

## CPP 38: Polymer Networks and Elastomers

Time: Wednesday 11:30–12:45

Location: H18

CPP 38.1 Wed 11:30 H18

**Simulation and theory of model sliding-ring polymer systems** — ●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 Polymer- forschung Dresden — <sup>2</sup>Technische Universität Dresden

In order to understand the elasticity of polymers which are harnessed by slidable rings such as polyrotaxanes we consider a simple model system. Here two chains are connected by crosslinking two of the slidable rings which act as stoppers for the other rings threaded on the chains. For the case of ideal chain statistics the partition function for chains under constant force can be calculated exactly and the resulting force-extension relations are compared with Monte Carlo simulations using the bond fluctuation model. We observe a strong strain-softening of the double-chain system under force which sharpens towards a jump-like transition of the elastic modulus for longer chains. We show that the reason for this behavior is fact that the slidable rings form a 1D real gas which is compressed by the stoppers if the chains are extended. Only if the external force exceeds the internal pressure caused by the slidable rings the chains can respond with the elastic compliance of their full contour related with a jump-like decay in modulus. Using simple thermodynamic arguments we calculate the critical force, and from an analytic approximation of the partition function we obtain the modulus of the connected chains in the low force region. Our system provides insights into a new class of elastic matter where conformational and internal degrees of freedom act together. A possible extension of our model are 'sliding-ring' gels build-up from many sliding-ring polymers.

CPP 38.2 Wed 11:45 H18

**Microphase separation in cross-linked copolymers** — ●GAOYUAN WANG, ANNETTE ZIPPELIUS, and MARCUS MÜLLER — Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Using particle-based simulations of a soft, coarse-grained model in conjunction with the Single-Chain-in-Mean-Field algorithm we have studied the cross-linking of (diblock) polymer melts and the subsequent microphase separation the cross-linked systems upon increasing the incompatibility,  $\chi N$ , between the two blocks. Without cross-linking, the simulated order-disorder transition (ODT) between a lamellar and a disordered liquid is shifted away from the mean-field prediction  $\chi N = 10.5$  and is of first-order. With increasing cross-link density, the  $\chi N$ , at which the ODT occurs (for fixed cross-link density), shifts to larger values. Beyond the cross-link density of 1 per chain a gradual formation of a microemulsion-like structure (disordered gel) is formed, i.e., the morphology features a characteristic length scale but not long-range order. When we cross-link a lamellar liquid at  $\chi N > \chi_{ODT}$  and decrease  $\chi N$ , the  $\chi N$  at which the ODT occurs (i.e. long-range order is lost) differs from the previous one.

CPP 38.3 Wed 12:00 H18

**Reversible magnetomechanical collapse in a soft elastic matrix** — MATE PULJIZ<sup>1</sup>, SHILIN HUANG<sup>2</sup>, KARL A. KALINA<sup>3</sup>, JOHANNES NOWAK<sup>3</sup>, STEFAN ODENBACH<sup>3</sup>, MARKUS KÄSTNER<sup>3</sup>, GÜNTER K. AUERNHAMMER<sup>2</sup>, and ●ANDREAS M. MENZEL<sup>1</sup> — <sup>1</sup>Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — <sup>2</sup>Max-Planck-Institut für Polymerforschung, Mainz, Germany — <sup>3</sup>Technische Universität Dresden, Dresden, Germany

Embedding rigid particles in an elastic matrix hinders their motion. Under mutual attraction, their displacement leads to elastic deforma-

tions of the elastic environment. Counteracting restoring forces result.

Nevertheless, as we demonstrate, a reversible particle approach up to virtual touching is possible. For this purpose, the behavior of magnetizable nickel particles in a soft elastic gel matrix was analyzed in experiments [1]. Switching on and off an external magnetic field, the particles reversibly collapse towards each other and subsequently re-separate. Explicit analytical calculations and finite-element simulations describe and quantify these experimental observations [1].

The effect should be interesting from an application point of view. In magnetorheological elastomers, the overall material stiffness can be reversibly tuned by external magnetic fields acting on embedded magnetizable particles [2]. Induced formation of chain-like aggregates is possible. An associated material stiffening could be maximized by induced virtual touching of the embedded particles.

[1] M. Puljiz et al., *Soft Matter* **14**, 6809 (2018).

[2] G. Pessot et al., *J. Phys.: Condens. Matter* **30**, 125101 (2018).

CPP 38.4 Wed 12:15 H18

**FORCs diagrams for magnetoactive elastomers studying by molecular dynamics simulations** — ●ALLA DOBROSERDOVA<sup>1</sup>, PEDRO ANTONIO SANCHEZ ROMERO<sup>1,2</sup>, and SOFIA KANTOROVICH<sup>1,2</sup> — <sup>1</sup>Ural Federal University, Ekaterinburg, Russia — <sup>2</sup>University of Vienna, Vienna, Austria

Magnetic elastomers are the systems consisting of magnetic particles distributed in a nonmagnetic elastic matrix. We use the FORCs (first-order reversal curves) diagrams to study how the matrix influences internal magnetic interactions. We consider several models of magnetoactive elastomers. We use the Molecular Dynamics Simulations to study the different systems. In order to introduce the elastic interactions we consider fixed nonmagnetic particles which are connected with dipolar ones by springs. As the simplest case, we consider spherical magnetic particles in an elastic matrix. As an extension, we take into account the shape anisotropy of magnetic particles. We also study magnetic particles with flake-like shapes. In order to plot the FORCs distribution we use a classical method [C. R. Pike et al., *J. Appl. Phys.* **85**, 6660 (1999)]. The research was supported by the Ministry of Education and Science of the RF (project 3.1438.2017/4.6) and Austrian Science Fund (FWF, START-Project No. Y 627-N27).

CPP 38.5 Wed 12:30 H18

**Magneto-active elastomeric (MAE) films and their properties** — ●SOFIA KANTOROVICH<sup>1,2</sup>, ELENA MININA<sup>1,2</sup>, ELENA KRAMARENKO<sup>3</sup>, and PEDRO SANCHEZ<sup>1,2</sup> — <sup>1</sup>University of Vienna — <sup>2</sup>Ural Federal University — <sup>3</sup>Moscow State University

Due to advances in synthesis, it is nowadays possible to prepare thin layers of elastomers with relatively high loading of magnetic particles. Such layers show a dramatic change of the hydrophobicity when an external magnetic field is applied. This effect is a consequence of the conventional chain formation of magnetic particles aligned along the magnetic field that causes not only the matrix deformation of the layer, but also roughens its surface. We study structural, magnetic and mechanical properties of such MAE layers by means of MD computer simulations. We develop a model of a MAE layers that captures the dependence of its surface roughness on the elastic properties of the polymer matrix and the magnetic interactions [1]. To examine elastic properties of these layers we consider them under action of an external magnetic field of different strength. We observe that the magnetic field stiffens the layer making it more robust to deformations. [1] P.Sanchez et al, *Soft Matter* 2018.