CPP 98: Composites and Functional Polymer Hybrids

Time: Thursday 15:00–17:00 Location: ZEU 114

CPP 98.1 Thu 15:00 ZEU 114

A mesoscopic approach to magnetostriction of magnetic gels and elastomers — Lukas Fischer and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Our focus is on magnetic gels and elastomers, consisting of rigid magnetizable particles embedded in an elastic polymeric environment. While the particles are discrete objects on the mesoscopic scale, the polymeric body represents an elastic continuum. When magnetized, the particles are subject to magnetic forces and push against the polymeric environment, inducing macroscopic magnetostrictive distortions.

Using analytical theory and numerical evaluations, we determine the overall distortion resulting for different discrete particle arrangements enclosed by a finite-sized, linearly elastic sphere [1]. Overall changes in volume and shape are evaluated. In contrast to many other approaches, our formalism includes the basically infinite number of internal degrees of freedom of deformation, which can play a qualitative role [2].

We assume identical, well-separated particles, all identically magnetized from outside [1]. Depending on the discrete particle arrangement and the compressibility of the elastic material, overall contraction or elongation along the magnetization axis results. For randomized particle arrangements, a trend of elongation along the magnetization axis is found, in line with previous experiments [3]. We presume that our approach can support the design of magnetostrictive actuation devices.

[1] L. Fischer and A. M. Menzel, *J. Chem. Phys.* **151**, 114906 (2019).
[2] G. Pessot et al., *J. Chem. Phys.* **141**, 124904 (2014).
[3] C. Gollwitzer et al., *J. Chem. Phys.* **128**, 164709 (2008).

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Self-Structuring formation of filler particles in low concentration magnetoactive polymers — •Dirk Sindersberger, Nina Prem, and Gareth Monkman — OTH Regensburg, Regensburg, Deutschland

The formation of micro-structures in magnetoactive polymers (MAP) is a recently discovered phenomenon found only with very low filler particle concentrations (less than 3 wt%). Due to the degassing process, filler particles collect around an ascending bubble, which dissolves at a certain point leaving particulate rings within the matrix. The formation of toroidal micro-structures commences as filler concentration approaches 1wt%. The development of coherent parallel aligned rings with a compact order continues as particle concentrations increase toward 2 wt%. Between 2 and 3 wt% capillary doublets develop, while mass percentages higher than 3 wt% results in increasing entropy as the random order of particle agglomeration found in higher concentration MAP dominates. Self-structured samples of different filler material and concentrations between 1 and 3 wt% have been investigated using X-Ray tomography, where the emerging structures can be observed and visualized. Additionally, this work utilizes a range of spectroscopic analysis methods (UV/VIS and FTIR) and their applicability to MAP characterization at wavelengths ranging from 200 nm to 25 μm.

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Magneto-sensitive elastomer beyond the linear magnetization regime — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

Magneto-Sensitive Elastomer (MSE) describes a composite material of a soft-elastic polymer network with embedded micron-sized magnetizable particles. Upon applying an external magnetic field, it can undergo large deformations. Due to the long-range nature of the magnetic interactions, the pronounced sensitivity to preparation conditions and a complex interplay of different mechanisms, such as deformation- and field-induced particle rearrangements, the theoretical description of MSE represents a challenging task. Accordingly, various simplifying assumptions are introduced. A very prominent simplification is the restriction to an exclusive linear magnetization behavior. Often in experiments, and in order to yield pronounced effects, rather large magnetic fields are applied where the linear approximation regime is no longer justified. We will present a generalized theoretical approach which correctly describes the low and the large field limit, and also provides a reasonable approximation for intermediate field strengths. Furthermore, we show how this formalism can be adopted to account additionally for different MSE sample forms.

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Molecular dynamics simulations of magnetoactive elastomers — •Alla Dobroserdova[1], Malte Schümann[2], Dmitry Borin[2], Pedro Sanchez[1,3], Stefan Odenbach[2], and Sofia Kantorovich[1,4] — [1]Ural Federal University, Ekaterinburg, Russia — [2]Technische Universität Dresden, Dresden, Germany — [3]Helmholz-Zentrum Dresden-Rosendorf, Dresden, Germany — [4]University of Vienna, Vienna, Austria

Magnetic elastomers are the systems consisting of magnetic particles distributed in a nonmagnetic elastic matrix. We perform Molecular Dynamics Simulations to investigate the influence of particle shape, their magnetic interactions, their coupling with polymer matrix and external magnetic field on the structural and magnetic properties of these systems. In order for the results to be predictive for a realistic class of magnetic elastomers, we match simulation parameters to those obtained from theological, tomographic and magnetic measurements. Based on the qualitative agreement between simulations and experiment, we can explain asymmetry of magnetic hysteresis loops, particle orientational ordering in field and shift of the FORC diagram maxima.

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Simulations of complex nanoparticles in block copolymer ultrathin films: colloidal anisotropy and inhomogeneity — •Javier Diaz[1], Marco Pinna[2], Andrei V. Zvelindovsky[2], and Ignacio Pagonabarraga[1] — [1]École polytechnique fédérale de Lausanne, Switzerland — [2]School of Maths and Physics, University of Lincoln,UK

Block copolymers (BCPs) are perfect candidates to control the position (and orientation, for anisotropic colloids) of nanoparticles (NPs) due to the microphase separation in several ordered morphologies: lamellar, cylinders, etc. Moreover, the presence of nanoparticles can modify the properties of the hosting BCP, including its morphology [1] and result in ordered co-assembled structures.

Anisotropic nanoparticles can display a high ordering within block copolymer ultrathin films, with a rich phase behaviour both in terms of NP position and orientation, depending on relative lengths and interactions with the BCP. We present a computational model [2] that allows to study anisotropic NPs with different shapes (rectangles, ellipsoids and rhomboids), comparing with recent experiments on nanorods and nanoplates.

Chemically inhomogeneous Janus NPs(JNPs) possess an additional orientational degree of freedom that can lead to ordered co-assembled phases with JNPs forming lamellar-like structures within the BCP [3].

[1] Diaz, J., Pinna, M., Zvelindovsky, A. and Pagonabarraga, I., 2019 Soft Matter, 15, 9325-9335 [2] Diaz, J., et al, 2019. Macromolecules 52, 21, 8285-8294 [3] Diaz, J., et al, 2019 Soft matter, 15(31), 6400-6410

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Dipolar Molecular Rotors in Surface-Anchored Metal Organic Frameworks — •Xianghui Zhang[1], Sebastian Hamer[2], Ritesh Haldar[3], Daniel Reuter[4], Florian Paneff[1], Dirk Volkmer[4], Peter Lunkenheimer[4], Ian Howard[3], Rainer Herges[2], and André Beyer[1] — [1]Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany — [2]Otto-Diels-Institute for Organic Chemistry, Christian-Albrechts-University of Kiel, 24098 Kiel, Germany — [3]Karlsruhe Institute of Technology (KIT) Institute of Functional Interfaces (IFG) and Light Technology Institute (LTI), 76344 Karlsruhe, Germany — [4]Experimental Physics V, University of Augsburg, 86135 Augsburg, Germany

Molecular rotors arranged in ordered two- and three-dimensional lattices are an emergent quantum mechanical system. We use dipolar molecular rotors as building blocks to synthesize surface-anchored metal-organic framework (MOF), which serves as a structural architecture to arrange the molecular rotors precisely in ordered arrays. The torsional barrier of single rotors was computed by ab initio DFT calculations, while dipole-dipole interactions were estimated from classical calculations. Dielectric spectroscopy was used to investigate the rotation dynamics of molecular rotors, where thermally activated reorientations of the dipolar rotors lead to an enhanced dissipation when the driving frequency is close to the natural fluctuation rate of the dipolar rotors. Both the activation energy and relaxation rates were determined experimentally and compared with theoretical calculations.

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Model cement systems studied by Colloidal-Probe AFM (CP-AFM) — •Simon Becker and Regine von Klitzing — Soft Matter at Interfaces, Institut für Festkörperphysik, TU Darmstadt, Germany

In nowadays construction industry due to ecological and financial reasons the tailored rheology of building materials such as concrete and therefore cement is of great importance. Especially the rheology of cement pastes in the early stage can be influenced by additives such as polycarboxylate ether (PCE) type super plasticizers in a viscosity reducing manner. For tuning the system a better understanding of the interplay between the nanoscopic forces on cement particles and the macroscopic rheology is of essential importance.

In the present study the interaction between model particles is investigated with colloidal-probe atomic force microscopy (CP-AFM). Thereby micrometer scaled spherical silica beads are used as model cement grains to imitate the silicate phases of cement clinker. Furthermore spray dried clinker particles are used for a more application-related approach. The latter ones are restricted to measurements in non-aqueous solutions to prevent hydration. The influence of the interaction forces in presence of different pH and different ionic strength and ion types such as KCl and $CaCl_2$ is investigated for these model systems.

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Calorimetric study on the vitrification kinetics, molecular mobility and rigid amorphous fraction in epoxy-based nanocomposites — •Paulina Szymoniak, Xintong Qu, and Andreas Schönhals — Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany

It was found for inorganic/polymer nanocomposites that a so-called rigid amorphous phase (RAF) is formed in the interfacial region by adsorption of polymer segments onto the nanoparticles. The segmental dynamics of RAF is expected to be altered, as compared to the pure matrix, which might percolate into the entire system, affecting the overall PNC properties. Here, the structure and molecular mobility of epoxy-based PNCs with different nanofillers (layered double hydroxide and boehmite) was studied by a combination of calorimetric and X-Ray scattering techniques. Temperature modulated DSC (TMDSC) showed that depending on the nanofiller, RAF can reach up to 40 wt % of the system or, on the contrary, the overall mobility of the matrix might increase due to the presence of particles. Such contrasting results, including the high amount of RAF, which was never shown before for epoxy-based PNCs, emphasize the importance of interfaces. Additionally, glass transition and glassy dynamics were investigated by a novel technique, Flash DSC (heating rates up to 10 kK/s) employed for the first time to a thermosetting system. It was used to study both the vitrification kinetics and glassy dynamics of the PNCs, for instance further confirming the presence of RAF and its impact on the overall material properties.