CPP 73: Functional Polymer Hybrids and Composites

Time: Thursday 15:00–16:30 Location: PC 203

CPP 73.1 Thu 15:00 PC 203

Morphology Control of Low Temperature Fabricated ZnO Nanostructures for All Solid-State Transparent Dye-Sensitized Solar Cells — •Kun Wang[1], Volker Körstgens[1], Dan Yang[1], Nuri Hohn[1], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]1TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, 22607 Hamburg — [3]3KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

In the last decade dye-sensitized solar cells (DSSCs) have received considerable interest for solar energy conversion due to their convenient and low-cost fabrication. Solid state DSSCs show great promising since they are generally free from electrolyte leakage and corrosion problems compared with the traditional liquid electrolyte solar cells. For the n-type semiconductor ZnO offers higher electron mobility and lower crystallization temperature as compared to titania. A low-temperature route based on a sol-gel method with diblock copolymer templating is demonstrated, through which ZnO films are prepared which have a tunable morphology including foam-like, worm-like and sphere-like structures. The morphologies are probed using SEM and grazing incidence X-ray scattering. Based on the controlled nanostructured ZnO films all solid-state transparent DSSCs are fabricated, which paves the way for building integration of the solar cells.

CPP 73.2 Thu 15:15 PC 203

In-situ GISAXS during sputter deposition of metal nanolayers on functional polymer thin films for lithium-ion batteries — •Simon Schaper[1], Franziska C. Löhrer[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel

Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-flim morphologies on the nanoscale and offers a superior adhesion of the deposited material.[1] We use in-situ grazing incidence small angle X-ray scattering (GISAXS) to investigate the formation, growth and self-assembled structuring on polymer thin films used in LIBs.[2] Different polymer films are compared with respect to the metal layer growth.

[1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017);
[2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

CPP 73.3 Thu 15:30 PC 203

Characterization of gold nanoparticle loading and distribution within polymer brushes by neutron reflectometry — •Dikran Kesal[1], Larissa Braun[1], Oliver Löhmann[1], Emanuel Schneck[2], Marcus Trapp[3], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Department of Physics, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — [2]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Polymer brushes are promising candidates for the design of smart surfaces. Exposed to specific stimuli, these systems undergo structural changes. Furthermore, they can be used as a matrix for the uptake of particles. Incorporating gold nanoparticles (AuNPs) in polymer brushes results in nanocomposite materials with interesting nanosensor properties due to the fact that AuNPs exhibit surface plasmon resonance (spr). Here, the interparticle distance can be used to shift the spr in a certain way. The aim is to correlate the AuNP distribution with optical properties. In the present study neutron reflectometry is used for studying the distribution of AuNPs.

The focus is on the concentration profile of AuNPs within the polymer brush, which were incubated at different pH values. The sensitivity of the method is enhanced by the use of contrast variation. The reflectivity data are analyzed with a self-written fitting procedure based on volume fraction profiles of all chemical components.

CPP 73.4 Thu 15:45 PC 203

Influence of particle microstructure on the effect of magnetostriction in magneto-sensitive elastomers — •Dirk Romeis, Vladimir Toshchevikov, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

Magneto-sensitive elastomers (MSEs) are field-controllable composite materials with magnetically switchable properties. They consist of a soft-elastic polymer network with immersed magnetizable microparticles. Under external magnetic field these composites can significantly change their mechanical properties. Recently, we developed a dipolar mean field approach [1] to predict the effective material behavior of MSE in the magnetic field. Especially for random isotropic distribution of the magnetizable particles we find a quantitative agreement with micro-scale continuum simulations [2]. Presently, the mean field approach is limited to special situations, such as a conservation of the particle microstructure and specific orientation of the magnetic field. However, for ultra-soft elastomer we expect the particles to rearrange into different structures if the external field is applied. We will present some modifications in order to describe the mechanical behavior of MSEs under more general conditions. This will help us to gain an enhanced understanding of this type of field-controllable polymer composites. This work was supported by DFG (Project GR 3725 / 7-2).

Literature
[1] *Romeis D. et. al.* Soft Matter **12**, 9364-9376 (2016)
[2] *Romeis D. et. al.* Physical Review E **95**, 042501 (2017)

CPP 73.5 Thu 16:00 PC 203

Density functional theory for ferrogels and magnetorheological elastomers — Peet Cremer[1], Marco Heinen[2], •Andreas M. Menzel[1], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]Universidad de Guanajuato, Guanajuato, Mexico

Locking the positions of magnetic or magnetizable colloidal particles in an elastic polymer matrix leads to an interesting class of composite materials. One remarkable feature is that their overall mechanical properties can be reversibly tuned from outside by magnetic fields.

Our scope was to establish a statistical approach to this situation in terms of classical density functional theory, including thermal fluctuations [1]. To lower the complexity, we mapped the problem to a suitable one-dimensional dipole-spring model. A central issue is that classical density functional theory was constructed to describe liquid-like states, in contrast to our fixed particle positions in the elastic matrix. We solved this problem by introducing suitable particle pair and external potentials to mimic corresponding elastic interactions. Comparison with Monte-Carlo simulations showed good agreement. In parts, the theory uses input from explicit analytical calculations of the elastic response of the polymer matrix [2,3].

The theory allows to calculate, for instance, the change in the elastic modulus for varying strengths of the magnetic particle interactions.

[1] P. Cremer et al., *J. Phys.: Condens. Matter* **29**, 275102 (2017).
[2] M. Puljiz et al., *Phys. Rev. Lett.* **117**, 238003 (2016).
[3] M. Puljiz et al., *Phys. Rev. E* **95**, 053002 (2017).

CPP 73.6 Thu 16:15 PC 203

Photodegradation Evaluation in PVC Films and Resonance Raman Spectroscopic Insights into the Patterns of UV Light-Induced Polyene Defects — •Patrice Donfack[1], Elena A. Sagitova[2], Gulnara Yu. Nikolaeva[2], Alexandra Costa[3], Simon J. Shilton[3], Dmitry I. Mendeleyev[4], Kirill A. Prokhorov[2], and Arnulf Materny[1] — [1]Jacobs University, Bremen, Germany — [2]A.M. Prokhorov General Physics Institute of the Russian Academy of Sciences, Moscow, Russia — [3]University of Strathclyde, Glasgow, Scotland, UK — [4]A.V. Topchiev Institute of Petrochemical Synthesis of Russian Academy of Sciences, Moscow, Russia

Polyvinylchloride (PVC) is among the most popular components in modern industrial composite polymer materials, whose structure can be purposefully tuned within a wide range to feature new interesting physical and chemical properties. Typical application-relevant properties of PVC-based materials are affected by the formation of conjugated double bond defects (polyene) as the result of e.g. mechanical, thermal, chemical, or optical factors. In the present contribution, the PVC structure and especially the UV irradiation-induced polyene formation in the PVC matrix are studied using a combination of several techniques, including resonance Raman spectroscopy. The latter has proven very powerful in providing structural insights in both the small crystalline and the predominantly amorphous phases in PVC. Our results uncover the size distribution and content of polyene defects in a photodegraded PVC matrix as a function of UV-irradiation doses, yielding important information relevant for PVC-based insulating materials.