DS 13: Optical Analysis of Thin Films I

Time: Thursday 9:30–11:00 Location: SCH A 316

Invited Talk DS 13.1 Thu 9:30 SCH A 316

Towards Catalytic Applications of Infrared Laser Polarimetry — •Andreas Furchner[1] and Karsten Hinrichs[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Division Energy and Information, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V.

Infrared (IR) polarimetry and ellipsometry are well-established non-destructive spectroscopic techniques for studying the refractive and absorptive properties of thin films and surfaces with monolayer sensitivity. This spectral range is particularly suited for investigating chemical composition, molecular interactions, anisotropy, conductivity, as well as changes and reactions at surfaces and interfaces.

The incorporation of quantum cascade lasers (QCLs) in novel IR polarimeter designs has pushed the boundaries of the achievable spatial and temporal resolution well into the sub-mm and sub-second range, respectively. Laser-based polarimeters thus enable hyperspectral and time-resolved amplitude–phase measurements with novel application potential. Probing individual laser pulses delivers time resolutions of 10 μs, spectral sweeps in 100 ms, and hyperspectral maps in minutes.

This presentation focuses on recent instrumental developments, such as the combination of QCLs with single-shot designs, that pave the way towards the application of IR laser polarimetry in thin-film catalysis. Here, surface reactions have to be studied *in situ* and *operando* in order to resolve the evolution of surface species and temporary adsorbates.

DS 13.2 Thu 10:00 SCH A 316

Large area functional thin film properties mapping using in-line hyperspectral imaging during roll-to-roll magnetron sputter deposition — Florian Gruber[2], Patrick Schlenz[1], Steffen Bieder[4], Eric Schneider[4], Jolanta Szelwicka[1], Julio Hernandez[3], Christian Sternemann[4], and •Steffen Cornelius[1] — [1]Fraunhofer FEP, Winterbergstrasse 28, 01277 Dresden, Germany — [2]Fraunhofer IWS, Winterbergstrasse 28, 01277 Dresden, Germany — [3]Norsk Elektro Optikk AS, Ostensjoveien 34, 0667, Oslo, Norway — [4]Fakultät Physik/DELTA, Technische Universität Dortmund, August-Schmidt-Straße 1, 44227 Dortmund, Germany

Roll-to-roll (R2R) coating processes of flexible substrates are established for cost-efficient thin film functional materials production for applications like energy efficient windows and solar cells. However, even small variations of thickness and/or composition homogeneity may affect the final product performance. Due to the high throughput of coated surface area in R2R coating the ex-situ material characterization is very time consuming, often destructive and offers no possibility for in-situ process monitoring and/or quality control.

The NanoQI EU-H2020 project develops a powerful in-line technology combining hyperspectral imaging with X-ray reflectivity via a machine learning algorithms, enabling large area (0.5m x 100m) high resolution (<1mm) high speed (m/min) thin film properties imaging. The combinatorial thickness mapping of a binary metal-oxide double layer (thickness up to 120nm) on PET substrate will be discussed in detail - aiming to achieve a thickness accuracy of only a few %.

DS 13.3 Thu 10:15 SCH A 316

Developing an open source ellipsometry analysis workflow — •Florian Dobener[1], Marius Müller[2], Carola Emminger[1,3], Chris Sturm[3], Tamás Haraszti[4], Marius Grundmann[3], and Sandor Brockhauser[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Germany — [2]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [3]Felix-Bloch Institut für Festkörperphysik, Universität Leipzig, Germany — [4]DWI Leibniz Institute for Interactive Materials, Aachen, Germany

Optical and geometric characteristics of multilayer material stacks are not accessible from ellipsometric data in a direct way. The optical model applied to the data is the key, which allows understanding of these properties. Accordingly, there exist a lot of different software tools to construct such models, which vary in their model implementation and are often closed source. Comparing, reproducing and using data from literature can therefore be challenging. Here, we present the open source ellipsometry software pyElli. It implements specific dispersion models from manufacturers and from literature. Furthermore, it allows for easy construction of non-standard measurement tasks, e.g. combining different measurements or using uncommon measurement parameters. Together with the recent NeXus ellipsometry standard, the NOMAD research data management platform and its interactive Jupyter based toolkit, we show how pyElli contributes to an open ellipsometry workflow. This open workflow is a standardised and reproducible way of analysing ellipsometry data and adds to the goal of making ellipsometry data FAIR.

DS 13.4 Thu 10:30 SCH A 316

IR dual-comb polarimetry of anisotropic nanofibers — •Karsten Hinrichs[1], Brianna Blevins[2], Andreas Furchner[3], Nataraja Sekhar Yadavalli[2], Sergiy Minko[2], Raphael Horvath[4], and Markus Mangold[4] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Department of Chemistry, The University of Georgia — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Division Energy and Information, Schwarzschildstraße 8, 12489 Berlin, Germany — [4]IRsweep AG, Laubisruetistrasse 44, 8712 Staefa, Switzerland

In this work an anisotropic nanofiber scaffold is investigated non-invasively under ambient conditions by infrared dual-comb polarimetry (IR - DCP). Amplitude and phase spectra at various azimuthal sample rotations are correlated with the orientation of characteristic vibrational transition dipole moments. IR - DCP is proven as a new method for the spectral analysis (here 1200 cm-1 to 1300 cm-1) of such anisotropic samples in very short measurement times (0.065 ms) at 1.4 cm-1 spectral resolution. Such capabilities are in particular interesting for imaging applications, time resolved studies and hyperspectral spectroscopy of anisotropic samples. In difference to classical ellipsometry which measures phase differences, IR - DCP can measure s- and p-polarized phases separately. We acknowledge financial support by the EU through EFRE 1.8/13 and the Horizon 2020 grant 820419 and by the BMBF through CatLab (03EW0015A/B).

DS 13.5 Thu 10:45 SCH A 316

Orientation in thin spider silk films at silicon substrates evidenced by dichroic FTIR spectroscopy — •Martin Müller[1,2], Mirjam Hofmaier[1,3], Sarah Lentz[4], Thomas Scheibel[4], and Andreas Fery[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Institut für Physikalische Chemie und Physik der Polymere, Dresden, Germany — [2]Technische Universität Dresden, Lehrstuhl für Makromolekulare Chemie, Dresden, Germany — [3]Technische Universität Dresden, Lehrstuhl für Physikalische Chemie Polymerer Materialien, Dresden, Germany — [4]Universität Bayreuth, Lehrstuhl für Biomaterialien, Bayreuth, Germany

Biomedically relevant spider silk films were deposited on unscratched and parallelly scratched silicon substrates and checked for conformation and orientation by dichroic transmission (T-) and ATR-FTIR spectroscopy. Films (d=0-200 nm) were casted from hexafluoroisopropanol solutions of recombinantly engineered spider silk proteins. Both FTIR methods revealed little b-sheet (<10%) and much disordered structure (>80%) from Amide I band analysis. Dichroic ratios R of Amide I components close to isotropic films were found by T- and ATR-FTIR indicating no orientation. Whereas, silk films after swelling in MeOH vapor revealed higher b-sheet (>30%) and lower disordered structure amounts (<60%). By T-FTIR isotropic R values of Amide I components assigned to antiparallel b-sheet were found indicating no in-plane orientation, while ATR-FTIR revealed R values significantly deviating from isotropy indicating out-of-plane orientation. Orientation was independent on scratching and increased decreasing d.