

CPP 40: Nanoparticles and Composite Materials I

Time: Thursday 9:30–12:45

Location: H48

CPP 40.1 Thu 9:30 H48

Investigation of Structure and Miscibility Patterns of Gold-Platinum Nanoparticles — ●LINN LEPPERT and STEPHAN KÜMMEL

— Institute of Theoretical Physics, University of Bayreuth, Germany
Gold-platinum nanoparticles (NPs) immobilised within spherical poly-electrolyte brushes have been proven to be excellent catalysts of oxidation reactions, being more efficient than pure NPs from gold or platinum [1]. However, little is known about their geometrical and electronical structure, as well as about the way the catalytic mechanism works. The theoretical treatment of these systems is complicated by the large number of electrons and the necessity to account for relativistic effects.

We present structure and miscibility patterns of small gold-platinum NPs obtained from numerical calculations. Our technique combines density functional theory based Simulated Annealing and local optimization methods and offers numerical efficiency as well as the inclusion of scalar relativistic effects.

[1] M. Schrunner et al., *Advanced Materials* 2008, 20, 1928-1933.

CPP 40.2 Thu 9:45 H48

Fibre-like polymer-metal nanocomposites - the morphology of a gold layer on curved polymer surfaces — ●STEPHAN V. ROTH¹, RAINER GEHRKE¹, ULLA VAINIO¹, KAI SCHLAGE¹, RALF RÖHLSBERGER¹, MANFRED BURGHAMMER², CHRISTIAN RIEKEL², VOLKER KÖRSTGENS³, EZZELDIN METWALLI³, and PETER MÜLLER-BUSCHBAUM³ — ¹HASLYAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — ²ESRF, 6rue Jules Horowitz, F-38043 Grenoble, France — ³Physik-Department E13, TU München, James-Frank-Str. 1, D-85748 Garching, Germany

Polymer-metal nanocomposites are used in many areas of sensor techniques, information technology and biotechnology [1]. These devices exploit the plasmon resonances of the confined electron gas in the metal nanostructures and typically exhibit a flat geometry. However, using aligned cylindrical, wire- or stripe-like arrays of nanoparticles enables to install plasmon waveguide devices which allow for guiding electromagnetic energy below the diffraction limit of light [2]. In our approach we use a two step technique to produce a scalable stripe-like flexible geometry. We indent a scalable biofibre in a polymer film - creating a polymeric channel - and subsequently deposit metal via sputter-deposition [3]. We follow the topography of the metal layer through the cross-section of the polymeric channel. Our findings show a strong correlation of nanoparticle morphology and cross-sectional position.

[1] Wolkenhauer et al., *Appl. Phys. Lett.* 89 (2006) 054101 [2] Maier et al., *Nature Mat.* 2, 229 (2003) [3] Metwalli et al., *Langmuir* 24, 4265 (2008)

CPP 40.3 Thu 10:00 H48

Directed Self-Assembly of Nanoporous Metallic- and Bimetallic Nanoparticle Thin Films — ●TORSTEN PIETSCH¹, NABIL GINDY², and AMIR FAHMI² — ¹Fachbereich Physik, Universität Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany — ²Department of Mechanical, Materials and Manufacturing Engineering, University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom

Nanoporous thin films attracted considerable interest due to potential applications in optical coatings, catalysis, sensors as well as electronic devices. Recently, such films were prepared by post deposition treatments. The present study is focused on the fabrication of nanoporous thin films via directed self-assembly of hybrid materials.[1] Due to the nature of this process no additional treatments are necessary to develop the pores.[2] Hierarchical nanoporous structures are fabricated directly via deposition of polymer templated Au-nanoparticles onto hydrophilic substrates.[3] These films exhibit two different pore diameters and a total pore density of more than 10^{10} holes per cm^2 . Control over the pore size is achieved by changing the molecular weight of the PS-b-P4VP diblock copolymer. Moreover, the porous morphology is used as a template to fabricate bimetallic nanostructured thin films. Such well-defined nanostructures, not only exhibit unique physical properties but also provide control over the hydrophobicity of the coated surfaces.

[1] Pietsch T et al., *Macromol. Chem. and Phys.* 210 (2009) 864

[2] Pietsch T et al.; *Soft Matter* 5 (2009) 2188

[3] Fahmi A et al.; *Macromol. Rap. Comm.* 38 (2007) 2300

CPP 40.4 Thu 10:15 H48

Real time GISAXS study of magnetic nanoparticle assemblies on polymer templates — ●EZZELDIN METWALLI¹, KAI SCHLAGE², VOLKER KÖRSTGENS¹, SEBASTIEN COUET², ROBERT MEIER¹, GUNAR KAUNE¹, STEPHAN V. ROTH², RALF RÖHLSBERGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physikdepartment E13, 85747 Garching — ²HASLYAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Hybrid materials consisting of metal nanoparticles dispersed in a polymer matrix[1,2] open pathways for engineering composites that exhibit advantageous electrical, optical, and magnetic properties. Using a portable DC magnetron sputtering deposition system, the incorporation of cobalt atoms into a microphase-separated polystyrene-block-polyethylene oxide P(S-b-EO) diblock copolymer film with parallel cylinder morphology is achieved. Time-resolved in situ grazing incidence small angle X-ray scattering (GISAXS) allows successfully to systematically investigate the formation and growth of Co nanoparticles into the polymer template. Cobalt atoms were found to wet selectively the polystyrene domains of the microphase-separated polymer film and then aggregate to form surface metal nanopatterns. Upon increasing the amount of metal content, the selectivity nature of the sputtering process was found to diminish with the formation of a pseudo-uniform metal layer. [1] E. Metwalli et al., *Langmuir* 24, 4265 (2008) [2] E. Metwalli et al., *Langmuir* 25, 11815 (2009)

CPP 40.5 Thu 10:30 H48

Manufacturing of barium titanate thin films with designed microstructure by a sol-gel process: in-situ SAXS investigation of the precursor system — ●TOMASZ STAWSKI, SJOERD VELDHOUIS, JOHAN TEN ELSHOF, OLE GÖBEL, HESSEL CASTRICUM, and DAVE BLANK — University of Twente, Inorganic Materials Science group, P.O. Box 217, 7500 AE Enschede, The Netherlands

Barium titanate (BTO) is used as a high-k dielectric material in multilayer ceramic capacitors. The minimum BTO layer thickness that can be achieved commercially with the state of the art tape casting methods is about 1 μm , which implies the use of starting powders with a particle size of ca. 200 nm. Further downsizing requires finer powders. Wet-chemical methods based on sol-gel reactions are among most thoroughly investigated, and can also be applied to make BTO. Knowledge of the size, shape and kinetics of primary sol-gel derived oligomeric nanostructures in solution is crucial to optimize the processing of functional oxide thin films from these solutions. The barium titanate sol-gel precursor system was analyzed by small angle X-ray scattering analysis at the DUBBLE beamline at the ESRF in Grenoble. BTO sols were formed in the reaction of barium acetate, titanium isopropoxide and water in glacial acetic acid and 2-methoxyethanol. The relationship between size and dimensionality of the oligomers, and the influence of synthesis conditions (temperature, concentrations of reactants) were investigated. Evolutionary, systematic changes in the radii of gyration (R_g) and internal structure of colloidal sols (characterized by the fractal dimension, D_f) were monitored as a function of time.

15 min. break

CPP 40.6 Thu 11:00 H48

Dynamics of entangled Polyisoprene-POSS Nanocomposites studied by Dielectric Spectroscopy and Linear Rheology — ●THOMAS GLOMANN^{1,2}, KLAUS NUSSER^{1,2}, GERALD JOHANNES SCHNEIDER², WIM PYCKHOUT-HINTZEN¹, REINER ZORN¹, LUTZ WILLNER¹, JUERGEN ALLGAIER¹, and DIETER RICHTER¹ — ¹IFF, Forschungszentrum Jülich GmbH, 52425 Jülich — ²Jülich Centre for Neutron Science at FRM2, 85747 Garching

Filler particles can tremendously improve the macroscopic properties of polymeric substances attributing to the enormous technological importance of composite materials. Recently, it was found that the addition of nanosized particles can lead to new and unexpected effects like a huge drop in viscosity. The microscopic details of the complex polymer-filler interactions still lack a general understanding.

We investigated the dynamics of entangled polyisoprene in the presence of POSS (polyhedral oligomeric silsesquioxanes) nanoparticles at

different filler loadings by means of dielectric spectroscopy and linear rheology. The dielectric measurements reveal that the particles do not alter the observed microscopic chain dynamics at all. However, the mechanical properties show a strong increase in modulus strength with increasing filler concentration. Moreover, the liquid-like behavior at low frequencies changes to a solid-like behavior above a certain critical filler level.

CPP 40.7 Thu 11:15 H48

Influence of the nanoparticles on the structural relaxations in epoxy nanocomposites as seen by rheological spectroscopy

— ●MATTHIEU THOMASSEY, JÖRG BALLER, JAN KRISTIAN KRÜGER, and ROLAND SANCTUARY — Université du Luxembourg, Laboratory of Physics of Condensed Matter and Advanced Materials (LPM), 162a Avenue de la Faïencerie L-1511 Luxembourg

Due to their large surfaces nanoparticles are well known to have a dramatic influence on the glass transition behavior of nanocomposites made of oligomer matrices and inorganic fillers. Generally one distinguishes between topological and surface induced effects of the nanoparticles. By changing the concentration of the filler particles, topological constraints are expected to have an influence on the glass transition of the composite. By modifying the state of their surfaces the interaction between the oligomer molecules and the nanoparticles and hence the mechanisms leading to the glass transition are also altered. This paper presents a rheological study of an epoxy resin (DGEBA) filled either with alumina particles with a hydrophilic surface or silica with a hydrophobic surface. Topological and surface-induced effects of the nanoparticles on the glass transition behavior of the composite are elucidated. Rheological spectroscopy is used to study the temperature and frequency dependencies of the shear moduli for the two types of nanocomposites. Special attention is paid to an abnormal behavior of the real and imaginary parts of the shear modulus.

CPP 40.8 Thu 11:30 H48

Polymer-grafted Silica Nanoparticles: a Structural Characterization in Solution and Bulk — ●MATHIAS MEYER¹, EIKE HÜBNER¹, WIM PYCKHOUT-HINTZEN¹, JÜRGEN ALLGAIER¹, AUREL RADULESCU², DIETER RICHTER^{1,2}, PIETER J. IN 'T VELD³, and HORST WEISS³ — ¹Institut für Festkörperforschung, Forschungszentrum Jülich GmbH — ²Jülich Centre for Neutron Science, Garching, Forschungszentrum Jülich GmbH — ³BASF SE, Ludwigshafen

Though nanocomposites with their astonishing properties are of great interest for research and industry, microscopic details of the polymer-interface have been scarcely investigated. Therefore a model system basing on grafted silica nanoparticles is designed and studied. From TEM, SANS and SAXS experiments, particle sizes and their distribution were determined independently. Despite surface stabilization, attractive inter-particle interactions, formerly neglected in literature, lead to small dynamic aggregates, which we described microscopically in a consistent manner. The influence of the grafting density and the chain length and type of the graft as well as of the dispersing medium were investigated in terms of a polydisperse core-shell-type model. Our experimental results are compared to multiscale simulations within an EU FP7 project (NanoModel), focussing on the radial density profile of the polymer shell. Due to our newly developed "grafting to" approach a labelling of the grafted chains is now possible, which allows for the first time to investigate the chain conformation in the shell. Unlike with other grafting methods (i.e. ATRP), also polymers with a low entanglement molecular weight can be grafted to.

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Functionalization and Characterization of SWCNTs for Electronics Applications — ENGIN KARABUDAK^{1,2}, CLAUDIA BACKES³, FRANK HAUKE³, ANDREAS HIRSCH³, and ●WENDEL WOHLLEBEN¹

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We report the application of a novel multiwavelength analytical ultracentrifuge (AUC) to the correlation between hydrodynamic size and absorption in CNT dispersions. The statistical relevance is high due to the evaluation of 10^{11} colloids in one experiment. The machine operates at up to 60 krpm and records $c(r,t,\lambda)$ with a 100-fold speed improvement over commercial AUCs. Single-wall CNTs are notoriously difficult to disperse, not only because of their high tendency to agglomerate, but also due to insufficient understanding of the CNT-ligand interactions. Here we prepare an up to 88 percent efficient dispersion of SWCNTs (HiPco and CoMoCAT) by non-covalent ligands (perylene bisimides with Newkome dendrimers) and intercalant agents (perylene). Without previous purification we quantify from a single 1h-experiment the coexistence of debundled, ligand-encapsulated CNTs; CNT bundles with few ligands attached; hydrolyzed intercalant; intercalant - ligand micelles, with the absorption profiles and anhydrous specific volume for each component. Bulky dendritic groups on the surfactants systematically reduce the adsorption density on the CNT surface, which is on the order of 1 mmol surfactant / g SWCNT.

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Modelling of electric conductivity in sheared CNT/polymer composites — ●MARINA SAPHIANNIKOVA¹, TETYANA SKIPA², DIRK LELLINGER², INGO ALIG², and GERT HEINRICH¹ — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden — ²Deutsches Kunststoff Institut, Schlossgartenstr. 6, 64289 Darmstadt

Theoretical description of electric properties of the polymer melts, filled with attractively interacting conductive particles, represents a great challenge. Such filler particles tend to build a network-like structure [1] which is very fragile and can be easily broken under steady shear flow with shear rates of about 1/s. In the quiescent state of melt the particles agglomerate again, slowly restoring the network structure. The agglomeration process can be facilitated by application of shear flow with small shear rates of about 0.01/s [1]. In this study, the shear-induced changes in electric conductivity of polymer composites are described using a Bethe-lattice percolation theory [2] which enables the modelling of filler network conductivity. Additionally, we take into account the matrix conductivity enhanced by the presence of single filler particles. The percolation theory is coupled with a kinetic equation for the scalar structural parameter which describes the instantaneous state of filler network at particular flow conditions. The coupling approach is verified in transient shear experiments carried out on polycarbonate composites filled with multi-wall carbon nanotubes.

This work was supported by the BMBF grant No.03X0504E.

[1] T. Skipa et al. Phys. Stat. Sol. B 246, 2453 (2009)

[2] F. Semeriyonov et al. J. Phys. A: Math. Theor. 42, 465001 (2009)

Invited Talk

CPP 40.11 Thu 12:15 H48

Novel Nanocomposites in Industrial Applications - Chances and Challenges — ●PÉTER KRÜGER — Bayer MaterialScience AG, Chempark Geb. Q23, 51368 Leverkusen

Zur Zeit nicht verfügbar