

## CPP 51: P16: New Instruments and Methods

Time: Wednesday 10:00–13:00

Location: Poster A

CPP 51.1 Wed 10:00 Poster A

**Theoretical analysis of vibrating microstructures using dynamic scanning electron microscopy (DySEM)** — ●MARIA SCHRÖTER<sup>1</sup>, MATTHIAS HOLSCHNEIDER<sup>2</sup>, MARTIN RITTER<sup>3</sup>, CHRISTIANE WEIMANN<sup>1</sup>, and HEINZ STURM<sup>1,4</sup> — <sup>1</sup>BAM 6.9, Federal Inst. Materials Research, Berlin — <sup>2</sup>Inst. Mathematics, Univ. Potsdam — <sup>3</sup>Electron Microscopy, TU Hamburg-Harburg — <sup>4</sup>Faculty V, TU Berlin

The poster presented shows the development and verification of a theory, with which the results of a newly developed measuring method (DySEM technique) can be described.

Dynamic Scanning Electron Microscopy is used for measuring the vibrational dynamics of a microscale oscillator at flexural and torsional resonance. In addition to the classical secondary electron (SE) signal, the dynamic part of the signal can be obtained using a lock-in amplifier synchronized to the excitation frequency.

The model of imaging generating mechanism relates the experimental images to the spatio-temporal interaction between electron beam and periodically vibrating microstructure. Furthermore, the material properties of the micro-oscillator as well as the contributions of energy loss mechanisms must be considered for imaging, especially for tapping mode microscopy of soft matter.

The analysis of the imaging of oscillating microstructures by means of scanning electron microscopy is thereby achieved in this poster presented as a combination of experiment, theory and simulation (1).

(1) Schröter, Dissertation TU Berlin (2014)

CPP 51.2 Wed 10:00 Poster A

**Force field conversion and comparison** — ●VOLKER LESCH<sup>1</sup>, CARLOS E. S. BERNARDES<sup>2</sup>, JOSE NUNO CANONGIA LOPES<sup>2</sup>, MARCELLO SEGA<sup>3</sup>, OTHMAR STEINHAUSER<sup>3</sup>, CHRISTIAN SCHRÖDER<sup>3</sup>, LUIS MIGUEL VARELA CABO<sup>4</sup>, HADRIAN MONTES<sup>4</sup>, TRINIDAD MENDEZ-MORALES<sup>4</sup>, and ANDREAS HEUER<sup>1</sup> — <sup>1</sup>Westfälische Wilhelms-Universität Münster — <sup>2</sup>Universidade de Lisboa — <sup>3</sup>Universität Wien — <sup>4</sup>University of Santiago de Compostela

Force fields are the core of each molecular dynamics (MD) simulation but each MD-simulation package has its advantages and drawbacks. Therefore, sometimes a conversion of force fields is necessary which is very tedious and error-prone. Here, we present the conversion tool ForConX (force field based on XML structure). ForConX is written in Python and organized in different modules for each of the following MD packages: Gromacs, Amber, Charmm, DL\_POLY.

Several studies focused on the effect of polarization on simulation results. Here, for the first time we compare two optimized force field and elucidate the real gaps between non-polarizable and polarizable MD-simulations. More specifically, we focus on the limits describing structure and dynamics of the optimized non-polarizable force field OPLS-AA and the optimized polarizable force field APPLE&P.

CPP 51.3 Wed 10:00 Poster A

**3D-cross correlated light scattering in combination with small-angle neutron scattering** — ●YVONNE HERTLE<sup>1</sup>, ANNEGRET GÜNTHER<sup>1,2</sup>, FANGFANG CHU<sup>2</sup>, DANIEL CLEMENS<sup>2</sup>, MATTHIAS BALLAUFF<sup>2</sup>, and THOMAS HELLWEG<sup>1</sup> — <sup>1</sup>Universität Bielefeld, PC III, Universitätsstr. 25, 33615 Bielefeld — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, EM-ISFM, Hahn-Meitner-Platz 1, 14109 Berlin

For researchers, particularly from the field of soft condensed matter, scattering techniques are an important element for the characterization of a wide variety of systems. Light scattering (LS) is suitable to determine the overall particle shape and size, however, small-angle

neutron scattering (SANS) provides information of the internal structure. The big difference between these two methods is the concentration range in which the samples are characterized. Conventional LS-experiments can only be performed on diluted samples to assure that only single-scattered light is detected, while for a SANS-measurement highly concentrated samples are required. In order to measure highly concentrated samples with LS, a 3D-LS setup is used, where multiple scattering is eliminated by performing two simultaneously light scattering experiments. Currently a combination of 3D-LS with a small-angle neutron scattering instrument (V16) at the Helmholtz-Zentrum in Berlin is build up to measure simultaneously two different scattering experiments on the same sample.

CPP 51.4 Wed 10:00 Poster A

**Glassy dynamics of polymer brushes: employing an equivalent circuit model to analyze broadband dielectric spectroscopy data** — ●MARTIN TRESS<sup>1</sup>, NILS NEUBAUER<sup>1</sup>, RENE WINKLER<sup>2</sup>, PETRA UHLMANN<sup>2</sup>, EMMANUEL URANDU MAPESA<sup>1</sup>, MANFRED REICHE<sup>3</sup>, and FRIEDRICH KREMER<sup>1</sup> — <sup>1</sup>University of Leipzig, 04103 Leipzig, Germany — <sup>2</sup>Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — <sup>3</sup>Max Planck Institute of Microstructure Physics, 06120 Halle (Saale), Germany

The glassy dynamics of poly(2-vinylpyridine) (P2VP) polymer brushes is investigated by means of Broadband Dielectric Spectroscopy (BDS). For that, P2VP brushes are grafted onto an ultra-flat, highly conductive silicon electrode. The latter is part of a recently developed nano-structured electrode arrangement which has been refined to achieve an electrode-to-electrode distance of only ~40 nm. Since the studied brushes exhibit thicknesses between 1.8 to 7 nm, a major fraction of the capacitor volume is empty. To consider the impact of this partial filling as well as the other components in the capacitor (e.g. nano-structure spacers) a sophisticated equivalent circuit model is implemented in the fit function. This enables to unravel polarization effects, charge transport and molecular relaxation.

CPP 51.5 Wed 10:00 Poster A

**Determination of Volatility of Ionic Liquids at the Nanoscale by means of Ultra-Fast Scanning Calorimetry** — ●MATHIAS AHRENBERG<sup>1</sup>, MARTIN BECK<sup>2</sup>, CHRISTIN SCHMIDT<sup>3</sup>, SERGEY P. VEREVKIN<sup>3</sup>, OLAF KESSLER<sup>2</sup>, UDO KRAGL<sup>3</sup>, and CHRISTOPH SCHICK<sup>1</sup> — <sup>1</sup>Institut für Physik, Universität Rostock — <sup>2</sup>Maschinenbauakultät, Universität Rostock — <sup>3</sup>Institut für Chemie, Universität Rostock

Ionic Liquids (ILs) are intended to be used as quenching media in the heat treatment of metallic materials, e.g. aluminum alloys, even the solution annealing temperature of such alloys is 800 K. The most thermally stable ILs exhibit an onset temperature of decomposition at about 620 K as measured with slow scanning methods, e.g. TGA. Since in a real quenching process the IL is exposed to high temperature only shortly and in a thin layer surrounding the alloy gives reason to investigate the IL at such small scales in time and space. Here we present a new method for the determination of the mass loss rate of such liquids using differential fast scanning calorimetry. We have developed and proven this method using [EMIm][NTf2] and [BMIm][NO3] at temperatures of up to 750 K and in different atmospheres to distinguish between decomposition and evaporation. It was demonstrated that evaporation is still the dominating process of mass loss even at such highly elevated temperatures. In addition, since the method allows very high heating rates (up to 10,000,000 K/s), much higher temperatures can be reached in the measurement of the mass loss rate as compared to common devices without significant decomposition of the ionic liquid.