

CPP 13: Composites and Functional Polymer Hybrids

Time: Monday 15:00–18:00

Location: ZEU 255

Invited Talk

CPP 13.1 Mon 15:00 ZEU 255

Nanocomposites and polymer thin films: from gas phase synthesis to functional applications — ●FRANZ FAUPEL, STEFAN SCHRÖDER, ALEXANDER VAHL, SALIH VEZIROGLU, CENK AKTAS, and THOMAS STRUNSKUS — Chair for Multicomponent Materials, Faculty of Engineering, Kiel University, Kiel, Germany

Highly filled particulate metal-dielectric nanocomposites films have unique functional properties with hosts of applications. To explore collective interactions between the particles, we control the particle separation on the nm scale by employing vapor phase deposition, which is a scalable approach permitting, inter alia, excellent control of the filling factor. For deposition of functional polymer thin films, we have recently used initiated chemical vapor deposition (iCVD) to avoid decomposition of the functional groups. Examples include highly stable electrets for electret microphones and magnetoelectric sensors, 3D superhydrophobic coatings, nanoscale gradient copolymers, and strain-invariant conductors for soft robotics. For the fabrication of the nanocomposites, the nanoparticles can form during gas phase co-deposition via self-organization or by means of high-rate gas aggregation cluster sources, which provide independent control of filling factor and size as well as in situ monitoring and control of composition. Recent examples of nanocomposites range from plasmonic meta-materials through photoswitchable molecular plasmonic systems to memristors and memsensors for neuromorphic electronics. We also explored nanoscale synergetic effects of plasmonics and photocatalysis, e.g. for photoinduced enhanced Raman spectroscopy (PIERS).

CPP 13.2 Mon 15:30 ZEU 255

Rheological optimization of filler packings using micro scale simulations — ●OLIVER ROSER^{1,2}, ANDREAS GRIESINGER³, and OTHMAR MARTI² — ¹Center for Heat Management (ZFW), Stuttgart — ²Institute of Experimental Physics, Ulm University — ³Baden-Wuerttemberg Cooperative State University (DHBW) Stuttgart

In a wide range of applications, polymers are modified with granular fillers to improve thermal or electric conductivity. The higher the amount of filler, the higher the conductivity. However, the attainable conductivity is restricted by processing limitations as the amount of filler also affects the composites viscosity. Only a clever combination of filler with multimodal size distributions can shift this limit and allow for higher amounts of filler without significant viscosity increase. The effect of multimodal packing structures on viscosity has already been investigated in several experimental and numerical studies, however common calculation techniques are mainly restricted to spherical and equal-sized filler particles. We extended common approaches with new packing simulations, considering the actual size distribution and shape of different filler materials. We implemented numerical packing optimization to find the best filler compositions for highly filled polymers with up to 80 v%. In this talk we will introduce the new packing simulations and their use for packing optimizations and present the acquired results and experimental validations.

CPP 13.3 Mon 15:45 ZEU 255

Increasing the Electrical Conductivity of Polymer Thin Films for Thermoelectric Applications — ●MARIE SIEGERT¹, MARKUS HÖNIG², MICHAEL SOMMER², and JENS PFLAUM^{1,3} — ¹University of Würzburg — ²Chemnitz University of Technology — ³ZAE Bayern

Thermoelectric generators based on sustainable, low-cost organic materials harbor great potential for waste heat recovery. Polymer thin films in particular can be easily upscaled to meet industrial standards and display aptly low thermal conductivity κ , but lack high electrical conductivity σ . However, the augmentation of σ imposes a major challenge as an increase in charge carrier concentration is usually accompanied by an unintentional decrease of the Seebeck coefficient S , which is detrimental for efficient thermoelectrics. Hence, we compare two possible strategies to enhance the charge carrier transport in such disordered systems. Firstly, doped polymer thin films utilizing the temperature activated n-type dopant TAM have been characterized regarding their thermoelectric properties. Secondly, composite films have been investigated, combining well studied polymers with metallic additives. Both approaches will be evaluated with respect to the enhancement in σ and the underlying transport mechanisms. First estimations of the resulting power factors indicate future strategies to

further refine the electronic properties and thus, the thermoelectric figure of merit.

The Deutsche Bundesstiftung Umwelt (DBU) is acknowledged for financial support.

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Conductivity of filled diblock copolymer systems. — ●ALEXANDER CHERVANYOV — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Münster, Germany

The reported work looks into the effect of stimuli-induced morphological changes in the composite consisting of insulating diblock copolymers (DBC) and conductive nanoparticles (NP) on the conductivity of this composite. The relation between the nano-structure of the described composite and its conductivity is studied by developing and making use of the multiscale computational approach. This approach relies on the consistent phase-field model of DBC, Monte-Carlo simulations of the filler distribution in DBC, and the resistor network model of the composite conductivity. The dependencies of the conductivity on the temperature of the composite, DBC morphology, and the affinities of fillers for copolymer blocks are studied in detail. In particular, the order-disorder transition in the host DBC system is found to be accompanied by the conductor-insulator transition in the filler network. The order-order transition between the lamella and cylindrical microphases of DBC proves to co-occur with a spike of the composite conductivity caused by restructuring of the conductive filler network.

15 min. break

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Modeling micro-structure evolution and its impact on moduli in magneto-active elastomers — ●MEHRAN ROGHANI, DIRK ROMEIS, and MARINA SAPHIANNIKOVA — Leibniz-Institut für Polymerforschung Dresden, Germany

Magneto Active Elastomers (MAEs) are field-controllable composites made of micron-sized, magnetizable particles embedded into a soft elastomeric matrix. These materials show a strong coupling between their mechanical properties and an applied magnetic field. The coupling can be directly related to magnetic interactions between the particles, which lead to the evolution of microstructure under the field. In the case of initially isotropic MAEs, this micro-structure evolution results in chains forming from the magnetized particles. This in turn causes a huge increase in the mechanical moduli along the field direction, leading to anisotropic behavior. We consider a transversely isotropic material model for the mechanics, and magnetic interactions are taken into account by the dipolar mean field approach. To couple the mechanical and magnetic effects, a restructuring parameter is introduced which is a function of material magnetization and moduli. This modeling approach improves our understanding of how microstructure evolution affects magnetically induced material deformation and stiffness. The first predictions are in good agreement with experimental results available in the literature. We thank the DFG for financial support through RTG-2430.

CPP 13.6 Mon 16:45 ZEU 255

Magneto-active elastomers: From composite structure to effective susceptibility — ●DIRK ROMEIS and MARINA SAPHIANNIKOVA — Leibniz-Institute of Polymer Research Dresden e.V.

Embedding magnetizable particles into elastic polymer network yields a field-controllable material known as magneto-active elastomer (MAE). In order to describe macroscopic samples of such composite material it is useful to develop an effective macro-continuum model. Based on the dipole approximation, we derive analytic relations for the effective magnetization behavior in MAEs, spanning from linear to saturation regime, for isotropic and anisotropic particle arrangements. In the limiting case of linear magnetics and isotropic distributions we reproduce an expression known from previous works. Accordingly, we believe that the present homogenization scheme provides a general description of the effective magnetic behavior with high practical relevance also in case of anisotropic distributions and beyond the linear magnetization. For a given particle arrangement and magnetization model on microscale, the solutions are obtained with low computational effort. Furthermore, the present formulation can be directly im-

plemented into a macroscopic material model for a composite sample of specified shape. It turns out, that an anisotropic particle distribution has an equivalent effect as an anisometric sample shape.

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Tuning the thermal conductivity of magnetic gels and elastomers — GUSTAV J. L. JÄGER, ●LUKAS FISCHER, TYLER LUTZ, and ANDREAS M. MENZEL — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

When an external magnetic field is applied to magnetic gels or elastomers—composite materials consisting of magnetic or magnetizable particles inside an elastic matrix—these materials typically exhibit interesting deformational (magnetostrictive) responses or changes in rheological properties (magnetorheological effect).

We study how the induced magnetic interactions lead to an internal restructuring of the magnetic particles, mainly the formation of particle chains along the direction of the external magnetic field. This behavior is not only connected to the aforementioned effects, it can also change the thermal conductivity of the magnetic gels and elastomers, which we focus on here. We analyze this phenomenon numerically for 2D mesoscopic (particle-resolved) models of magnetic gels and elastomers [1], thus characterizing thin elastic films and membranes.

Our results indicate significant magnetically induced changes in the thermal conductivity. The influence of several parameters on this effect is investigated, such as the density and number of magnetizable particles, the amplitude of their magnetization, and the aspect ratio of the systems. Similar changes in the electric conductivity of magnetic gels and elastomers are expected.

[1] G. J. L. Jäger, L. Fischer, T. Lutz, A. M. Menzel, *J. Phys.: Condens. Matter* **34**, 485101 (2022).

CPP 13.8 Mon 17:15 ZEU 255

Morphology evolution and nanoparticle localization in printed hybrid nanoparticle-diblock copolymer thin films investigated by in situ GISAXS — ●CHRISTOPHER R. EVERETT¹, GUANGJIU PAN¹, MANUEL A. REUS¹, DAVID KOSBAHN¹, FRANK HARTMANN², MARTIN BITSCH², MATTHIAS OPEL³, MARKUS GALLEI², MATTHIAS SCHWARTZKOPF⁴, and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹TUM, TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — ²Saarland University, LS Polymer Chemistry, 66123 Saarbrücken — ³Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — ⁴DESY, 22607 Hamburg — ⁵MLZ, TUM, 85748 Garching

The diblock copolymer (DBC) PS-*b*-PMMA forms films with periodic ordered nanostructures that can act as scaffolds for inorganic magnetic nanoparticles. These films have application as magnetic sensors and in magnetic data storage devices. Film formation and the resulting magnetic properties both depend on the localization of the nanoparticles in the DBC domains. In this investigation, ultra-high molecular weight PS-*b*-PMMA films containing two types of nanoparticles, cobalt ferrite and nickel, are fabricated by a slot-die coating technique. Grazing incidence small-angle X-ray scattering (GISAXS) is used to monitor in situ the morphological evolution of the DBC films and nanoparticle segregation in the films during the deposition and drying process. The magnetic properties of the hybrid films are investigated with a SQUID

magnetometer.

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Tunable mesoporous zinc titanate films via diblock copolymer-directed cooperative self-assembly and a sol-gel technique — ●YANAN LI¹, NIAN LI¹, SHANSHAN YIN¹, CONSTANTIN HARDER², YUSUF BULUT², APOSTOLOS VAGIAS³, STEPHAN V. ROTH^{2,4}, and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²DESY, 22607 Hamburg, Germany — ³MLZ, TUM, 85748 Garching, Germany — ⁴Department of Fiber and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden

Mesoporous ordered films have broad applications ranging from sensors to supercapacitors and biodevices due to their large specific surface area and pore accessibility of their porous nanostructures. Here, we investigate the evolution and formation mechanisms of morphologies of mesoporous zinc titanate films obtained by changing the ratio of two inorganic precursors after calcining hybrid films consisting of organic-inorganic materials. The amphiphilic diblock copolymer self-assembles into micelles in a mixture of N,N-dimethylformamid/hydrogen chloride playing the role as structure directing template. The inorganic precursors are loaded in the micellar shell due to hydrogen bonds between PEO and precursors. We combine a sol-gel route with a spin coating to prepare hybrid films, and investigate the influence of the different weight fractions of precursors and polymer concentration on the film morphologies. The inner and surface morphologies of the hybrid films are characterized using grazing incidence small-angle X-ray scattering and scanning electronic microscopy, respectively.

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Gold Nanoparticle/Polymer Brushes Composites: Controlling the Structure via Ion-Specific Effects — ●PHILIPP RITZERT and REGINE V. KLITZING — Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

Nanocomposite materials based on inorganic gold nanoparticle (AuNP) inclusions inside an organic matrix (e.g. polymer brushes) are employed in various fields: medical technology, catalysis, materials engineering. Combining the properties of both material classes facilitates high versatility of mechanical, optical and chemical properties, while simultaneously covering obvious drawbacks, e.g. stability of one compound. To provide the wide range of applications, nanocomposite materials usually require a specific internal structure. Yet, the understanding of the formation of internal structure and control over formation process is still lacking. Therefore, we aim to provide an approach to manufacture nanocomposite materials with controlled structure. Our model system utilizes various sodium salts (anion: F, Cl, Br, I, SCN) as stimuli for the assembly of citrate-capped gold nanoparticles in a poly-(N-isopropylacrylamide) brush. In a first step, we characterize the effect of sodium salts on pure AuNP suspensions. In a second step, we investigate adsorption parameters of AuNPs from suspension to brush, e.g. adsorption time. The third step involves the structure control of the composite materials with the characterized stimuli. Optical measurements reveal distinct differences between the sodium ions and concentration dependent aging behaviour.