

## CPP 17: Poster: Polymer Networks and Dynamics

Time: Monday 18:30–21:00

Location: P1C

CPP 17.1 Mon 18:30 P1C

**Shear deformation of model networks: A Monte-Carlo-Study** — ●TONI MÜLLER<sup>1,2</sup>, MICHAEL LANG<sup>1</sup>, and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden — <sup>2</sup>Technische Universität Dresden

Using the bond-fluctuation model, we compare the elastic properties of end-linked model networks with model systems where either entanglements or both entanglements and excluded volume were switched off in the computer simulation. In our simulations we apply a shear-stress to the periodic simulation box and calculate the deformation in equilibrium. The goal of this study is to consider the contribution of connectivity and of topological constraints to the shear modulus separately. We expect further insight into the influence of network defects and the impact of excluded volume on the elasticity. As a result we can make a reasonable estimate for the entanglement degree of polymerization.

CPP 17.2 Mon 18:30 P1C

**Theoretical and experimental investigations of sealing systems** — ●FELIX SENF<sup>1</sup>, ROBIN FONK<sup>2</sup>, SEAN SCHNEEWEISS<sup>2</sup>, ULRICH SIMON<sup>2</sup>, and OTHMAR MARTI<sup>1</sup> — <sup>1</sup>Institut für Experimentelle Physik, Ulm — <sup>2</sup>Ulmer Zentrum für wissenschaftliches Rechnen, Ulm

The following investigation is about leak tightness between surface structures as well as material data to describe critical leakage systems. In technical applications the sealing of hardware components is described with leakage rates based on different boundaries of the system. In general, physical rules state that an absolutely sealed system is not possible. Different parameters like materials, surface structures, roughness parameters, closing forces and not least the design of the sealing system influence the function of the sealing joint. Engineer standards to describe the surface influence of sealing are only based on roughness parameters of the hardware surface. They don't consider that roughness parameters are only statistical parameters with limited information to the real sealing behavior of the joint. Therefore the real systems can show high tolerances in sealing limits. The research program is about understanding the alignment between elastomers and metal surface structures and the resulting open volumes. The theory of contact problems, FEA simulation tasks and compression experiments help us to describe this alignment. An experimental set up for leakage measurements and the combination with CFD simulation are the main part to understand the leakage nature more detailed. Out of this toolbox we want to create a new practical understanding on how sealing works.

CPP 17.3 Mon 18:30 P1C

**Low-frequency dynamics of anisotropic magneto-sensitive elastomers** — DMYTRO IVANEYKO, ●VLADIMIR TOSHCHÉVIKOV, and MARINA SAPHIANNIKOVA — Leibniz-Institut für Polymerforschung Dresden

The low-frequency dynamics of magneto-sensitive elastomers (MSEs) with isotropic, chain-like and plane-like distributions of magnetic particles is studied under a uniform magnetic field  $H$ . A coarse-grained network model is used, in which the magnetic particles are positioned on the sites of a tetragonal lattice [1]. The lattice anisotropy is defined by the ratio  $\alpha$  of average distances between neighboring particles along and perpendicular to the symmetry axis of an MSE. In our calculations we take into account the influence of the elastic network and magnetic interactions between the particles under the magnetic field. It is shown that the relaxation spectrum of MSE depends on  $\alpha$ . The dynamic storage  $G'$  and loss  $G''$  moduli are calculated for three different geometries of application of the oscillating shear strain with respect to the symmetry axis of MSE, coinciding with the direction of  $H$ . The application of the magnetic field leads to a strong anisotropy of  $G'$  and  $G''$  moduli. Moreover,  $G'$  and  $G''$  can change up to several orders of magnitude in agreement with recent experiments.

[1] Ivaneyko D. et al., *Soft Matter*, 2015, 11, 7627-7638; Ivaneyko D. et al., *Soft Matter*, 2016, submitted.

CPP 17.4 Mon 18:30 P1C

**FORC measurements in magnetic elastomers using molecular dynamic simulations** — ●ALLA DOBROSERDOVA<sup>1</sup>, PEDRO ANTONIO SANCHEZ ROMERO<sup>2</sup>, JULIA LINKE<sup>3</sup>, THOMAS GUNDERMANN<sup>3</sup>, SOFIA

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Magnetic elastomers consists of magnetic particles distributed in a non-magnetic elastic matrix. We use the FORC (first-order reversal curves) diagrams [C. R. Pike et al., *J. Appl. Phys.* 85, 6660 (1999)] to study how the matrix influences the internal magnetic interactions. Following the protocol of experimental measurements, we use Molecular Dynamics Simulations to model the system. We consider two different systems. In the first one, fixed nonmagnetic particles are connected with dipolar ones by springs to mimic magneto elastic coupling. In the second system, dipolar particles are replaced by magnetisable colloids. The first step is to get the main hysteresis loop of this system (changing the direction and intensity of an external magnetic field). The second part of the study includes the computer simulations to obtain the first-order reversal curves. In the result, we have the FORC diagrams in dependence of the coercive and the reversal fields. The research was supported by the RFBR Grant 16-52-12008 and the DFG Grant Od18/24-1 within the German-Russian Research Collaboration PAK907.

CPP 17.5 Mon 18:30 P1C

**Nitrogen-doped graphene as an alternative to eco-toxic zinc oxide in rubbers** — YULIA GLEBOVA<sup>1,2</sup>, ●NIKOLAI SEVERIN<sup>1</sup>, VLADIMIR SHERSHNEV<sup>2</sup>, and JÜRGEN P. RABE<sup>1</sup> — <sup>1</sup>Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — <sup>2</sup>Moscow State University of Fine Chemical Technologies, Russia

Zinc Oxide (ZnO) is an essential ingredient of industrial rubber production, it regulates the vulcanization onset, accelerates vulcanization kinetics, and improves the mechanical properties of rubber. However, environmental pollution with ZnO is of concern, since it is recognized to be significantly eco-toxic, and it might have also adverse effects on human health. One of the major sources of ZnO environmental pollution is rubber items, in particular tires. Nitrogen (N-) doped graphene is a promising next generation catalyst comparable in its efficiency to platinum. We show that replacement of 3 phr (weight parts per hundred weight parts of polymer) of ZnO by just 0.1 phr of N-doped graphene in styrene-butadiene rubber reduces the vulcanization onset time by more than a factor of two while keeping the fast vulcanization kinetics and enhancing the tensile strength as compared to the rubber with just ZnO. Shorter vulcanization time implies saving energy, which together with the non-toxicity of N-graphene should make the resulting rubbers substantially more environmentally friendly.

CPP 17.6 Mon 18:30 P1C

**Topological interactions in polymers under shear** — MACIEJ KAWECKI<sup>1</sup>, FRANZ ADLMANN<sup>1</sup>, PHILIPP GUTFREUND<sup>2</sup>, SUDIPTA GUPTA<sup>3</sup>, PETER FALUS<sup>2</sup>, DAVID UHRIG<sup>3</sup>, and ●MAX WOLFF<sup>1</sup> — <sup>1</sup>Department for Physics and Astronomy, Uppsala University, Sweden — <sup>2</sup>Institut Laue-Langevin, Grenoble, France — <sup>3</sup>Oak Ridge National Laboratory, Oak Ridge, TN, USA

Since decades topological interactions as described by the reptation theory of DeGennes, Doi and Edwards are among the most successful concepts in physics. The scaling laws and viscoelastic properties in polymers are predicted correctly. However, currently no such generalized theory is available for large deformations, where shear thinning occurs. Even more, until now, no experimental approach allowed to test possible extensions of the reptation theory, such as convective constrain release, which would have the potential to theoretically predict the shear thinning transition. We present a neutron spin echo based method to directly measure and quantify nanoscale dynamics in flowing liquids and we extract the chain dynamics in a polymeric melt beyond the shear thinning transition. Under flow we find an additional relaxation process, which we attribute to shear thinning and which is in line with the theory of convective constrain release.

CPP 17.7 Mon 18:30 P1C

**Thermal, collective and self-diffusion of linear and cross-linked PMMA** — ●BASTIAN PUR<sup>1</sup>, WERNER KÖHLER<sup>1</sup>, MARTIN SCHNEIDER<sup>2</sup>, KLAUS HUBER<sup>2</sup>, ALEXEI F. PRIVALOV<sup>3</sup>, and MAX SCHÄFER<sup>3</sup> — <sup>1</sup>Physikalisches Institut, Universität Bayreuth, 95440

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Present theories for polymer thermophoresis discuss two theoretical models: draining coil (Rouse) and nondraining coil (Zimm). In order to discriminate between these models we have started a comparative investigation of linear chain polymers and cross-linked polymers (microgels). The linear polymer samples are poly(methyl-methacrylate) (PMMA) and the microgel samples are PMMA cross-linked with different amounts of ethylenglycole-di-methacrylate (EGMA). In either case toluene is used as solvent. By means of a transient holographic grating technique we obtained the Fickian diffusion coefficient  $D$ , the thermal diffusion coefficient  $D_T$  and the Soret coefficient  $S_T$  as functions of the polymer concentration  $c$ . Using NMR diffusometry in ultrahigh static magnetic field gradients we have determined the self-diffusion coefficient  $D_s$ . For  $c \rightarrow 0$  the thermophoretic mobilities of the linear polymers and the microgels with 3.5% EGMA are identical within experimental accuracy. The concentration dependence of  $D_T$  is, however, different, with a more pronounced slowing down of the microgel. Against our assumption,  $D_s$  of the microgel shows an even stronger concentration dependence, indicating different friction mechanisms.

CPP 17.8 Mon 18:30 P1C

**Influence of Structure on the Slip Boundary Condition of Polymeric Liquids: Experiments and MD-Simulations —**

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In the classic case of a liquid running through a pipe, the flow velocity is usually the fastest in the center and decreases towards the walls. On small scales, the importance of this interface grows. In fact, on a microscale and under certain conditions, a liquid can reach a velocity at the interface (slippage). We study slippage of thin polymer films on two differently ordered types of self-assembled silane monolayers (SAM), as well as on an amorphous PTFE surface. The influence of the liquid\*s and substrate\*s structure on slippage is examined in dewetting experiments of polymers with various side groups. It turns out that PS on a SAM of relatively low degree of order shows an usual high slip length, whereas slip is reduced if PMMA or polyvinylpyridine (PVP) is used instead of PS. The specific kind of order plays a major role. Insights on the structure are gained with the help of X-ray reflectometry and MD-simulations. MD-simulations could mimic experimentally observed structural and dynamical data and enabled new insights to the mechanisms at the solid/liquid interface.

CPP 17.9 Mon 18:30 P1C

**Non-monotonic effect of small molecules on the glass tran-**

**sition temperature of entangled polymers —** •ELIAS MAHMOUDINEZHAD and FATHOLLAH VARNIK — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), IC 02-753, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

Using molecular dynamics simulations, we aim to study how the presence of small particles within a polymer melt affects its glass transition temperature,  $T_g$ . In this study,  $T_g$  is determined via standard cooling simulations from the liquid state to the glassy phase. We use a variant of a well-established fully flexible polymer model, first proposed by Kremer and Grest [1], extended by the attractive part of the Lennard-Jones interactions. The chain length,  $N_p$  is chosen larger than the entanglement length of the model ( $N_p=64 > N_e=32$ , see Refs. [1, 2]). The size of small particles is smaller than the monomer diameter and is varied in a wide range. It is found that the size of small particles plays a crucial role for the  $T_g$  of the investigated polymer-particle mixture. Importantly, the glass transition temperature of the system changes in a non-monotonic way with the size of small particles. Our results are in qualitative agreement with experiments on polymers. The present observations can also be rationalized in terms of a recent mode coupling theory for binary mixtures [3], thus highlighting the generic character of the observed non-monotonic behavior [4].

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**Simulation study of a PMMA chain with azobenzene side**

**groups near a silica surface —** •MARKUS KOCH<sup>1,2</sup> and OLGA GUSKOVA<sup>1,3</sup> — <sup>1</sup>Leibniz-Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden — <sup>2</sup>Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden — <sup>3</sup>Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden

In recent years, azobenzene-containing hybrid materials have been of high scientific interest due to their strong responses under external illumination with light. The most striking feature of azobenzenes (azo) is a fully reversible photoisomerization between its trans- and cis-states. When azo-groups are coupled to polymeric systems, this isomerization reaction induces conformational changes and stresses on larger length scales. This makes such materials very promising for applications in nano- and microtechnology.

Here, we present the results of a simulation investigation approach to model the systems with Ångström resolution. Our study combines DFT calculations for a comprehensive analysis of the electronic and optical properties of specific azo-compounds with all-atom MD simulations to investigate the dynamical behavior of polymers with covalently attached azo side-groups. In particular, we present the dynamic behavior of a PMMA chain with covalently attached side groups of Disperse Red-1 acrylate, which is grafted to a silica substrate.

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