CPP 13: Focus: Field Controllable Functional Polymers II

Time: Monday 15:00–18:30 Location: C 264

CPP 13.1 Mon 15:00 C 264

Multiscale Finite Element Modeling of Magnetoactive Materials — •Philipp Metsch, Christian Spieler, and Markus Kästner — Institute of Solid Mechanics, Technische Universität Dresden, 01062 Dresden, Germany

Magnetorheological elastomers feature mechanical moduli that become strongly enhanced by an applied external magnetic field as well as the ability to generate magnetically induced deformations and mechanical actuation stresses. Typically, these materials represent a two-component system, in which micron-sized magnetizable particles are embedded in a cross-linked polymer network. Since the effective material behavior of magnetorheological elastomers is essentially determined by the constitutive properties of the individual components and their geometrical arrangement in the composite, this contribution will apply a homogenization approach for coupled magneto-mechanical problems. Starting from the properties of the magnetizable particles and the polymeric matrix, a weakly coupled model based on a continuum formulation of the problem is presented.

The governing equations are solved using the extended finite element method that allows the use of non-conforming, structured meshes which do not have to be adapted to the particle-matrix interfaces. This is advantageous if complex systems representing stochastic and structured particle distributions are considered. The obtained results are compared to those from other modeling approaches and experimental investigations.

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Theoretical study of Janus-like magnetic particles at low temperature — •Ekaterina Novak[1], Elena Pyanzina[1], and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — [2]University of Vienna, Sensengasse 8, 1090, Wien, Austria

Application of complex innovation methods in the field of magnetic materials led to a synthesis of magnetic Janus particles [Zhao and Gao, Adv. Mat., 2009; Smoukov et al., Soft Matter., 2009]. The two faces of magnetic Janus particles are the magnetic and nonmagnetic hemispheres. Applying an external electric or magnetic field one can assemble such magnetic Janus particles in staggered chains, chain-like or mesh-like superstructures and double and staggered chains. Driving the rotations of such colloids opens new perspectives in biomedical and technological applications. Here we present a theoretical study of Janus-like magnetic particles at low temperature. We would aim at investigating only one possible dipolar orientation and use the shift of the dipole, which in Janus particles correspond to the size of the magnetic side, as a control parameter to investigate both ground state structures and thermodynamically equilibrium self-assembly. To describe the basic features of the Janus-type magnetic colloids, we put forward a simple model of a spherical particle with a dipole moment shifted outwards the centre and oriented perpendicular to the particle radius. Using direct calculations and molecular dynamics computer simulations, we investigate the ground states of small clusters and the behaviour of bigger systems at low temperature.

CPP 13.3 Mon 15:30 C 264

Magnetic gels - The influence of the sample shape on the deformation behaviour — •Rudolf Weeber and Christian Holm — Institut fuer Computerphysik, Allmandring 3, 70569 Stuttgart

Magnetic gels are hybrid materials, consisting of magnetic particles immearsed in a hydrogel or elastomer. They are of interest due to the intricate interplay between elastic and magnetic forces observed in them. For example, magnetic gels can change their elasticity and shape, when an external magnetic field is applied. This property makes them interesting for applications in medicine and engineering.

It has been shown that two mechanisms exist by which a magnetic gel can deform in a homogeneous magnetic field. The first one is present only in magnetic gels in which the magnetic particles act as the cross-linker. It relies on a coupling of the orientation of the magnetic nanoparticles to the polymer matrix. The second mechanism, which will be the focus of this contribution, is based on the change of the average dipole-dipole interaction between the nanoparticles as they align to an external field.

Here, we discuss a recently developed coarse-grained simulation model for magnetic gels to study this deformation mechanism. It allows us to examine both, the influence of the local configuration of magnetic nanoparticles and the shape of the entire gel sample on the material's deformation in an external magnetic field.

CPP 13.4 Mon 15:45 C 264

Magneto-Sensitive Elastomers — •Sahbi Aloui and Manfred Klüppel — German Institute of Rubber Technology, Hannover, FRG

Magneto-sensitive elastomers (MSE) consist of a non-magnetic polymer matrix in which magnetic filler particles are embedded. These adjustable materials are able to ensure adaptability to changing environmental conditions by varying in-operando their dynamical properties. MSE have proven themselves in several practical applications like adaptive vibration control systems, a recently patented sensor for temperature measurements and industrial adhesives.

We study the non-linear dynamical-mechanical behavior and the magnetorheological response of MSE. Considerable influences on the properties of the MSE exert the magnetic fillers. Basic parameters like filler volume fraction in the prepared MSE, chemical composition and size distribution of magnetic particles play a major role. We focus on an optimization of mechanical and magnetic properties of MSE by preparing an anisotropic MSE, whose stiffness and hysteresis behaviors show magnetic orientation dependence. Combining highly reinforcing magnetic nanoparticles with micro-sized particles is advantageous to obtain a MSE with high switch ability in a magnetic field and reasonable mechanical properties.

References Aloui S., Klüppel M. *Magneto-Rheological Response of Elastomer Composites with Hybrid-Magnetic Fillers*, Smart Materials and Structures (submitted) Karl C., McIntyre J., Alshuth T., Klüppel M., Kautsch. Gummi Kunstst. 66/1-2 (2013), 46-53

Invited Talk CPP 13.5 Mon 16:00 C 264

Magnetic particles in polymer harness: Modeling mesoscopic magnetomechanics of polymer composites — •Yuriy Raikher[1,2] and Oleg Stolbov[1,2] — [1]Institute of Continuous Media Mechanics, Ural Branch of RAS, Perm, 614013, Russia — [2]Perm National Research Polytechnic University, Perm, 614990, Russia

Weakly-linked rubber-like materials filled with micron-size multidomain grains are nowadays considered as the most technologically desirable media. They are sufficiently soft elastically and sufficiently loaded magnetically as to display strong magnetomechanical effects like field-induced strains, tuning of the elastic modulus, etc. In now discussed and tested applications of these soft magnetic elastomers (SMEs), a usual working element is a 3D sample. Here we consider SME films, which are more flexible mechanically and, thus, more sensitive to the field than the 3D ones. The macroscopic behavior of a SME film comes out as a net result of the particle-matrix interaction. In such samples, the particle displacements crucially depend on the direction of the applied field. Moreover, in the numerical modeling, we use, instead of the customary dipole-dipole potential, another one, which much better accounts for the magnetic softness of the multi-domain particles. The field-induced response of SME films at the mesoscopic scale is discussed and projected to the macroscopic observations. Support by RFBR grants 13-01-96056 and 14-02-96003 and project MIG S26/617 from the Ministry of Education and Science of Perm Region are acknowledged.

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Influence of the dipole moment orientation inside particles on the macroscopic behaviour of magnetic ellipsoids systems — Anna Gudkova and •Elena Pyanzina — Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia

Magnetic anisotropic particles in the last years became an independent fast-emerging branch of dipolar soft matter research. In this contribution we focus our attention on the magnetic ellipsoids, which have the orientation-dependent steric interparticle interaction. The magnetic part of the interaction will be characterized by simple magnetic dipole-dipole interaction, with the dipole moment being always fixed in the particle's centre of mass, but with different orientation (along/perpendicular to the main axis). The theoretical study and results of computer simulations for microstructure and magnetic, rheological and structural properties for the systems with different dipole orientation and particle anisotropy are presented. It was shown that all aforementioned characteristics strongly depend on the particle anisotropy and the dipole orientation as well as external magnetic field. As a result one can drastically change macroscopic responses of the systems. This may prove to be very important in various medical and industrial applications, where a bottom up design of materials plays a crucial part.

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Interplay between thermo-mechanical and functional properties of inductively heated nanomagnetite filled shape-memory polymers — •Kazakeviciute-Makovska Rasa and Steeb Holger — Ruhr-Universität Bochum Universitätsstr. 150 D-44780 Bochum

One of the main problems in development of thermo-responsive shape-memory polymer (SMP)-based devices for engineering and medical applications is the design of a safe and effective method of thermal actuation. The conventional method of actuation involves the direct heating. A novel alternative to this method is the inductive heating. This may be achieved by the addition of ferromagnetic particles to a polymer matrix and exposing SMPs to an alternating magnetic field to cause the volumetric and remote heating. Based on the data available in open literature, we discuss the bulk thermo-mechanical and functional properties and performance of nanomagnetite reinforced SMPs. The analysis includes a wide range of filler parameters, induction parameters, and filler distribution configurations with the aim to understand the effects of particle size and shape on the thermal, pseudo-elastic, and rheological properties of this class of SMP nanocomposites. A parallel analysis of the functional behavior of nanomagnetite reinforced shape memory polymers is concerned with the shape fixity and shape recovery properties as well as the maximum recovery stress.

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Branched structures in dipolar hard sphere fluids: junctions revisited. — •Sofia Kantorovich[1,2], Alexey Ivanov[2], Lorenzo Rovigatti[1], Jose Maria Tavares[3], and Francesco Sciortino[4] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]University of Lisbon, Lisbon, Portugal — [4]University of Rome "La Sapienza", Rome, Italy

To clarify the scenario of temperature-induced structural transitions in magnetic nanocolloids of moderate concentrations we developed a theoretical approach and performed an extensive Monte Carlo simulations study. Our theoretical approach is based on the density-functional theory, where single nanoparticles can self-assemble in primary "defect-free" chains and rings as well as in "defect structures" in which primary structures are merged with the help of specific "defect particles". We are able to limit the amount of possible branching points (defects) to three main types, using a thorough numerical and visual analysis of simulation results (Rovigatti et al., J. Chem. Phys., 2013). The defects of types X and Y are serving as cross-linkers between primary structures, whereas defect of type Z could only appear within chains and rings. One of the key findings here is that at high dipolar strength (very low temperature) all Y defects are to be replaced by more energetically advantageous and infinitesimally magnetoresponsive defect structures made of two rings cross-linked by X defect (in contrast to the predictions of Tlusty and Safran, Science, 2000).

CPP 13.9 Mon 17:30 C 264

Equilibrium behavior of ferromagnetic supramolecular brushes — •Pedro A. Sánchez[1], Joan J. Cerdà[2], Tomás Sintes[2], and Sofia S. Kantorovich[1,3] — [1]University of Vienna, Sensengasse 8, 1090, Wien, Austria — [2]Instituto de Física Interdisciplinar y Sistemas Complejos (UIB-CSIC), E-07122 Palma de Mallorca, Spain — [3]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia

We present our recent progress on the characterization of the equilibrium structural behavior of ferromagnetic supramolecular brushes. These systems consist of a polymer brush-like structure formed by grafted supramolecular ferromagnetic filaments instead of molecular polymers. In general, magnetic filaments are obtained by crosslinking magnetic colloids by means of macromolecules to form a permanent magnetoresponsive chain structure. The grafting of magnetic filaments on surfaces is a promising strategy to create field controllable coatings with many potential applications.

Our study is focused on the determination of the dependence of the brush structure on the interplay between the steric repulsions and the magnetic interactions of the colloids, and is based on extensive molecular simulations and analytical theories.

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The study of the diffusion coefficient in the magnetic fluids: theory and computer simulation — •Alla Muratova[1] and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — [2]University of Vienna, Sensengasse 8, 1090, Vienna, Austria

We present the results on the mobility and diffusion coefficients in the systems of magnetic dipolar particles. Of course, there were several attempts to study diffusion [Yu. A. Buyevich et al., Physica. A 190, 276 (1992); P. Ilg, Phys. Rev. E 71, 051407 (2005); J. Jordanovic et al., Phys. Rev. Lett. 106, 038301 (2011)], but the detailed theoretical description is still missing. We consider the ferrofluids with chain aggregates of dipolar spheres. In our study, we combine theoretical approach and computer simulation. In theoretical study, we use Density Functional Approach to obtain the chain concentrations. Then we can calculate the mobility and diffusion coefficients. We know that the self-diffusion coefficient decreases with growing particle volume fraction and dipole-dipole magnetic interaction parameter in the three-dimensional samples of magnetic fluids. In this case, we have good agreement between the theory and computer simulation. So we can expand our theory to the cases of bidisperse ferrofluids and magnetic fluids with geometrical constraints. Thus, we study how the mobility and diffusion coefficients depend on the system polydispersity, granulometric composition, geometrical constraints and dipolar stregths.

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Dynamic mechanical response of dielectric elastomer actuators for the control of optical elements — •Gunnar Gidion, Matthias Kollosche, Werner Wirges, and Reimund Gerhard — Applied Condensed-Matter Physics, Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm, Germany

Dielectric Elastomer Actuators (DEA) consisting of an elastomer membrane with compliant electrodes are investigated with respect to their voltage-induced dynamic mechanical response. The in-plane deformation of prestretched acrylic and silicone membranes in a rectangular frame is captured with a high-speed camera and analysed with respect to the frequency response of the device. The geometry is examined for different pre-stretches at frequencies of up to 300 Hz. The AC driving voltage is applied in combination with various DC-bias voltages. The results are compared to the shear moduli obtained by means of dynamic mechanical analysis (DMA) of the respective materials. In addition, it has been observed that the sinusoidal electrical excitation is not translated into a purely sinusoidal motion of the actuator membrane. This observation is discussed in terms of viscoelastic creep and harmonic distortion. The results can be used to understand and modify the dynamic electromechanical response of soft actuators for optical applications such as e.g. the control of the grating period in soft diffractive optical elements.

CPP 13.12 Mon 18:15 C 264

Tuning elastomer membranes: Materials design and electrical stability of acrylic and silicone elastomers — •Matthias Kollosche[1], Martin Blümke[2], Gunnar Gideon[1], Miriam Biederman[2], Hartmut Krüger[2], and Reimund Gerhard[1] — [1]Institute of Physics and Astronomy, Universitiy of Potsdam, Potsdam, Germany — [2]Fraunhofer Institute for Applied Polymer Research Fraunhofer IAP, Potsdam, Germany

Soft dielectrics are sensitive to multiple stimuli, such as changes in e.g.temperature or pH value, and to control parameters such as mechanical stretch or electrostatic pressure. The latter two mechanisms are employed in Dielectric Elastomer Actuators (DEAs) - capacitors that consist of an elastomer sandwiched between two compliant electrodes. Many researchers have focused on the optimization of dielectric-elastomer and conductive-electrode materials with particular emphasis on higher permittivities, lower elastic compliances, and higher electric-breakdown strength as well as on high electrode conductivities and stretchability. Nevertheless, the stability and the durability have not yet been studied in detail. Here soft dielectric materials such as the industrial acrylic (3M, VHB 4905) and silicone (Wacker, Elastosil) elastomers are compared to specifically modified silicones with enhanced permittivity and reduced stiffness. The resulting transducers are characterized without and with pre-stretch over relatively long periods of time and under high electric fields. Results will be discussed in terms of durability and failure mechanisms of the materials under investigation for possible use in advanced elasto-optical devices.