

CPP 33: Poster: Charge Effects in Soft and Biological Matter

Time: Wednesday 17:30–19:00

Location: Poster C

CPP 33.1 Wed 17:30 Poster C

A Transport Model for an All Solid State Lithium Ion Battery — STEFAN FUNKEN and MANUEL LANDSTORFER — Institut für Numerische Mathematik, Universität Ulm, Ulm, Germany

New developed solid electrolytes indicate some big advantages for rechargeable lithium ion batteries, e.g. heat and cycling stability. These features yield benefits for cell coupled solar cell/rechargeable battery devices. A priori knowledge of some of the cell parameters is of great interest to eliminate poor material combinations and reduce experimental work.

A continuum mechanical modeling framework at cell level will be presented which takes into account the deintercalation and intercalation of lithium, transport of lithium through the solid electrolyte and electrochemical reactions on the flat phase interfaces. Furthermore the potential drop across the rigid double layer is modeled as Robin boundary condition. The derivation of the transport equation for lithium ion concentration $c_{Li^+}(x, t)$ in the solid electrolyte is done by a free energy functional $F[c_{Li^+}]$ which takes into account repulsive ion-ion interaction. Defining the chemical potential as Frechet derivative of the free energy with respect to concentration, $\mu_{Li^+} = \frac{\delta F[c]}{\delta c}$, and the Flux as $\vec{\Gamma}_{Li^+} = D \cdot \nabla \mu_{Li^+}$ one obtains a diffusion equation with a concentration dependent, non-linear diffusion coefficient.

The full model is a coupled non-linear partial differential equation system which is solved with COMSOL® and own code. Numerical results for discharge behavior of an example cell will be presented.

CPP 33.2 Wed 17:30 Poster C

X-Ray and Neutron Reflectometry Study of Polyelectrolyte Multilayers under Mechanical Stress — JOHANNES FRÜH¹, ADRIAN RÜHM², RUMEN KRASTEVA^{1,3}, and RALF KÖHLER^{1,4} — ¹MPI für Kolloid- und Grenzflächenforschung, Am Mühlenberg 1, 14424 Potsdam, Germany — ²MPI für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — ³Naturwissenschaftliches und Medizinisches Institut an der Universität Tübingen Markwiesenstraße 55, 72770 Reutlingen, Germany — ⁴Helmholtz-Zentrum Berlin, Lise Meitner Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Polyelectrolyte (PE) multilayers (PEM) produced by layer-by-layer (LbL) self assembly technique find application in different fields of the technique. Often the PEM are exposed to mechanical stress which they have to sustain. This makes the studies on mechanical properties of PEM important. Especially interesting is the crossover of internal interactions of PE molecules on molecular level and their mechanical properties as their "macroscopic" representation. Our investigation focuses on the changes of the thicknesses and the roughnesses of thin PEM films when the film is exposed to uniaxial mechanical stress. The PEM were prepared from poly-styrene sulphonate (PSS) and poly-diallyldimethyl-ammonium chloride (PDDA) using LbL technique on sheets of homogeneous and molecularly flat poly-dimethylsiloxane (PDMS) and on glass slides as substrates. A modified reflectometry technique on the substrates was used to investigate the thickness changes of the PEM. The films exhibit ranges of elastic and plastic deformation according to the strength of the applied stress.

CPP 33.3 Wed 17:30 Poster C

Application of Transient Current Measurements at High Voltages to salt containing poly(ethylene oxide) — JENS BALKO, PETER KOHN, KLAUS SCHRÖTER, and THOMAS THURN-ALBRECHT — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany

Poly(ethylene oxide) (PEO) based solid polymer electrolytes attract great interest due to their potential use in battery technology. Though conductivity measurements of salt-polymer complexes are frequently reported the independent determination of the charge carrier density and the mobility of ions is difficult. We studied these two quantities by a recently proposed method using transient current experiments at high voltages. The applicability of this method relies on the complete depletion of ions in the bulk as well as the use of blocking electrodes, i.e. the absence of electrochemical reactions at the metal-polymer interface. At low ion content we find consistent values for the charge carrier density, mobility and conductivity. However at higher lithium salt concentrations electrochemical reactions take place that limit the application of the method. We discuss the influence of salt concentra-

tion, electrode material and applied voltage.

CPP 33.4 Wed 17:30 Poster C

Properties of terminally-charged dendrimers with flexible spacer-chains and explicit counterions: A Monte Carlo study — JAROSLAW KLOS^{1,2} and JENS-UWE SOMMER^{1,3} — ¹Leibniz Institute of Polymer Research Dresden e. V., 01069 Dresden, Germany — ²Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — ³Institute for Theoretical Physics, Dresden University of Technology, 01069 Dresden, Germany

We study the properties of terminally-charged dendrimers of generations $G = 5, 6$ with flexible spacers of length $S = 1, 2, 4, 8$ accompanied by explicit counterions in an athermal solvent using Monte Carlo simulations based on the Bond Fluctuation Model. In our study both the full Coulomb potential and the excluded volume interactions are taken into account explicitly with the reduced temperature τ as the main simulation parameter. Our calculations confirm that counterions get localized in the molecules' interior and, in particular, condense on the terminal group as τ is lowered. This, in turn, affects the conformational properties of the molecules that weakly swell at intermediate τ due to dominating repulsion between the terminal groups and shrink in the limit of high and low τ , respectively. Like for neutral dendrimers, we find a substantial decrease of monomer densities with the radial distance from the dendrimers' center of mass and backfolding of the terminal groups towards the molecules' interior. Furthermore, by means of the radius of gyration tensor we conclude that the mean instantaneous shape of dendrimers is spherical for all τ inspected.

CPP 33.5 Wed 17:30 Poster C

The diffusion of charged nanoparticles at the air/water interface — TOBIAS GEHRING and THOMAS FISCHER — The University of Bayreuth

We measure the electrostatic effects on the diffusion of nanoparticles at the air/water interface. Using particle tracking of fluorescent nanoparticles on air/water interfaces of different ionic strength we are able to determine the change of diffusion of the particles and hence their immersion into the interface with the salt content. First measurements of those electrostatic effects will be presented.

CPP 33.6 Wed 17:30 Poster C

Dynamics of a tethered polymer chain in an oscillating shear flow: a fluorescence microscopy study — MARYAM KHAKSAR^{1,2}, ANDRE SCHRODER¹, THOMAS GISLER², and CARLOS MARQUES¹ — ¹Institut Charles Sadron, rue du Loess Strasbourg Cedex 2 — ²Universität Konstanz, Fachbereich Physik, D-78457 Konstanz

Advances in fluorescence microscopy of single-molecule DNA and the preparation of well defined surfaces with end-tethered DNA chains has allowed unprecedented scrutiny of the behaviour of single polymer chains near an impenetrable wall in equilibrium as well as out of equilibrium. In this contribution we study the response of single end-tethered DNA molecules to an oscillatory shear flow of frequency ω and shear amplitude γ , using fluorescence microscopy and image processing. At moderate shear amplitude γ the chain behaviour is expected to be controlled by the dimensionless Deborah number $De = \omega\tau$, where τ is the longest relaxation time of the polymer chain. At low frequencies $De \ll 1$ a chain can relax faster than the flow cycle and the deformation is expected to be equivalent to the one of a chain in a stationary flow. At large frequencies $De \gg 1$ the chains cannot relax within an oscillation period and one expects the chains to move coherently with the flow. Using fluorescence microscopy we study the dynamic response of end-tethered λ DNA to the flow in the range $0.1 \ll De \ll 10$, thus exploring not only the small and large Deborah number regimes but also the full crossover region.

CPP 33.7 Wed 17:30 Poster C

Einfache Herstellung eines Dreischicht Ferroelektrets und Charakterisierung mittels dielektrischer Resonanzspektroskopie — LARS HOLLÄNDER, WERNER WIRGES and REIMUND GERHARD — Universität Potsdam, Institut für Physik und Astronomie, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Deutschland

Ferroelektrete sind sehr nützliche Wandlermaterialien für elektromechanische und elektro-akustische Sensoren und Aktoren. Hier wird ein

neues und einfaches Verfahren zur Herstellung piezoelektrisch aktiver Polymerschichtsysteme vorgestellt. Die Mittelschicht ist eine weiche, doppelseitig klebende Folie (3M 468MP), aus der mittels Laserschneiden eine Netzstruktur erstellt wird. Auf diese Mittelschicht werden von beiden Seiten, einseitig metallisierte, kommerziell erhältliche Polykarbonat-Filme (BayerMaterialScience Makrofol DE 6-2) aufgeklebt, wobei sich die metallisierte Seite jeweils außen befindet. Danach werden die Proben mit einer hohen elektrischen Spannung in direktem Kontakt gepolt. Eine Polungsspannung von etwa 4 kV reicht aus, um

einen piezoelektrischen d_{33} -Koeffizienten von ca. 150 pC/N (aus der Resonanzkurve bestimmt) zu erhalten. Durch Veränderung der Hohlraumdurchmesser lässt sich die Dickenresonanzfrequenz der Ferroelektrite in einem Bereich von ca. 15 bis 30 kHz variieren. Mit der gleichen Methode lässt sich durch zusätzliches Anlegen einer Gleichspannung das innere elektrische Feld der Probe bestimmen.

Durch das einfache Aufkleben der äußeren Schichten können viele verschiedene Polymer Materialien zur Herstellung der piezoelektrischen Sensoren und Aktoren verwendet werden.