if the polymer is stretched, which can be explained by a combination of chain stretching and conformational changes of single PEG-monomers. Our findings challenge the basic notion of polymer science, according to which polymers are entropic springs, which react to stretching with a loss of conformational entropy. Generalizing our results might be of great importance to other water soluble systems as well.