

## CPP 27 POSTER Polymer Physics and Materials

Time: Thursday 17:00–19:00

Room: P2

CPP 27.1 Thu 17:00 P2

**Microfocus-Infrared Synchrotron Ellipsometry for analysis of laterally patterned organic thin films** — ●MICHAEL GENSCH<sup>1</sup>, ERNST HEINER KORTE<sup>2</sup>, NORBERT ESSER<sup>1</sup>, ULLRICH SCHADE<sup>3</sup>, and KARSTEN HINRICHS<sup>1</sup> — <sup>1</sup>ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — <sup>2</sup>ISAS - Institute for Analytical Sciences, Bunsen-Kirchhoff-Str. 11, 44131 Dortmund, Germany — <sup>3</sup>Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

A purpose-build infrared spectroscopic ellipsometer is presented that enables to investigate sample areas of less than 1 mm<sup>2</sup> with monolayer sensitivity. This sensitivity is achieved for films on metallic as well as on semiconducting substrates by utilizing radiation from an infrared synchrotron beamline at BESSY II. Measurement principle and performance of the instrument are discussed on selected examples and an outline of the recently performed upgrade of the set-up is given. It is shown how thickness, structure and composition of patterned nanofilms can be characterized by evaluation of the infrared ellipsometric parameters [2]. This is of technological relevance to investigate the functionality of e.g. stimuli responsive 1D polymer brush gradient films, biodiagnostic arrays or monomolecular films for solar cell applications. [1] M. Gensch, K. Roodenko, K. Hinrichs, R. Hunger, A. Merson, U. Schade, Y. Shapira, Th. Dittrich, J. Rappich, N. Esser, J. Vac. Sci. Technol. B 23, 1838 (2005). [2] K. Hinrichs, M. Gensch, N. Esser, Appl. Spectrosc. 59, 272A (2005).

CPP 27.2 Thu 17:00 P2

**IR-VIS Ellipsometry for characterization of ultra-thin polymer films** — ●K. HINRICHS<sup>1</sup>, M. GENSCH<sup>1</sup>, N. ESSER<sup>1</sup>, L. IONOV<sup>2</sup>, M. STAMM<sup>2</sup>, S. MINKO<sup>3</sup>, and K.-J. EICHHORN<sup>2</sup> — <sup>1</sup>ISAS - Institute for Analytical Sciences, Department Berlin, — <sup>2</sup>Leibniz Institute for Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden — <sup>3</sup>Chemistry Department, Clarkson University, Potsdam, New York 13699, USA

Mid infrared (MIR) spectroscopic ellipsometry [1] and Visible (VIS) ellipsometry have been jointly used for the study of mixed polystyrene-poly(2-vinylpyridine) and polystyrene-poly(ter-butyl acrylate) polymer grafted films (mixed brushes) with gradually changing composition (1D gradient mixed brushes). In the first step from ellipsometric measurements the optical constants of the single polymers in thin films (PS, P2VP, PBA) have been evaluated. In a second step the thickness and composition of mixed polymer brush films (d<10nm) of these compounds were determined. It is evident that infrared optical properties of polymer thin films are correlated to the chemical structure of the thin film and can be used for lateral compositional analysis, whereas conventional VIS ellipsometry is limited by the similarity of refractive indices of different polymers. Present limitations of IRSE are due to the signal to noise ratio and restricted lateral resolution. This can be improved at the synchrotron ellipsometer at BESSY/Berlin, which is presently upgraded for mapping experiments.

[1] K. Hinrichs, M. Gensch, N. Esser, Appl. Spectrosc. 59 (2005) 272(A)-282(A). [2] L. Ionov, A. Sidorenko, K.-J. Eichhorn, M. Stamm, S. Minko, K. Hinrichs, Langmuir 21 (2005) 8711.

CPP 27.3 Thu 17:00 P2

**Optical and mechanical anisotropy of oriented PET films studied by reflectance difference spectroscopy** — ●KLAUS SCHMIDEGG<sup>1</sup>, LI DONG SUN<sup>1</sup>, GÜNTHER MAIER<sup>2</sup>, JOZEF KECKES<sup>2</sup>, and PETER ZEPPENFELD<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenbergerstr. 69, A-4040 Linz — <sup>2</sup>Erich Schmid Institut für Materialwissenschaften, Jahnstr. 12, A-8700 Leoben

A new method for the characterization of molecular orientation in polymers is presented, which is based on the determination of the optical anisotropy by reflectance difference spectroscopy (RDS). Its advantages are the sensitivity to birefringence, spectroscopic information, high time resolution and superior measurement precision as compared to refractive index measurements. The capabilities of RDS are presented for the special case of biaxially oriented poly(ethylene terephthalate) (PET) films, for which both magnitude and direction of the optical anisotropy can be determined. The data are consistent with refractive index measurements

using spectroscopic ellipsometry and wide-angle X-ray scattering. The high time resolution and the simple setup enabled us to perform in-situ measurements during tensile testing of thin PET films. A clear correspondence of the initial optical and mechanical anisotropy directions can be seen. The RDS signal depends linearly on the applied strain and the gradient shows the same angular behavior. A closer look reveals that not only the size of the optical anisotropy changes, but also the position of the axes is rotated towards the drawing direction, which is a consequence of the reorientation of the molecules in the polymer.

CPP 27.4 Thu 17:00 P2

**Surface roughness and adsorption isotherms of molecularly thin liquid films** — ●MICHAEL PAULUS<sup>1</sup>, CRISTIAN GUTT<sup>2</sup>, and METIN TOLAN<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Dortmund, D-44221 Dortmund, Germany — <sup>2</sup>Deutsches Elektronen Synchrotron (HASYLAB), Notkestraße 85, D-22607 Hamburg, Germany

We present an x-ray reflectivity study of molecularly thin adsorbed isobutane films on liquid glycerol. The interaction between the isobutane and the liquid glycerol is usually dominated by long-range van der Waals interaction which gives rise to the formation of thin films of gas molecules on the glycerol surface. Surfaces of liquids are modulated by thermally excited capillary wave fluctuations. Concerning thin films, this capillary wave fluctuations are strongly suppressed by the substrate-film interaction. This leads to a layer thickness dependent roughness of thin adsorbed films. The x-ray reflectivity measurements provide both, the adsorption isotherms and the rms roughness of the adsorbed film. The measured surface roughness of the isobutane film is smaller than expected from a calculation based on a harmonic approximation of the interaction potential. It turned out that the calculation of surface roughness of molecularly thin adsorbed films leads to good agreement with experiment, only when higher order terms of the interaction potential are considered. This is causally connected by the strong coupling between the glycerol and layer surface at low layer thickness.

CPP 27.5 Thu 17:00 P2

**Phase properties of confined dipolar fluids** — ●MATHIAS GRAMZOW<sup>1</sup> and PD DR. SABINE H. L. KLAPP<sup>1,2</sup> — <sup>1</sup>Stranski Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin — <sup>2</sup>TU Berlin, Institut für Theoretische Physik, Hardenbergstrasse 36, 10623 Berlin

The phase behavior and structural properties of various dipolar model fluids confined to a slit pore are investigated using density functional theory in meanfield (MF) and truncated modified meanfield (MMF) approximation. As a first step we approximate the inhomogeneous number density in the pore as a constant and consider only the orientational structure. Our focus lies on the description of isotropic and anisotropic fluid phases.

In the MF calculations we find first- and second-order isotropic-to-ferroelectric as well as isotropic liquid-to-gas phase transitions. For both types of phase transitions the confinement shifts the critical points towards lower temperatures. It also shifts the chemical potential, where the direction of the shift depends on the model considered. Moreover, in very narrow pores the isotropic liquid-to-gas phase transition is entirely suppressed.

Finally, we compare our MF results for the phase behavior to those from the more sophisticated MMF approach. The latter also provides information on the local orientational structure which turns out to be anisotropic even in globally isotropic phases.

CPP 27.6 Thu 17:00 P2

**Gradient nanotubes by wetting** — ●MARC MILBRADT<sup>1</sup>, PAUL MICHAEL<sup>1</sup>, ANDREAS GREINER<sup>2</sup>, and RALF WEHRSPHORN<sup>1</sup> — <sup>1</sup>Physics Department, University of Paderborn — <sup>2</sup>Philipps University Marburg

Using the wetting-assisted templating (WASTE) process for the preparation of single homogenous nanotubes we produced gradient nanotubes. The WASTE process is based on the spontaneous wetting of high-energy surfaces (macroporous silicon or porous alumina) by low-surface energy materials (organic compounds, here: polymers). The wetting can be done in solution or in melt state. With modifications on the WASTE-process it is possible to prepare nanotubes with a longitudinal gradient. The so-called "face-to-face"-wetting allows wetting of two different ma-

terials placed on the opposite ends of the template pores.

We prepared gradient nanotubes by the use of PMMA and a fluorescent PMMA/9-Vinylanthracene copolymer. The gradient is formed at the point of contact of the two polymers. Another way to prepare gradient nanotubes is to use a mixture of polystyrene and a fluorescent dye (here: DANS) on the one side and polystyrene on the other side of the template pores. In this case the gradient is formed by diffusion of the dye into the polymer. The gradient nanotubes were investigated by fluorescence microscopy.

The gradient nanotubes can be used for graded-index optical fibers or waveguides and gradients in the surface-energy can be used to direct fluids on a given path.

CPP 27.7 Thu 17:00 P2

**Unexpected preparative effects on the properties of thin polymer films** — ●ANATOLI SERGHEI<sup>1</sup>, HEIKO HUTH<sup>2</sup>, CHRISTOPH SCHICK<sup>2</sup>, and FRIEDRICH KREMER<sup>1</sup> — <sup>1</sup>University of Leipzig, Institute for experimental physics I, 04103 Leipzig, Germany — <sup>2</sup>University of Rostock, Physics Department, , 18051 Rostock, Germany

Thin supported PS films dewet a solid substrate when kept above  $T_g$  in vacuum ( $\sim 3$  mbar), while in high vacuum ( $10^{-6}$  mbar), under identical experimental conditions, i.e. same thickness, temperature and annealing time, no dewetting takes place. When sandwiched between two thin metal electrodes a characteristic pattern is developed in ambient air above  $T_g$ , whereas no changes are observed in high vacuum or in a pure nitrogen atmosphere. These two seemingly unrelated phenomena are suggested to have a common physical origin: due to the presence of remanent oxygen in the immediate vicinity of the polymer films, chain scissions are induced, which result in a pronounced decrease of the average molecular weight. This causes an enhancement of the molecular mobility and a reduction of the corresponding glass transition temperature  $T_g$ , as proven by Broadband Dielectric Spectroscopy, AC-calorimetry and capacitive dilatometry. No shifts of the glass transition in thin PS films down to a thickness of 20 nm are detected when the samples are annealed in high vacuum and measured in a pure nitrogen atmosphere.

A. Serghei et al., Phys. Rev. E 71, 061801 (2005).

CPP 27.8 Thu 17:00 P2

**Spin-Echo Neutron Reflectivity on Diblock-Copolymer Films** — ●MAX NÜLLE<sup>1</sup>, ADRIAN RÜHM<sup>2</sup>, JANOS MAJOR<sup>1</sup>, ULRICH WILDGRUBER<sup>2</sup>, and HELMUT DOSCH<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — <sup>2</sup>Max-Planck-Institut für Metallforschung, ZWE Neue Forschungsneutronenquelle Garching, Lichtenbergstr. 1, 85747 Garching bei München

SERGIS (Spin-Echo Resolved Grazing Incidence neutron Scattering) is a recently developed novel neutron scattering technique which will be routinely employed at the new X-ray/neutron reflectometer N-REX+ at FRM-II. In contrast to conventional scattering methods, SERGIS measures the lateral structure and morphology of surfaces and thin film systems in real space. The spatial resolution is achieved by measuring the total polarization of the scattered beam, without the usual need to collimate the beam in the direction of interest. Therefore SERGIS combines a high neutron flux with the ability to characterize structures from the nanometer scale up into the micron range, and can thus yield novel information about both equilibrium and time-dependent phenomena on these length scales. One typical example is morphologies produced by dewetting phenomena. First results of experiments on diblock-copolymer films will be presented.

CPP 27.9 Thu 17:00 P2

**Bottom-Up Lithography: Growing Layout-Defined 3-dimensional Micro- and Nano-Structures by Molecular Self-Assembly** — ●MATTHIAS BARCZEWSKI<sup>1,2</sup>, ALFRED BLASZCZYK<sup>1</sup>, MARCEL MAYOR<sup>1,3</sup>, THOMAS SCHIMMEL<sup>1,2</sup>, and STEFAN WALHEIM<sup>1</sup> — <sup>1</sup>Institute for Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — <sup>2</sup>Institute of Applied Physics, University of Karlsruhe, 76131 Karlsruhe (Germany) — <sup>3</sup>Chemistry Department, University of Basel, 4056 Basel (Switzerland)

We present a novel soft-lithographic approach for the formation of metal-organic micro- and nanostructures on surfaces. The structures are grown from bottom up, instead of removing material from a resist layer [1]. This can be achieved by making use of an anisotropic molecular self-assembly process which leads to the formation of a metal-organic film which we call Substrate-Consuming Metal-Organic Layer (SCMOL). This growth can be laterally controlled by the pre-deposition of a mono-

molecular two dimensional pattern, by Micro-Contact Printing. This patterned self-assembled monolayer (SAM) acts as a lateral stencil mask for the growth process of the SCMOL film. This process yields structures with perpendicular walls and a lateral resolution of about 20 nm. The height of the structures reaches up to 600 nm - hundred times the height of the constituent molecules.

[1] S. Walheim, M. Barczewski, A. Blaszczyk, M. Mayor, Th. Schimmel Patent application: DE 102005025693.7 (2005)

CPP 27.10 Thu 17:00 P2

**Mixed monolayers of phospholipids and amphiphilic block copolymers at the air/water interface** — ●S. RALEVA<sup>1</sup>, H. HUSSAIN<sup>2</sup>, J. KRESSLER<sup>2</sup>, V. SCHÖN<sup>3</sup>, P. HUBER<sup>3</sup>, and B. STÜHN<sup>1</sup> — <sup>1</sup>TU Darmstadt, D-64289 Darmstadt — <sup>2</sup>MLU Halle-Wittenberg, D-06099 Halle — <sup>3</sup>University of Saarland, D-66041 Saarbrücken

We have investigated the behaviour of mixed monolayers of phospholipids and amphiphilic block copolymers at the air/water interface by measuring the surface pressure/area isotherms in conjunction with x-ray reflectivity measurements. The samples are the synthetic phospholipid diphtanoylphosphatidilcholine (DPhPC) and amphiphilic di- and tri-block copolymers of poly(ethylene oxide) and poly(perfluorohexylethyl methacrylate). From the isotherms we obtain information about the monolayer conformation as a function of the degree of compression. From the x-ray reflectivity measurements we obtain information about the surface roughness, film thickness and electron density variation along the surface normal. We discuss the results as a function of the film composition and the surface pressure. DPhPC isotherms show that the phospholipid exists in the liquid-expanded phase at all surface pressures. The results of monolayer thickness at the air/water interface are in agreement with the results for monolayer of DPhPC on solid substrate. Analysis of the surface pressure/area isotherms shows that the addition of polymer results in homogeneously mixed as well as of non mixed films, depending on the concentration of the added polymer, its composition and surface pressure. X-ray reflectivity measurements results show clear change in the thickness of the film after addition of the polymer.

CPP 27.11 Thu 17:00 P2

**Polarized Fourier Transform Infrared Spectroscopy on Thin Chiral Liquid Crystal Elastomer Films** — ●MICHAEL TAMMER<sup>1</sup>, PATRICK KÖLSCH<sup>1</sup>, BIN CHEN<sup>2</sup>, HEINO FINKELMANN<sup>2</sup>, and FRIEDRICH KREMER<sup>1</sup> — <sup>1</sup>Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig — <sup>2</sup>Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie, Stefan Meier Str. 31, 79104 Freiburg

Liquid crystalline elastomers (LCE) are consisting of crosslinked polymers with mesogenic units connected to the polymer network. Embedding an anisotropic liquid crystals in an elastic polymer network results in a variety of remarkable features. Their macroscopic form changes strongly with temperature, they are birefringent due to the alignment of the mesogens or they change volume in electric fields, just to name a few of the sophisticated features of this relatively new class of material. The potential applications range from soft contact lenses, artificial muscles, multicolor laser devices to electro-mechanical devices. Polarized Fourier Transform Infrared Spectroscopy (FTIR) is applied to investigate the molecular response of thin liquid crystal elastomer (LCE) films with a cholesteric mesogen structure to an external mechanical stress. The analysis of the absorbance bands for molecular vibrations of the main chain, the spacer groups and bands of the mesogens yields the mean orientations and the order parameters of these molecular units. The influence of the applied strain on the orientation and order is determined.

CPP 27.12 Thu 17:00 P2

**Structural and mechanical properties of thin PMMA films prepared by pulsed laser deposition** — ●ANDREAS MESCHEDÉ, ERIK SÜSKE, THORSTEN SCHARF, and HANS-ULRICH KREBS — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Thin polymer films were grown by pulsed laser deposition (PLD) at 248 nm in ultra high vacuum (UHV). In the case of poly(methyl methacrylate) (PMMA), the observed films consist of two components which differ in chemical and mechanical properties as molecular mass or amount of crosslinking. These properties can be controlled by deposition parameters like substrate temperature and laser fluence or by using absorption optimized target material. In this contribution the deposition mechanism with respect to the film characteristics, as for example microstructure and mechanical properties, which have been ex-

amined by scanning electron microscopy, mechanical spectroscopy and nano-indentation measurements, will be discussed.

CPP 27.13 Thu 17:00 P2

**Faster dynamics in thin polymer films?** — ●ANATOLI SERGHEI<sup>1</sup>, LUTZ HARTMANN<sup>1</sup>, YULIA MIKHAILOVA<sup>2</sup>, KLAUS-JOCHEN EICHORN<sup>2</sup>, BRIGITTE VOIT<sup>2</sup>, and FRIEDRICH KREMER<sup>1</sup> — <sup>1</sup>Leipzig University, Institute for Experimental Physics I, Leipzig, Germany — <sup>2</sup>Leibniz Institute of Polymer Research, Dresden, Germany

The molecular dynamics in thin films of polymers with different macromolecular architectures (linear and hyperbranched structures) are investigated by Broadband Dielectric Spectroscopy. Pronounced confinement-effects are detected: the average relaxation rate of the dynamic glass transition increases with decreasing film thickness, indicating a faster dynamics in thin films. The molecular mechanism of these effects is revealed by the quantitative determination of the relaxation time distribution in dependence on the confinement size. It turns out that: a) the increase in the average relaxation rate is caused by a gradual suppression (freezing-out) of the slower relaxation modes in confinement; b) at a molecular level no polymer segments are found to relax faster in thin films than in the bulk.

L. Hartmann et al., Eur. Phys. J. E 8, 145 (2002). A. Serghei et al., Eur. Phys. J. E 17, 199 (2005).

CPP 27.14 Thu 17:00 P2

**Mechanical Properties of Free Standing Liquid Filaments** — ●ALEXANDRU NEMES, ALEXEY EREMIN, and RALF STANNARIUS — Institute of Experimental Physics, University of Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Stable free standing filaments with slenderness ratios (length to diameter ratio) of more than 1000 can be prepared in some mesophases of liquid crystals. In our work, the mechanical properties of such structures are described. With a special excitation technique, we pluck the filaments and excite damped oscillations. Experimental relaxation times and oscillation frequencies of such liquid chords are discussed within a model that describes the damped vibrations of a liquid string under the influences of surface tension, inertial, viscous, and elastic forces. Reference: R. Stannarius, A. Nemes and A. Eremin, Phys. Rev. E, 72 020702(R) (2005)

CPP 27.15 Thu 17:00 P2

**AFM-Nanolithography on self-assembled monolayers** — ●HARALD GRAAF<sup>1</sup>, MAIK VIELUF<sup>1</sup>, MASATO ARA<sup>2</sup>, and HIROKAZU TADA<sup>2</sup> — <sup>1</sup>Optische Spektroskopie und Molekülphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — <sup>2</sup>Division of Materials Physics, Graduate School of Engineering Science, Osaka University, Osaka 560-8531 JAPAN

We report on the anodic oxidation of self-assembled monolayers (SAM) on silicon surfaces by Atomic Force Microscopy (AFM). These SAM are prepared by heat-induced chemical reaction of an alkene with a hydrogen terminated silicon surface. They are characterized by a high order of the molecules and a strong physical as well as chemical stability. By varying the headgroup of the alkenes the properties of the surface can be easily tuned, e.g. from hydrophobic to hydrophilic. By anodic oxidation the SAM can be locally degraded and the below silicon oxidized leading to silicon oxide nanostructures. These silicon oxide structures can either be modified by attaching different silane molecules or can be selectively removed by chemical etching followed by chemical modification of the formed ditch.

CPP 27.16 Thu 17:00 P2

**Molecular Editing of Polymer Brushes with the Tip of an AFM** — ●ROLAND GROEGER<sup>1</sup>, INGO SAMERSKI<sup>1</sup>, THOMAS SCHIMMEL<sup>1,2</sup>, and STEFAN WALHEIM<sup>1</sup> — <sup>1</sup>Institute for Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — <sup>2</sup>Institute of Applied Physics, University of Karlsruhe, 76131 Karlsruhe (Germany)

Polymer brushes prepared from low molecular-weight carboxyl-functionalized polystyrene and polybutadiene were prepared on silicon oxide surfaces. Their topography and their adhesion properties are investigated by Atomic Force Microscopy (AFM). We describe how these ultra-thin polymer films can be mechano-chemically removed by the tip of an AFM at pre-defined locations and subsequently replaced by another polymer species. In this way it was possible to generate polymeric surfaces with a pre-defined chemical pattern. This opens perspectives for generating specifically functionalized nano-scale patterns, e.g. for

nano-biology.

CPP 27.17 Thu 17:00 P2

**Thin Films of Crystalline Diblock Copolymers** — ●CHARLES DARKO<sup>1</sup>, I. BOTIZ<sup>2</sup>, G. REITER<sup>2</sup>, and C. PAPADAKIS<sup>1</sup> — <sup>1</sup>Physik Department E13, Technische Universität München, James-Frank Str. 1, 85748 Garching — <sup>2</sup>Institut de Chimie des Surfaces et Interfaces, CNRS, Mulhouse, France

In thin films of diblock copolymers having one crystallizing block, a number of surface structures have been observed, e.g. edge-on or flat-on lamellae with high persistence lengths, spirals and dendrites, allowing the structuring of organic surfaces on a large range of length scales. The crystallization growth process in thin films of lamellar poly(styrene-*b*-ethyleneoxide) diblock copolymer was followed by in-situ optical microscopy. Using grazing-incidence small-angle X-ray scattering (GISAXS) and grazing-incidence X-ray diffraction (GIXD), we investigate the orientation of the mesoscopic structures with respect to the substrate as well as the orientation of the crystalline chains with respect to lamellar interfaces. This information on the structure inside the film is compared to the surface texture obtained by atomic force microscopy with the focus on the effect of crystallization temperature.

CPP 27.18 Thu 17:00 P2

**Electrostatic field induced patterning: a method for controlling the anisotropy of films of polar organic molecules** — ●SVEN VERPOORT<sup>1</sup>, ANSGAR DRAUDE<sup>1</sup>, RAFAEL MEINHARDT<sup>1</sup>, HILMAR FRANKE<sup>1</sup>, and ROGER A. LESSARD<sup>2</sup> — <sup>1</sup>Fachbereich Physik / Angewandte Physik, Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg, Germany — <sup>2</sup>COPL, department de physique, génie physique et optique, Université Laval, Québec, Canada G1K7P4

The presence of electrostatic charges on the surface of electrically isolating substrates like glass or polymers is able to control the orientation of vapor deposited polar organic molecules.

Different methods for the fabrication of charge patterns have been used with inorganic glass: friction, Corona, contact charging, e-beam charging...

Optically anisotropic layers of the azo dye DR1 have been prepared. The anisotropy is detectable by a change in the optical transparency and the pattern reflects the previously recorded charge distribution.

CPP 27.19 Thu 17:00 P2

**AFM as a Tool for Observation and Nanomanipulation** — ●ALEXANDER SCHMATULLA<sup>1</sup>, DIETER MEINHARD<sup>2</sup>, BERNHARD RIEGER<sup>2</sup>, and OTHMAR MARTI<sup>1</sup> — <sup>1</sup>Department of Experimental Physics, University of Ulm, 89069 Ulm, Germany — <sup>2</sup>Department of Anorganic Chemistry II, University of Ulm, 89069 Ulm, Germany

We show the possibility of a custom built Atomic Force Microscope (AFM) as an useful tool for observation and nanomanipulation in material science. In particular we have analysed spin coated polymer networks. First we demonstrate an appropriate preparation of the polymer sample. Using the AFM, particular polymer strains have been pulled over several well defined distances. Further we will compare our results with SEM images, GPC results and other methods. Finally the corresponding changes on the sample will be discussed.

CPP 27.20 Thu 17:00 P2

**Solvent Effect in NMR Spectra of Nucleic Bases from Hybrid QM-MM Simulations** — ●SITTIPONG KOMIN and DANIEL SEBASTIANI — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

We present a study of structural properties and <sup>1</sup>H NMR chemical shifts of nucleic bases in aqueous solution using hybrid quantum mechanics/molecular mechanics(QM/MM) molecular dynamics simulations. The purpose of this work is to study the solvent effect in NMR shifts. We benchmark our computational setup by applying it to water dimer, methanol dimer and ethanol-water dimer, which is particularly relevant to the development and validation of model in QM scheme comparing with QMMM scheme. The method is used to compute the <sup>1</sup>H NMR chemical shifts of Adenine, Guanine, Adenine-9methyl, Guanine-9Methyl in aqueous solution.

CPP 27.21 Thu 17:00 P2

**Investigation of spatially confined polyelectrolytes using fluorescence microscopy** — •DANIEL RAPOPORT<sup>1</sup>, DAN ANGHEL<sup>2</sup>, HELMUTH MÖHWALD<sup>1</sup>, and REGINE V. KLITZING<sup>3</sup> — <sup>1</sup>MPI für Kolloid- und Grenzflächenforschung, D-14224 Potsdam — <sup>2</sup>Institute of Physical Chemistry, Spl. Independentei 202, RO-77208 Bucharest — <sup>3</sup>Institut für Physikalische Chemie, CAU Kiel, Ludewig-Meyn-Strasse 8, D-24118 Kiel

Confinement phenomena are common to a vast number of natural and technical processes, such as the transfer of proteins or DNA through a narrow pore, filtration or nanoencapsulation. The effect can be intermolecular like an increased ordering of the molecules or it can be intramolecular like conformational changes. In the case of aqueous solutions of polyelectrolytes it is largely unknown, how these respond to the restrictions of geometrical confinement. Although numerous investigations of integral thermodynamic values have been carried out, a detailed molecular picture is still missing. Here we report on fluorescence measurements with pyrene labeled poly(acrylic acid) inside thin free standing liquid films, which were formed using sodium dodecylsulfate (SDS) as a surfactant. Upon film formation we found an increase of the excimer/monomer fluorescence intensity ratio. Moreover, at high pH stratification of the film leads to an additional rise of the excimer/monomer ratio, thereby directly proving the confinement effect on a molecular level.

CPP 27.22 Thu 17:00 P2

**Manipulation of the smectic layer spacing in liquid crystal elastomer films by mechanical stress** — •VICTOR AKSENOV<sup>1</sup>, JÜRGEN BLÄSING<sup>1</sup>, RALF STANNARIUS<sup>1</sup>, MARTIN RÖSSELE<sup>2</sup>, and RUDOLF ZENTEL<sup>2</sup> — <sup>1</sup>Otto-von-Guericke-Universität Magdeburg, Inst. für Experimentalphysik — <sup>2</sup>Johannes-Gutenberg-Universität Mainz, Inst. für Organische Chemie

Liquid crystal elastomers (LCEs) are rubbers with anisotropic elastic moduli. For deformations in the plane of smectic layers, they behave like two-dimensional isotropic rubbers, with elastic moduli close to those of conventional rubber materials. For deformations perpendicular to the layers, the elastic moduli can be two orders of magnitude higher than for conventional rubbers, comparable to the smectic layer compression modulus. It was observed earlier that deformations of SmA LCE parallel to the smectic layers do not change the sample thickness, this corresponds to a Poisson ratio close to 1 parallel to smectic layers, and zero perpendicular to it [1]. In our material, the measured Poisson ratio is close to 1/2. Simultaneous optical reflectometry and small angle X-ray scattering reveal that in-plane deformations of the LCE sample cause changes of the smectic layer spacing [2]. SmA and SmC\* phases show similar elastic behaviour, comparable to isotropic rubber. A layer compression up to 30 % was achieved mechanically. Such an effect has been observed for the first time in smectic LCE.

[1] E. Nishikawa and H. Finkelmann, *Macromol. Chem. Phys.* 200, 312 (1999). [2] V. Aksenov et al., *Liq. Cryst.* 32, 805 (2005).

CPP 27.23 Thu 17:00 P2

**Freestanding polyelectrolyte multilayer membranes as pressure sensors and separation membranes** — •INGO DÖNCH, MARC NOLTE, BJÖRN SCHÖLER, and ANDREAS FERY — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, 14424 Potsdam

Polyelectrolyte multilayer membranes can be prepared with thicknesses on the nanoscale and they are semipermeable. This makes them interesting candidates for miniaturized osmotic pressure sensors or separation membranes. We demonstrate first steps towards such devices and applications.

A method has been developed that allows the transfer of membranes onto topographically structured PDMS substrates, so that parts of the membrane are freestanding. In the case of cylindrical cavities, the deformation of the resulting circular freestanding membrane patches can be readily described by continuum mechanical approaches. Experimentally, we probe the deformation using AFM (for small deformations) and osmotic pressure differences (for large deformations). In the latter case, we can quantitatively describe our findings which show an extraordinarily high sensitivity of these membranes towards pressure differences. Similarly, we show that large molecular weight molecules can be entrapped in the cavities and discuss possible uses of such systems in combinatorial chemistry.

CPP 27.24 Thu 17:00 P2

**A Scanning Probe Microscope (SPM) with quasi *in-situ* Sample Treatment Capabilities: Solvent vapor treatment of thin polymer films in the presence of high electric fields** — •VIOLETTA OLSZOWKA, MARKUS HUND, LARISA TSARKOVA, ALEXANDER BÖCKER, and GEORG KRAUSCH — Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth

We have investigated a block copolymer thin film undergoing treatments with solvent vapor and high homogenous electric fields (E-fields,  $\approx 40 \frac{\text{V}}{\mu\text{m}}$ ). E-fields can be used to control the domain orientation which in turn ends to an important role in fabricating and controlling nanostructures. Due to the high electric field it is not possible to perform *in-situ* scanning. The E-field would produce SPM image artifacts caused by additional electrostatic forces between tip and sample. Moreover the applied high voltage could destroy the microscope by flashovers and could damage the scanner. Performing the sample treatments 'ex situ' would require time-consuming re-positioning protocols. We therefore have adapted an SPM with advanced quasi *in-situ* sample treatment capabilities to effectively study the influences of high electric fields on block copolymer films exposed to a controlled solvent vapor atmosphere.

CPP 27.25 Thu 17:00 P2

**Spreading of nematic liquid crystals** — •CHRISTOPHE POULARD — LPCP, Université de Mons-Hainaut, 20 place du Parc, B-7000 MONS, Belgique

The spontaneous spreading of nematic liquid crystals on silica substrates has been investigated at various scales by combining ellipsometry, profilometry and interferometry. While anchoring defects play a major role on hydrophilic substrates at the macroscopic scale, making the behaviour of films highly complex, they do not show up on these hydrophobic substrates.

Then, the main specificity of the nematic films is the elastic energy associated to the long range orientational order. Experiment shows that the macroscopic spreading laws differ from the ones of simple wetting liquids. Moreover, at the microscopic scale, a sharp transition between a mesoscopic, nematic film, and a molecularly thin precursor, is observed. The length of the precursor scales as the inverse of the macroscopic velocity, as expected for adiabatic wetting films.

CPP 27.26 Thu 17:00 P2

**Effect of high-frequency oscillatory shear on the force of detachment of an AFM tip from a solid surface** — •BINYANG DU<sup>1</sup>, SERGIY RUDENKIY<sup>1</sup>, PATRAWIN GASEMJIT<sup>1</sup>, LARS-OLIVER HEIM<sup>2</sup>, and DIETHELM JOHANNSMANN<sup>1</sup> — <sup>1</sup>Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 4, 38678, Clausthal-Zellerfeld — <sup>2</sup>Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

The force of detachment between an AFM-tip and a material surface, namely the pull-off-force, is a key parameter for characterization of adhesive interactions on the nanometer scale. Experiments have shown that the pull-off-force can depend on the loading rate, at which the force is ramped up. Kramer's theory also predicts a logarithmic dependence on the loading rate, which has indeed been found in various experiments. Here we report on the pull-off-force between an AFM tip and a quartz crystal under high-frequency oscillatory lateral shear as a function of shear amplitude. The pull-off-force (more precisely: the pull-off-distance) was determined repeatedly and automatically at a rate of 0.5 Hz, while the quartz crystal was swept through a resonance. The shear amplitude is typical in a range of nanometer. The pull-off-distance decreases with increasing the shear amplitude. By plotting the pull-off-distance versus the logarithm of shear amplitude, one finds a linear dependence over a range of more than a decade. This behavior can be rationalized by assuming a multicontact interface with an exponential distribution of peak heights.

CPP 27.27 Thu 17:00 P2

**Formation of thermoresponsive hydrogel films via electrochemically initiated polymerization** — •JOHANNA REUBER and DIETHELM JOHANNSMANN — Institute of Physical Chemistry, Arnold-Sommerfeld-Strasse 4, 38678 Clausthal-Zellerfeld

Electrochemically initiated polymerization has previously been employed to produce coatings on metals [1], where the interest mainly was in corrosion protection. We report on the extension of this technique to films of poly-(N-isopropylacrylamide) (p-NIPAM), which is a thermo-

responsive hydrogel.[2] A free-radical polymerization is initiated via an electron transfer from the electrode to an electrochemically active initiator. The progress of polymerization was monitored by means of the electrochemical quartz crystal microbalance (EQCM). Typical thicknesses are in the range of up to 100 nm. The water content varies between 20 and 80 %. AFM micrographs reveal a globular structure. The permeation of ions through the gel is possible, as proven by CV runs in the presence of  $K_3[Fe(CN)_6]$  in the bulk. First experiments have been performed to explore biomedical applications such as cell-sheet engineering [3] or stimulated drug release [4]. In cell culture, the layers show low-fouling properties. A second application are polymer metal composites: galvanic deposition of copper particles onto the polymer-covered surface has been demonstrated. References: [1] N. Baute, C. Jérôme, et al., *European Journal of Inorganic Chemistry* 2001, 1097. [2] H.G. Schild, *Progress in Polymer Science* 1992, 17, 163. [3] A. Kikuchi, T. Okano, *Journal of Controlled Release* 2005, 101, 69. [4] A. Kikuchi, T. Okano, *Advanced Drug Delivery Reviews* 2002, 54, 53.

CPP 27.28 Thu 17:00 P2

**Substrate-Consuming Metal-Organic Layers (SCMOLs) from Thiol Derivatives - a combined SAXS/SEM Study.** — ●BIRGIT RIEDEL<sup>1</sup>, MATTHIAS BARCZEWSKI<sup>1,2</sup>, JOCHEN GEERK<sup>3</sup>, THOMAS SCHIMMEL<sup>1,2</sup>, and STEFAN WALHEIM<sup>1</sup> — <sup>1</sup>Institute for Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — <sup>2</sup>Institute of Applied Physics, University of Karlsruhe, 76131 Karlsruhe (Germany) — <sup>3</sup>Institute for Solid-State Physics, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany)

Substrate-Consuming Metal-Organic Layers (SCMOLs) were prepared using a variety of thiol molecules. This new type of metal-organic dielectric films grow at room temperature from solution at the interface of the metal substrate and the newly formed metal-organic film. The resulting morphological characteristics of the various compounds were investigated by Small Angle X-Ray Scattering (SAXS) and Scanning Electron Microscopy (SEM). A strong correlation of the structural data and the molecular architecture could be observed and will be discussed. First results on the optical properties of these solid transparent films - with a thickness pre-selectable from a few nanometer up to 1 micrometer - will be presented.

CPP 27.29 Thu 17:00 P2

**Synthesis, structure and *ab initio* calculations of three-dimensional polymers of  $C_{60}$  fullerene.** — ●NAGESH KINI, AKIRA KUBO, and SHOJI YAMANAKA — Department of Applied Chemistry, Graduate School of Engineering, Hiroshima University, Higashi Hiroshima - 739-8527, Japan.

Solid  $C_{60}$  fullerene is known to polymerise in one, two or three dimensions under high pressure and high temperature (HPHT) conditions. Earlier, we have reported structures of orthorhombic and rhombohedral two-dimensional (2D) polymers determined by x-ray diffraction of single crystals synthesised under HPHT conditions. Recently we have obtained good quality single crystals of three-dimensional (3D) polymers of  $C_{60}$  fullerenes by a topochemical conversion under HPHT conditions. The three different types of single crystals of 3D polymers obtained are: an orthorhombic 3D polymer (polymerised from orthorhombic 2D polymer), a rhombohedral 3D polymer (polymerised from rhombohedral 2D polymer) and a 3D cubic (fcc) polymer (polymerised from monomer (fcc)  $C_{60}$ ). The structures of these 3D polymers were determined by single crystal x-ray diffractometry using a Rigaku R-axis diffractometer attached with an imaging plate (IP). The structures were geometrically optimised by *ab initio* calculations and the relative stabilities of the 3D polymer structures were compared.

CPP 27.30 Thu 17:00 P2

**Chemisorption of PTCDA on Ag(110): A quantum chemical study** — ●AFSHIN ABBASI, MICHAEL SCHREIBER, and REINHARD SCHOLZ — Institut für Physik, Technische Universität Chemnitz

Experimental studies of PTCDA monolayers on Ag(110) have revealed an adsorption geometry where each molecule is placed on top of 12 substrate atoms [1]. In the present work, we investigate a non-periodic approximant of this interface, including one PTCDA molecule and one or two layers of silver. Both in Hartree-Fock and DFT calculations, the anhydride oxygen atoms experience a strong interaction with the substrate, resulting in a bended geometry with an Ag-O bond length of about 2.4 Å. Several orbitals delocalized over the molecule and the topmost substrate layer result in a large positive net charge of the adsorbate. As most of the

negative charge in the topmost layer of the substrate resides below the positively charged perylene core, the Coulomb interaction between substrate and adsorbate contributes a substantial part to the total binding energy.

The calculated adsorption geometry is analysed in terms of the chemical hardness of the electronic orbitals, electronic excitations, and the infrared activity of the molecule along the substrate normal.

[1] C. Seidel, J. Poppensieker, and H. Fuchs, *Surf. Sci.* **408**, 223 (1998); M. Böhlinger, W. D. Schneider, K. Glöckler, E. Umbach, and R. Berndt, *Surf. Sci.* **419**, L 95 (1998).

CPP 27.31 Thu 17:00 P2

**Fabrication and electrical characterization of Polypyrrole nanowires** — ●JÖRN-HOLGER FRANKE, BIN DONG, LIFENG CHI, and HARALD FUCHS — Physikalisches Institut and CENTech, Wilhelm-Klemm Str. 10, WWU Münster

E-Beam Lithography is used to pattern a resist structure (PMMA-Resist on Silicon-Wafer) which is subsequently used as a mask for copolymerization of Pyrrole and N-(3-Trimethoxysilyl-Propyl) Pyrrole. The Trimethoxysilyl group of the latter one binds covalently to the Silicon Dioxide of the Wafer, thereby enabling the generated Polypyrrole nanowires to survive the following Lift-Off Process. Gold electrodes are evaporated on top of the resulting Polypyrrole to form easily accessible electrodes for conductivity measurements. The dependence of specific conductivity on nanowire diameter is studied.

CPP 27.32 Thu 17:00 P2

**Electrode Stability in Electrochromic Systems Based On Flexible Substrates** — ●ROLAND WAGNER<sup>1,2</sup>, ROLAND WEISS<sup>1</sup>, GOTTHARD RIEGER<sup>1</sup>, and JÜRGEN R. NIKLAS<sup>2</sup> — <sup>1</sup>Siemens AG Corporate Technology, Dept. CT MM 1, Erlangen, Germany — <sup>2</sup>Technical University Bergakademie Freiberg, Freiberg, Germany

Electrochromic (EC) systems use materials that change their color when an electrical voltage is applied. Due to redox processes the intra molecular electron configuration is affected causing different absorption spectra. Electrodes of this EC system are exposed to an aggressive environment, as electrons are exchanged at the interface of solvent based electrolytic EC material and flexible electrodes. Especially the transparent top electrode, which is typically ITO on thin PET films, degrades during device operation. Metals (e.g. Cu), TCO and polymer (e.g. PEDOT) based materials are tested as back and top electrode for its degradation under different conditions, e.g. accelerated lifetime tests and voltage cycling. Optical and electrical properties like contrast and current behavior are discussed as well as degradation processes and mechanisms.

CPP 27.33 Thu 17:00 P2

**Cyclo-olefin-polymer ferroelectrets: Electric charging, piezoelectric activity and thermal stability** — ●OLENA VORONINA, MICHAEL WEGENER, WERNER WIRGES, and REIMUND GERHARD-MULTHAUPT — University of Potsdam, Department of Physics, Am Neuen Palais 10, D-14469 Potsdam, Germany

Non-cellular cyclo-olefins are known for their good charge-trapping properties. Their charge stability is quite comparable to that of the best known polymer electrets FEP and PTFE [1]. Thus, cyclo-olefins are interesting candidates for the development of piezoelectric polymer foams, so-called ferroelectrets. Ferroelectrets are cellular polymer films containing air-filled voids. Their piezoelectricity is based on an optimized combination of bipolar internal charging of the voids (which thus become giant electric dipoles) and of a rather low elastic modulus. An applied mechanical stress changes the void size and leads to an electrical signal.

Recently, cyclo-olefin polymers were developed into ferroelectret polymer films [2]. We briefly describe the preparation process and discuss the electric charging, the piezoelectric properties and the thermal stability of the new ferroelectrets. The results demonstrate that the piezoelectric activity is thermally stable at least up to 110°C, which is a significant improvement of the service temperature in comparison to other ferroelectret polymers.

[1] G. M. Sessler, G. M. Yang and W. Hatke, Annual Report CEIDP, IEEE Service Center, Piscataway NJ, 467-470 (1997). [2] A.-M. Savijärvi, M. Paaajanen, E. Saarimäki, and H. Minkkinen, Proc. 12th Intern. Symp. on Electrets (ISE12), IEEE Service Center, Piscataway NJ, 75-78 (2005).

CPP 27.34 Thu 17:00 P2

**Electromechanics of organic Schottky like contacts, in between piezoelectricity and electrostriction** — ●REINHARD SCHWÖDIAUER<sup>1</sup>, SIEGFRIED BAUER<sup>1</sup>, GILLES DENNLER<sup>2</sup>, CHRISTOPH LUNGENSCHMIED<sup>2</sup>, NIYAZI SARICIFTCI<sup>2</sup>, and HOWARD REISS<sup>3</sup> — <sup>1</sup>Soft Matter Physics, Johannes Kepler University, Altenbergerstrasse 69, A-4040 Linz, Austria — <sup>2</sup>Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Johannes Kepler University, Altenbergerstrasse 69, A-4040 Linz, Austria — <sup>3</sup>Department of Chemistry and Biochemistry, University of California, 600 Charls E. Young Drive East, Los Angeles, CA90095, USA

Piezoelectricity and electrostriction are electromechanical effects at the heart of a variety of applications in transducers. In organic semiconductors an unusual voltage dependences of the electromechanical strain is observed: The converse electromechanical response follows a power law dependence  $S \sim V^a$  of the mechanical strain  $S$  versus the applied voltage  $V$ , with an exponent  $a=1.5$ . The power law exponent is in-between traditional linear piezoelectricity and quadratic electrostriction. The experimental finding is a direct consequence of the strongly nonuniform electric field distribution within the Schottky contact arrangement. Electromechanical responses of organic Schottky devices appear to be of fundamental interest for the investigation of non-uniform electric field distributions, and for potential practical applications as electromechanical transducers.

CPP 27.35 Thu 17:00 P2

**Luminescent characterization of perovskite-like layered strontium lanthanum titanate compounds** — ●VOLODYMYR CHUMAK<sup>1</sup>, YU TITOV<sup>1</sup>, M SLOBODYANIK<sup>1</sup>, S NEDILKO<sup>2</sup>, O CHUKOVA<sup>2</sup>, and P SMOLYAR<sup>2</sup> — <sup>1</sup>Chemistry faculty of Kyiv National Taras Shevchenko University, 64, Volodymyrska str., 01033, Kyiv, Ukraine — <sup>2</sup>Physics faculty of Kyiv National Taras Shevchenko University, 64, Volodymyrska str., 01033, Kyiv, Ukraine

First the peculiarities of the luminescent emission of the five-slab perovskite-like  $\text{SrLa}_{4-x}\text{Ln}_x\text{Ti}_5\text{O}_{17}$  ( $\text{Ln} = \text{Pr}, \text{Yb}$ ) compounds belonged to the  $A_nB_nO_{3n+2}$ -family are found and described. Photoluminescence and excitation spectra were obtained at 4.2, 77 and 300 K. Luminescence was excited by radiation from the  $\text{N}_2$ -laser, the Ar-laser, powerful xenon lamp DKsL-1000. The luminescence was registered using MDR-2 and DFS-12 diffraction spectrometers which cover wide spectral region. Reflection, excitation and luminescence spectra were also investigated using synchrotron radiation in the energy region 3.5-20 eV. Experiments with synchrotron radiation were carried on at SUPERLUMI station at HASYLAB (DESY), Hamburg, Germany. Results of experimental studies allowed us to conclude that mentioned above the sets of compound could be regarded as perspective phosphors, i. e. the transformers of the UV or IR emission into visible light, or the white-light-emitting and storage phosphors, perspective laser materials. When doped with the rare earth ions  $\text{Pr}^{3+}$  or  $\text{Yb}^{3+}$  they are considered as perspective fast-scintillation materials.

CPP 27.36 Thu 17:00 P2

**Ion Irradiation of Polystyrene - Sol Molecular Weight Distribution** — ●RALF DELTO and RÜDIGER BRENN — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, 79104 Freiburg

Irradiation of polymers with high energetic ions results in a change of molecular weight distribution. The formation of crosslinks produces a gel fraction (network) while breaking of chains leads to a soluble sol fraction. The change of the Mw distribution depends on the applied ion dose.

Theoretical and experimental work has been done on the production of networks. Here we concentrate on the sol part. Sol-Mw distributions are calculated with statistical methods and with numerical simulations. Measurements are performed on polystyrene (PS) thin films using 1 MeV protons for irradiation. The films consist of a deuterated and a protonated layer (dPS-hPS). The irradiated sol (dPS and hPS) diffuses into the opposite layer while heating above  $T_g$ . As the tracer diffusion constant depends on the molecular weight, chains of different length diffuse unequally fast. Thus the diffusion profiles contain information about the abundance of chains of different degrees of polymerisation in the sol. Diffusion depths profiles for the deuterated component are determined with  $^3\text{He}$  nuclear reaction analysis.

CPP 27.37 Thu 17:00 P2

**Struktur und mechanische Festigkeit eines nanostrukturierten Biomaterials zum Knochenaufbau** — ●SVEN RADEFELDT and THOMAS GERBER — Universität Rostock, August-Bebel-Str. 55, 18055 Rostock

Nanostrukturierte Biomaterialien, die dadurch charakterisiert sind, eine extrem hohe innere Oberfläche zu besitzen und deren innere Oberfläche so modifiziert ist, dass körpereigene Proteine während der Anwendung angelagert werden, bieten vollkommen neue Möglichkeiten in der regenerativen Medizin. Es wird eine im Sol-Gel-Verfahren hergestellte Hydroxylapatit-Keramik vorgestellt, die von den Zellen nicht als Fremdkörper angesehen wird und sofort in den natürlichen remodelling-Prozess des Körpers eingebunden wird. Dieses hochporöse Material, dessen Nanostruktur der des natürlichen Knochens nachempfunden ist, wurde in seiner Zusammensetzung so optimiert, dass zukünftig auch die Heilung von Defekten ermöglicht werden soll, die an sehr stark belasteten Knochen (z.B. Wirbelkörper der Wirbelsäule) aufgetreten sind. Zum Nachweis der Korrelation zwischen Struktur und Eigenschaften des Biomaterials wurden Untersuchungen mittels SAXS, WAXS, TGA, DTA, REM und TEM durchgeführt.

CPP 27.38 Thu 17:00 P2

**Nanofibrillar structure and molecular mobility in spider dragline silk** — ●TILO SEYDEL<sup>1</sup>, DANIEL SAPEDE<sup>1,2</sup>, TREVOR FORSYTH<sup>1</sup>, MAREK KOZA<sup>1</sup>, RALF SCHWEINS<sup>1</sup>, FRITZ VOLLRATH<sup>3</sup>, and CHRISTIAN RIEKEL<sup>2</sup> — <sup>1</sup>Institut Laue-Langevin, B.P.156, F-38042 Grenoble, France — <sup>2</sup>European Synchrotron Radiation Facility, B.P.220, F-38043 Grenoble, France — <sup>3</sup>Dept. of Zoology, University of Oxford, Oxford OX1 3PS, U.K.

Spider silk is a protein biopolymer known for its outstanding mechanical properties combining elasticity and strength. Spider dragline silk has been investigated by neutron diffraction and neutron spectroscopy techniques [1]. The results support a three-phase hierarchical model of the structure consisting of semicrystalline nanofibrils embedded in an amorphous polymer matrix. The mechanical properties of spider dragline silk fibres are strongly affected by the water content, and neutron spectroscopy provides information on the humidity-dependent polymer chain mobility as well as on a gradual melting of confined water. New instrumental developments in neutron spectroscopy will be presented alongside, as the feasibility of neutron experiments is often limited by the small available sample quantities.

[1] D.Sapede, T.Seydel, V.T.Forsyth, M.M.Koza, R.Schweins, F.Vollrath, and C.Riekkel; *Macromolecules* Vol.38, p.8447 (2005).

CPP 27.39 Thu 17:00 P2

**Gas Induced Dilation in Glassy Polymers - Combining Experiment, Phenomenological Models and Simulation** — ●OLE HÖLCK<sup>1</sup>, MARTIN BÖHNING<sup>1</sup>, MATTHIAS HEUCHEL<sup>2</sup>, and MARTIN R. SIEGERT<sup>2</sup> — <sup>1</sup>Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — <sup>2</sup>GKSS Forschungszentrum, Institut für Polymerforschung, Kantstrasse 55, 14513 Teltow, Germany

Dense amorphous polymers are utilised as barrier materials or membranes in a variety of applications. Considerable efforts have been made to describe and characterise solution and diffusion of small penetrants constituting the permeation process. However, little is known about the mechanisms which - at elevated concentrations and long term exposure - lead to plasticisation of the polymer matrix and subsequent structural rearrangements. In this joint research project a thorough kinetic analysis of sorptive dilation along with the evaluation in the framework of phenomenological models, such as the Site Distribution-model of Kirchheim, is utilised to relate the results of laboratory experiments to complementary investigations of detailed atomistic MM/MD-packing models. The results are based on established analysis methods as well as promising new approaches to overcome the discrepancies due to the different time scales of observation in experiment and modelling. Comparison is made between measured and simulated characteristics relevant to gas transport and dilation, such as diffusivity and solubility of the penetrant and free volume distribution of the polymer matrix.

CPP 27.40 Thu 17:00 P2

**Ion mobility in PMMA doped with small amounts of a Lithium salt** — ●P. KOHN, K. SCHRÖTER, and T. THURN-ALBRECHT — Department of Physics, Martin Luther University, Hoher Weg 8, 06120 Halle, Germany

Normally NMR techniques are used to determine the mobilities of ions in polymer electrolytes (via determination of diffusion coefficients and use of the Einstein relation). We discuss Time Of Flight (TOF) measurements in an electric field and parallel plate geometry as an alternative method to determine mobilities of ions. In a first step the ions of opposite charge are forced to separate and accumulate at the different electrodes by applying a constant voltage. As a consequence of a reversed voltage in the second step the ions migrate from one electrode to the other. The current measured during this process gives the transit time which is directly related to the mobilities of the charge carriers.

For an exemplary application we used this method to study ion mobility in polymethylmethacrylate (PMMA) doped with lithiumtrifluorosulfonate ( $\text{LiCF}_3\text{SO}_3$ ). The measurements were complemented by dielectric spectroscopy in the frequency domain. While the TOF measurements give the mobilities, the frequency dependent dielectric measurements give the temperature and salt-concentration dependence of the ohmic conductivity of the electrolyte.

CPP 27.41 Thu 17:00 P2

**Tailoring the material properties of Polypropylene by blending** — ●STEFAN FISCHER<sup>1</sup>, OTHMAR MARTI<sup>1</sup>, TOBIAS DIENSNER<sup>2</sup>, and BERND RIEGER<sup>2</sup> — <sup>1</sup>Department of Experimental Physics, University of Ulm, 89069 Ulm, Germany — <sup>2</sup>Department of Inorganic Chemistry II, University of Ulm, 89069 Ulm, Germany

Tailoring material properties like mechanical deformation behavior is of special interest for possible applications. Isotactic Polypropylene (iPP) is a low-cost polymer, showing a high modulus with the drawback of being brittle. By blending commercial available iPP with high molecular iPP (synthesized with metallocene catalysts) we intended to influence material properties like failure behavior, such broadening the range of accessible applications. This approach additionally has special advantages in the recycling process since there is no mixture of chemical different materials. We will present the results of different blending experiments, analyzed by DSC and mechanical measurements. For a target-oriented approach to tailoring material properties it is crucial to know the processes taking place on a microscopic level like crystallization. Preliminary results of measurements with AFM and X-ray scattering and their connection to the macroscopic behavior will be discussed.

CPP 27.42 Thu 17:00 P2

**Side chain crystallization in random copolymers containing octadecylmethacrylate** — ●E. HEMPEL<sup>1</sup>, H. BUDDÉ<sup>2,3</sup>, C. SCHICK-TANZ<sup>4</sup>, S. HÖRING<sup>2</sup>, and M. BEINER<sup>1</sup> — <sup>1</sup>FB Physik und — <sup>2</sup>FB Chemie, Universität Halle, D-06099 Halle/Saale — <sup>3</sup>Fraunhofer Pilotanlagenzentrum für Polymersynthese und -verarbeitung Schkopau, D-06258 Schkopau — <sup>4</sup>FB INW, Fachhochschule Merseburg, D-06217 Merseburg

The crystallization behavior of two series of random copolymers, poly(styrene-*stat*-octadecylmethacrylate) [P(S-*stat*-ODMA)] and poly(methylmethacrylate-*stat*-octadecylmethacrylate) [P(MMA-*stat*-ODMA)], has been studied by DSC and scattering techniques. Interestingly, side chain crystallization occurs in all copolymers containing more than 25mol% ODMA while only a single glass transition is observed for lower ODMA contents. This indicates that the alkyl groups of different ODMA units can aggregate and form small crystals if the ODMA content is large enough. Isothermal crystallization experiments show that the crystallization kinetics slows down and that the transformation interval broadens if the ODMA content decreases. The crystallization temperature  $T_c$  for samples containing 25mol% ODMA is 40K reduced as compared to values for PODMA homopolymers. This can be interpreted as a consequence of crystallization occurring in isolated ODMA compartments which must be nucleated separately. Scattering data measured during the isothermal crystallization process of P(S-*stat*-ODMA) copolymers are included in the discussion. The results for random copolymers are compared with the findings for PODMA homopolymers as well as P(S-*block*-ODMA) block copolymers.

CPP 27.43 Thu 17:00 P2

**Probing Micromechanical Behavior of Semicrystalline Polypropylene Films by Brillouin Spectroscopy** — ●OLGA PRIADILOVA<sup>1</sup>, WEI CHENG<sup>1</sup>, WERNER STEFFEN<sup>1</sup>, JOCHEN GUTMANN<sup>1</sup>, and GEORGE FYTAS<sup>1,2</sup> — <sup>1</sup>Max-Planck for Polymer Research, D-55128 Mainz, Germany — <sup>2</sup>Department of Materials Science and Technology, University of Crete and FO.R.T.H P.O.Box 1527, 71110 Heraklion, Greece

The elastic properties of polypropylene films crystallized under different conditions were investigated via Brillouin spectroscopy measure-

ments. It was found that elastic constants of the polypropylene films are dependent on their microstructure. Inelastic Brillouin light scattering from films reveals the presence of up to four bulk and surface phonons. The coexistence of amorphous and crystalline regions with at least submicron sizes allow for the propagation of two longitudinal and transverse elastic excitations. The relation of the acoustic excitations to the surface and bulk morphology of the semicrystalline films is supported by X-ray scattering techniques and optical microscopy images. Inelastic (Brillouin) light scattering from semicrystalline homopolymers can measure the high frequency elastic constant of the two microphases if the formed spherulites exceed the size of the wavelength of the probed phonons. In this case, the film is inhomogeneous over the relevant length scales and there is an access to the transverse phonon in the crystalline phase yielding the elastic constant as well.

CPP 27.44 Thu 17:00 P2

**Kinetics of isothermal crystallisation and melting-recrystallisation of iPP, iPS, PET and PBT** — ●J. HEEG, A. MINAKOV, and C. SCHICK — University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

Isothermal crystallisation and melting-recrystallisation were investigated by the help of Fast Scanning Chip Calorimetry and DSC (Differential Scanning Calorimetry). For the purpose of fast scanning a commercially available chip calorimeter was used. The implanted heater in combination with non-adiabatic operation gave the possibility for both controlled fast heating and cooling. Crystallization kinetics of the slowly crystallising iPS and PET were studied on a PerkinElmer PYRIS 1 DSC. PBT and iPP were investigated with the fast scanning chip calorimeter. In the case of iPP, in accordance with de Santis [1], two minima in isothermal melt crystallisation half time were observed. These can be explained by the formation of two different phases in iPP. Namely, the crystalline alpha-modification and the mesomorphic phase. Additionally isothermal cold crystallisation experiments gave no evidence for preferring a certain crystallising temperature in case of the alpha-modification. Only the mesomorphic phase gave again a pronounced peak in crystallisation half time. Surprisingly, for PBT two minima in crystallisation half time were found too, for both melt and cold crystallisation. The reason for this is not yet understood. Beside crystallization kinetics recrystallization kinetics will be discussed too.

[1] F. de Santis, C. Schick, in preparation for publication.

CPP 27.45 Thu 17:00 P2

**Crystallization/melting transition of polymer thin films probed by ellipsometry** — ●CHRISTA H.M. WEBER, ADRIANA M. MIHUT, SVEN HÜTTNER, ARNAUD CHICHE, and GEORG KRAUSCH — Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth

Ellipsometry has been used to investigate crystallization and melting of thin polymer films. This technique is sensitive to the sharp changes in film density and thickness that occur during these transitions. As a result, precise melting and crystallization points can be measured in-situ during thermal or solvent vapor treatments. We present example studies of model crystalline polymers and block copolymers thin films.

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**Relaxation behavior, physical aging and crystallization kinetics** — ●T.R. GOPALAKRISHNAN and M. BEINER — FB Physik, Universität Halle, D-06099 Halle/Saale, Germany

Recently the properties of amorphous pharmaceuticals attracted a lot of attention. We have studied the relaxation and crystallization behavior of amorphous acetaminophen produced by rapid quenching. DSC heating curves for this sample show a pronounced glass transition at  $T_g=23^\circ\text{C}$  before spherulites are formed during the cold crystallization process at temperatures around  $T_c=85^\circ\text{C}$ . Weak exothermal contributions in the range 110-130°C indicate a solid-to-solid transition to another polymorphic state which finally melts at  $T_m \approx 158^\circ\text{C}$ . In order to get more detailed information about the relaxation behavior of amorphous acetaminophen we have investigated the dynamic glass transition ( $\alpha$ ) between  $T_g$  and  $T_c$  by dielectric spectroscopy. A weak secondary relaxation ( $\beta$ ) has been found in  $\epsilon''$  isotherms measured at temperatures below  $T_g$ . The crystallization kinetics will be described based on isothermal crystallization experiments by dielectric spectroscopy at temperatures between 30°C and 55°C. We observed that isothermal crystallization affects mainly the  $\alpha$  relaxation strength  $\Delta\epsilon$  while shape and position of the  $\alpha$  peak in  $\epsilon''$  isotherms are nearly unaffected. This shows that the situation can be approximated by a two phase model. The dielectric results are consis-

tent with data from calorimetric measurements detecting the change of the strength of the thermal glass transition  $\Delta c_p$  after different periods of isothermal crystallization at  $T_c$ . Characteristic crystallization times  $\tau_c$  obtained by both methods are nearly identical.

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**Semi-flexible star-shaped molecules** — ●SIBYLLE GEMMING<sup>1,2</sup>, MICHAEL SCHREIBER<sup>2</sup>, MATTHIAS LEHMANN<sup>3</sup>, IGOR POPOV<sup>1</sup>, and GOTTHARD SEIFERT<sup>1</sup> — <sup>1</sup>Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden — <sup>2</sup>Institut für Physik, Technische Universität, D-09107 Chemnitz — <sup>3</sup>Institut für Chemie, Technische Universität, D-09107 Chemnitz

The structural prerequisites are investigated, which make star-shaped molecules suitable precursors for the formation of columnar liquid crystalline phases. Electronic structure calculations on smaller mesogens show, that not all conformers exhibit the atomistic structure, the stability against distortion, and additional dipole moments, which favour columnar stacking. For the presently studied compounds with short terminating alkyl chains, the calculations indicate that the steric factor becomes dominant with increasing star size. Thus, the optimised geometric structures were employed to generate a simplified mathematical model of the structures, which accounts only for the steric interaction in the larger stars. With the help of these diagrams, the most common conformers of star-shaped molecules can be derived in a systematic fashion.

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**Polymer-surfactant interactions: Effect of temperature on aggregation** — ●JOHN BOSCO STANISLAUS<sup>1</sup>, HEIKO ZETTL<sup>1</sup>, JEROME CRASSOUS<sup>2</sup>, MATHIAS BALLAUFF<sup>2</sup>, and GEORG KRAUSCH<sup>1</sup> — <sup>1</sup>Physical Chemistry II, Universität Bayreuth, Universitätstraße 30, 95440, Bayreuth, Germany — <sup>2</sup>Physical Chemistry I, Universität Bayreuth, Universitätstraße 30, 95440, Bayreuth, Germany

The interactions between an anionic surfactant sodium dodecyl sulphate (SDS) and hydrophobically modified non ionic polymer, methylcellulose (MC), in water have been investigated by fluorescence correlation spectroscopy (FCS) and rheology. FCS is used to study the dynamics of the aggregates. We are able to follow the solution properties over a wide concentration range of both polymer and surfactant via measurement of the diffusion time of single dye molecules. At constant MC concentration the diffusion time increases gradually with SDS concentration. Starting from certain SDS concentration it decreases again to a minimum when the SDS concentration is further increased. This behaviour is coinciding with the behaviour of the zero shear viscosity. Two possible aggregations can be identified above the critical aggregation concentration (CAC). The changes in diffusion time and aggregation states are studied as a function of temperature. Moreover the gelation of MC is studied by piezoelectric axial vibrator.

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**ATRP-Synthesis of Polymer Brushes in aqueous Solution for Silicon Surface Modification** — ●SEBASTIAN NETT<sup>1</sup>, GUNNAR KIRCHER<sup>1</sup>, MARKUS WOLKENHAUER<sup>1</sup>, and JOCHEN S. GUTMANN<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Ackermannweg 11, D-55128 Mainz — <sup>2</sup>Institute for Physical Chemistry, Johannes Gutenberg University, Welderweg 11, D-55099 Mainz

The aim of this project is the chemical modification of Micromechanical Sensors (MMS) for the use as temperature and chemical probes. The silicon-surface properties are changed by growing polymer brushes on top of the MMS.

Our approach make use of a Nanoplotter (GESIM) to "print" microstructures on micro cantilever sensors. The Nanoplotter is optimized for water as system liquid. Therefore the synthesis of the covalently bound polymer brushes has to be in aqueous solution. We performed ATRP (Atom Transfer Radical Polymerization) -Synthesis of PNIPAM (Poly(N-Isopropylacrylamide)) in a mixture of H<sub>2</sub>O and DMF both in bulk solution and small droplets. Ellipsometry measurements provided the characterization of the film. The brush thickness varies with molecular weight from 5 to 40 nm.

The synthesized PNIPAM shows a LCST (lower critical solution temperature) behavior at a critical temperature of 32°C.

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**Single DNA Molecules in Shear Flow** — ●DAVID STEINMETZ<sup>1</sup> and CHRISTIAN WAGNER<sup>2</sup> — <sup>1</sup>Geb. 38, 3. OG, Zi. 3.19, Universität des Saarlandes, 66041 Saarbrücken — <sup>2</sup>Geb. 38, 3. OG, Zi. 3.20, Universität des Saarlandes, 66041 Saarbrücken

We present investigations of single DNA molecules in an oscillatory shear flow, that is a typical form of a time dependent rheometric flow. The molecules are labelled with a fluorescent dye (POPO-3) and observed with a EPI fluorescence microscope. The viscosity of DNA solutions in oscillatory flows is a complex quantity and at the frequency corresponding to the inverse relaxation time of the single molecules, the elastic part of the viscosity should have a maximum. The microscopic response of the molecules to the oscillatory shear flow should also be maximal at this frequency. Our goal is to associate macroscopic behaviours with microscopic ones.

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**Molecular Dynamics of the Glass Relaxation Process of Block** — ●S. Z. MOHAMMADY<sup>1</sup> and S. KAHLE<sup>2</sup> — <sup>1</sup>Chemistry Department, Faculty of Science, Cairo University, P.O.12613 Giza, Egypt — <sup>2</sup>Max-Planck-Institut für Polymerforschung, Postfach 3148, D-55021 Mainz

The molecular dynamics of the relaxation processes of the soft blocks in different types of block copolymers having different molecular architectures have been investigated. Four model examples of block copolymers are investigated, namely, two styrene-butadiene-styrene (SBS) block copolymers and two styrene-styrene butadiene-styrene (S-SB-S). Samples were chosen, so that, in each pair of block copolymers one of them is linear triblock and the other is star asymmetric. In addition, two polybutadiene, PB, homopolymer samples having similar chain lengths to the PB blocks present in the SBS block copolymers have been investigated. Dynamic mechanical measurements have been done for the real and imaginary parts of the complex shear modulus ( $G'$ ,  $G''$ ) in the temperature and frequency ranges from -110 to 30°C and 10-2 to 15.9 Hz, respectively. Complete master curves have been constructed for all samples. Moreover, broad band dielectric spectroscopy has been carried out in wide temperature and frequency windows, -120 to 0°C and 10-1 to 107 Hz, respectively. Stress - strain and transmission electron microscopic (TEM) measurements were also conducted. The results show that the molecular dynamics of the glass process in the soft phase in block copolymers is dramatically changed as compared to the behavior in the bulk (for instance, PB homopolymers). In addition, the molecular architecture is found to be an important factor in determining the molecular mobility of the soft blocks. The results are explained in terms of the applied confinement of the counter phase (PS phase), block lengths, domain thicknesses and the type of end to end junctions between the different blocks. A correlation between the macroscopic and microscopic properties in the block copolymers was done.

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**Preparation and characterisation of Polystyrene-ZnO hybrid polymer particles.** — ●MUKESH AGRAWAL<sup>1</sup>, ANDRIJ PICH<sup>2</sup>, NICK ZAFEIROPOULOS<sup>1</sup>, and MANFRED STAMM<sup>1</sup> — <sup>1</sup>Leibniz Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany — <sup>2</sup>Institute of Macromolecular Chemistry and Textile Chemistry, Dresden University of Technology, Mommsen Straße 4, 01062 Dresden, Germany

We report on the preparation and characterisation of ZnO nanoparticles and PS-ZnO polymeric composite particles. ZnO nanoparticles with diameters from 8-50 nm are formed depending on the reaction time, temperature and NaOH concentration. Polymeric composite particles are prepared by two step method in which first step consists of preparation of the functionalised core polystyrene particles and during second step prepared ZnO particles were deposited on to core particles surface. The core particles PS/AAEM with a high monodispersity are prepared by the surfactant free emulsion polymerisation. Prepared ZnO particles are deposited in the form of nano crystals on to the PS/AAEM particle surface by heterocoagulation process. Effect of reaction parameters such as reaction temperature, Zn(CH<sub>3</sub>CO<sub>2</sub>)<sub>2</sub> concentration and NaOH concentration, on the thickness of inorganic shell is investigated. ZnO particles are characterised by SEM, AFM and WAXS. Morphology of polymeric composite particles is characterised by SEM and AFM. Inorganic content in the polymeric composite is determined by thermogravimetric analysis.