CPP 3: Interfaces and Thin Films I

Time: Monday 10:30–13:00 Location: ZEU 160

CPP 3.1 Mon 10:30 ZEU 160

Depinning of 2D Droplets in a Free Energy Model — •Daniel Herde, Stephan Herminghaus, and Martin Brinkmann — MPI for Dynamics and Self-Organization, Göttingen, Germany

While the problem of a moving contact line on an ideal substrate has been studied for some time, the dynamic behaviour on a heterogeneous substrate is not yet fully understood. Even the pinning behaviour of droplets, where they stay in place even though an external force is applied, is not characterised properly. We use a free energy approach to numerically describe the depinning of 2D droplets at single defects, on periodic and on randomly patterned substrates in the static limit.

The simulations for a single defect agree with a simple prediction for the force required for depinning, relating it to the maximum wettability contrast. Periodic substrate wettabilities lead to a set of new phenomena, as the system can display more than one stable pinned state. The determined depinning forces deviate strongly from the single pinning site case. These findings agree with our small Reynolds number fluid dynamics simulations.

CPP 3.2 Mon 10:45 ZEU 160

Order and phase behavior of cylinder forming diblock copolymers and nano-particles mixture in confinement : A Molecular Dynamics study — •Lenin Singh Shagolsem[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden — [2]Institute of Theoretical Physics, TU Dresden

We study a coarse grained model of cylinder forming diblock copolymers and nano-particles mixture confined between Lennard-Jones hard walls. Both non-selective and selective nano-particles cases are considered. For non-selective nano-particles two models of interactions between monomers and nano-particles are used. Here, we focused on the role of interfaces and particles clustering, uptake and segregation of particles as a function of temperature and overall particle volume fraction, and the influence of particles on morphology. On the other hand, for the case of selective nano-particles, we systematically explored the various ordered structures formed in this restricted environment.

CPP 3.3 Mon 11:00 ZEU 160

Mechanical Properties of Random Block Copolymer Melts in the Bulk and at Selective Substrates — •Birger Steinmüller and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, Göttingen

Random block copolymers are interesting materials to study since they show microphase separation, while lacking longer-ranged order, in a melt. We use two different coarse-grained models to access the properties of these systems via computer simulations:

The Single-Chain-in-Mean-Field simulation (SCMF), which uses a soft, density-dependent non-bonded interaction, and the Lennard-Jones bead-spring model. For the latter model we use LAMMPS, since simulating the melt via MD allows us to access the frozen state (glass) at low temperatures.

In order to determine the mechanical properties of the melt, we equilibrate the system, then quench it below the glass transition temperature. We use this glass to calculate, via a virial expansion, the local mechanical properties, e.g., local compressibility and local shear modulus. This approach is used for bulk systems, as well as for melts in contact with a selective substrate. We compare the mechanical properties of the interface and the interphase with those of the bulk. Another type of interface in the bulk, the boundary region between domains with a high concentration of the two different sorts of monomers, is additionally considered.

CPP 3.4 Mon 11:15 ZEU 160

Approach to polymer brushes of spherical monomers — •Dirk Romeis[1,2], Holger Merlitz[1,3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden — [2]TU Dresden, Fachbereich Physik, 01062 Dresden — [3]Department of Physics and ITPA, Xiamen University, Xiamen 361005, P. R. China

Recent experiments [1] for the creation of polymer brushes achieved considerable high grafting densities ($\sigma \geq 1/nm^2$) and subsequently chain stretchings up to $70 - 90\%$. In this range the behavior can no longer be approximated using the Gaussian chain model. Furthermore MD simulations [2] of brushes of densely grafted chains revealed significant instabilities of the brush surface upon slight variations of individual chains/chain ends. Analytical SCF approach for a polymer brush of spherical monomers [3] is not applicable to study these effects as it fully neglects fluctuations. We present a modified Scheutjens-Fleer method to account for a spherical shape of the monomers, compare the results with other approaches [2],[3] and give a quantitative analysis of the observed surface instabilities, which entail the behavior of a phase transition. [1] Devaux C. et. al. [*Macromolecules* **38** 4296, 2005]. [2] Merlitz H. et. al. [*Macromolecules* **41** 5070, 2008]. [3] Biesheuvel M. et. al. [*Macromolecules* **41** 6254, 2008].

CPP 3.5 Mon 11:30 ZEU 160

Ferrocene-Pyridine Block Copolymers at the Air/Water Interface and in Solution — •Martin Müller[1], Markus Gallei[2], Roland Klein[2], Bernd Stühn[1], and Matthias Rehahn[2] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Ernst-Berl-Institut für Technische und Makromolekulare Chemie, TU Darmstadt

Ferrocene-containing polymers attract much attention because of their unique mechanical, (electro)chemical, (opto)electronical or magnetic properties [1]. We present structural investigations of the block copolymer poly(vinylferrocene-*b*-(2-vinylpyridine)) (PVFc-*b*-P2VP) [2]. Langmuir technique and in-situ X-Ray reflectivity on the water/gas interface were used to investigate the surface properties and conformations as a function of molecular weight (brush regimes and mushroomlike structures). In addition time dependent X-Ray reflectivity revealed surface structure relaxations of the pyridine blocks at the air/water interface. SAXS was used to determine structure of the PVFc-*b*-P2VP solutions. The results indicate the formation of vesicles with relative narrow size distributions. Combining the different methods leads to a detailed understanding of PVFc-P2VP structures.

[1] G. R. Whittell, I. Manners, Adv. Mater. 2007, 19, 3439

[2] M. Gallei et al. Macromolecules, 2010, 43 (4), 1844-1854

CPP 3.6 Mon 11:45 ZEU 160

Polyoxazoline Brushes: Fabrication, Characterization and Applications — •Mukesh Agrawal[1], Juan Carlos Rueda[2], Petra Uhlmann[1], Martin Müller[1], Frank Simon[1], Carla Chung[1], and Manfred Stamm[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — [2]Laboratorio de Polimeros, Sección Física, DGI, Pontificia Universidad Católica del Perú, Lima, Perú

In this study, we explore the fabrication of poly(2-isopropyl-2-oxazoline) brushes on macroscopic surfaces by exploiting the *grafting-to* approach. Firstly, carboxyl functionalized poly(2-isopropyl-2-oxazoline) molecules have been synthesized by ring opening cationic polymerization and subsequently, resulting polymer chains have been grafted onto the underlined substrates in brush-like conformation. A wide range of analytical tools including ellipsometry, contact angle, X-ray photoelectron spectroscopy, attenuated total reflection infrared spectroscopy and atomic force microscopy have been employed to characterize the polyoxazoline brushes. Finally, fabricated polymer brushes have been used to control adsorption of inorganic nanoparticles and protein molecules on macroscopic surfaces.

CPP 3.7 Mon 12:00 ZEU 160

Reversible structuring of azobenzene polymer films by surface plasmons — Tobias König and •Svetlana Santer — Department of Experimental Physics, Potsdam

Our group is interested in interactions between nano-particles and nano-structured polymer surfaces. We have shown that it is possible to move adsorbed nano-objects with relative ease, in large number and simultaneously without using external devices. The essential idea is not to put more effort in fighting against the prevailing surface forces but rather to utilize them - in clear contrast to current techniques of nano-manipulation with AFM [Santer, Adv Mat 2006]. For this, the topography should be reversible switching by changing the morphology at the scale of objects to be moved. In this work, we choose light for changing the polymer topography. Here we present azo thin films [Seki, Chem Soc Jpn 2007] with integrated optically active elements supposed to support and steer the response of polymer films to external illumination. During irradiation surface plasmon polarizations (SPP) are generated on a metallic mask. The interaction of the SPP

with azo polymers results in printing of near field intensity distributions into topography with the pattern size below the diffraction limit. The topography can be driven reversible. This allows us to analyze different patterns by changing polarization or wavelength at the same position. We also examine the structuring process depending on different metallic patterns like nanogab, nanohole and hexagonal pattern. By confirmation with FDTD simulation we are able to analyze the forces which are responsible for the imprints at the azo air interface.

CPP 3.8 Mon 12:15 ZEU 160

Biomimetic crystalization of iron oxides at liquid interfaces studied by x-ray scattering experiments — •Florian Wieland[1], Patrick Degen[2], Steffen Bieder[1], Michael Paulus[1], Martin Schroer[1], Christoph Sahle[1], Johannes Möller[1], Heinz Rehage[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Germany — [2]Fakultät Chemie, Technische Universität Dortmund, Otto-Hahn-Str. 6, 44227 Dortmund, Germany

Biomineralization processes provide composite materials which show a hierarchical organization, complex and controlled shapes. In living organisms the biomineralization process is controlled by complex biological mechanisms and by the environment where the process takes place. We have investigated in-situ the mineralization of iron oxide at Langmuir monolayers at the aqueous solution-air interface. Information on the vertical density profile were obtained by x-ray reflectivity measurements where the structural evolution of the mineral layer could be observed. Furthermore grazing incidence diffraction measurements were performed in order to evaluate the crystal structure of the iron oxide and the lateral structure of the Langmuir layer. For the investigation of the local structure of the forming film surface sensitive extended x-ray absorption fine structure measurements were performed. The formation of a thin amorphous layer of iron oxide under Langmuir monolayers which posses a negative or positive headgroup was observed. The EXAFS data show that the iron coordination is similar to the coordination in maghemite, but without long range ordering.

CPP 3.9 Mon 12:30 ZEU 160

Surface templated orientation of α-helical poly(L-lysine)/ polyanion complexes on unidirectionally texturised substrates — •Martin Müller[1], Wuye Ouyang[2], Thomas Keller[3], and Klaus Jandt[3] — [1]Leibniz Institute of Polymer Research (IPF) Dresden — [2]Unilever, Shanghai, P.R. China — [3]Institute of Materials Science and Technology (IMT) , University Jena

Oriented polyelectrolyte complex layers of stiff α-helical poly(L-lysine) (PLL) and poly(styrenesulfonate) (PSS) or poly(vinylsulfate) (PVS) were deposited on either unidirectionally mechanically scratched silicon substrates (i) or thin unidirectionally melt-drawn (md) poly(ethylene) (PE) films (ii) applying the layer-by-layer concept. Based on ATR-FTIR dichroism of the Amide I/II band and SFM image analysis averaged cone opening angles γ of bundled α-PLL rods in the range $\gamma = 12° - 35°$ for both substrate types were found, from which high in-plane orientation was concluded. On the mechanically texturised Si substrates (i) fibrous rod-like deposits were aligned along the scratching direction and the orientation showed a significant molecular weight effect of PLL and of PSS, which can be interpreted by a topographical confinement effect of nanoscopic surface grooves on PLL/polyanion rods. Whereas, on the md-PE films (ii) fibrous rod-like deposits were aligned normal to the drawing direction, which can be interpreted by a templating effect of oriented lamellae and regular amorphous/crystalline patterns. Applications of such oriented PEL complex structures are enantiospecific surfaces for the separation of chiral drugs as well as templates for directed cell growth.

CPP 3.10 Mon 12:45 ZEU 160

Thermal tuning of micro-structured conducting polymer thin films — •Robert Meier[1], Hsin-Yin Chiang[1], Matthias A. Ruderer[1], Shuai Guo[1], Johannes Wiedersich[1], Volker Körstgens[1], Jan Perlich[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Conducting polymers have already shown their great potential for versatile applications such as organic light emitting diodes or thin film transistors. For such applications many routes have been invented to structure thin films on the micro- and even the nanoscale. Since conducting polymers often have a low glass transition temperature the shape of polymeric microstructures can be tuned by posterior annealing. In this work we present an in-situ grazing incidence small angle x-ray scattering study of the influence of thermal treatment on microchannels made of conducting polymers. These structures are fabricated via a new and easy fabrication routine combining a structured master and a film transfer technology. The temperature depending collapsing of the channels reveals a constant transition from sharp side walls to wavy surfaces. Such structured surfaces yield an increased light reflection and hence allow an enhanced optical absorption interesting for organic solar cells. The study is complemented with atomic force microscopy and scanning electron measurements of the polymeric microstructures before and after thermal treatment.