DS 8: Thin Film Characterisation: Structure Analysis and Composition I

Time: Monday 15:00–16:30 Location: H8

Invited Talk DS 8.1 Mon 15:00 H8

Materials characterization at the nanoscale by X-ray spectrometry — •Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

The development of efficient nanoscaled materials requires the correlation of the materials functionality with their chemical and physical properties. To probe these properties, analytical methods that are sensitive at the nanoscale are required. The reliability of most analytical methods is based on the availability of reference materials or calibration samples, the spatial elemental composition of which is as similar as possible to the matrix of the specimens of interest. However, there is a drastic lack of reference materials at the nanoscale. PTB addresses this challenge by means of an X-ray analytical method where all instrumental and experimental parameters are determined with known contributions to the uncertainty of the analytical results. This first-principle based approach does not require any reference materials but a complete characterization of the instrumental characteristics and, in addition, of the X-ray fundamental parameters related to the elements composing the sample. X-ray spectrometric methods allow for the variation of the analytical sensitivity, selectivity, and information depth needed to effectively reveal the spatial, elemental, and chemical specimen parameters of interest. Examples of interfacial speciation, elemental depth profiling, as well as layer composition and thickness characterizations in various materials will be given. Recent instrumental achievements provide access to liquid-solid interfaces as well as towards the in-situ speciation of battery materials.

DS 8.2 Mon 15:30 H8

Determination of growth quality of thin films by In-situ GISAXS during the deposition process — •Jörg Wiesmann[1], Peter Siffalovic[2], Karol Vegso[2], and Martin Hodas[2] — [1]Incoatec GmbH, Geesthacht, Germany — [2]Inst. of Physics, Slovak Acad. of Sci., Bratislava, Slovakia

We present how the growth of thin films can be investigated during the deposition by means of grazing incidence small angle X-ray scattering (GISAXS). These experiments are typically done only at synchrotrons. They are now also feasable in the home-lab by using modern microfocus sources like the air cooled IμS.

The IμS is explained in more detail. It is a high-brilliance X-ray source for diffractometry and available with Cr, Co, Cu, Mo, and Ag anodes. It is equipped with a 2-dim beam shaping multilayer optic. We can form either a collimated beam with low (below 0.5 mrad) or a focusing beam with higher divergence (up to 10 mrad) and very small focal spots below 100 μm.

In our presentation we give an overview of experiments and results demonstrating the potential of the IμS in in-situ GISAXS studies. We present 2 applications in detail:

1) Multilayers deposited by ion beam assisted deposition: This experiment was done only at synchrotrons. With an IμS it becomes feasible in the home-lab.

2) Growth of thin metallic layers on graphene: The difference between production by PVD and Thermal Deposition is discussed.

DS 8.3 Mon 15:45 H8

Real-Time Investigation at Metal-Polymer-Interfaces during Sputter Deposition. — •Matthias Schwartzkopf[1], Oleksandr Polonskyi[2], Alexander Hinz[2], Thomas Strunskus[2], Franziska Löhrer[3], Volker Körstgens[3], Peter Müller-Buschbaum[3], Franz Faupel[2], and Stephan V. Roth[1] — [1]DESY, Photon Science, Notkestr. 85, 22607 Hamburg — [2]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, Kaiserstr.2, 24143 Kiel — [3]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

The reproducible low-cost fabrication of functional metal-polymer-nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed the combination of in-situ time-resolved GISAXS [1] and GIWAXS with in-situ ellipsometry during sputter deposition of gold on thin polystyrene films. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of different deposition rates on the growth regimes with their specific thresholds and permits a better understanding of the growth kinetics of gold clusters on polymer substrates. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

DS 8.4 Mon 16:00 H8

Ion beam sputter deposition (IBSD) of cubic MgO and NiO — •Martin Becker, Robert Hamann, Mario Gies, Fabian Michel, Angelika Polity, and Martin Eickhoff — 1st Physics Institute, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Ion beam sputter deposited MgO and NiO thin films were grown on (0001) (c-cut), $(01\bar{1}2)$ (r-cut), $(11\bar{2}0)$ (a-cut) and $(10\bar{1}0)$ (m-cut) sapphire substrates. A pure Ni metallic target and a MgO ceramic target were processed with different gas mixtures of argon and oxygen at elevated substrate temperatures. X-ray photoelectron spectroscopy (XPS) and energy dispersive X-ray spectroscopy (EDX) were used to identify composition and stoichiometry. It is shown, that elevated temperatures favor crystallization in preferential orientations. The determined out-of-plane relationships were XO(111)$\|Al_2O_3(0001)$ (c-cut), XO(111)$\|Al_2O_3(11\bar{2}0)$ (a-cut) and XO(110)$\|Al_2O_3(10\bar{1}0)$ (m-cut) for X = Mg/Ni, whereas on $Al_2O_3(01\bar{1}2)$ (r-cut) no significant out-of-plane intensity was observed. XRD rocking curves indicated small full width at half maximum (FWHM) around 10-100 arcsec. X-ray pole figures and reciprocal space mapping (RSM) indicated distinct epitaxial in-plane relationships. The morphology was studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM), which reveal smooth and homogeneous surfaces for thin layers, enabling their use as appropriate buffer layers for established IBSD-sputtered materials like cuprous oxide and stannic oxide.

DS 8.5 Mon 16:15 H8

Determing the optical constants of NiO with Resonant X-Ray Reflectivity — •Katrin Fürsich[1], Volodymyr B. Zabolotnyy[1], Christian Schüssler-Langeheine[2], Maurits W. Haverkort[3], and Vladimir Hinkov[1] — [1]University Würzburg, Am Hubland, 97074 Würzburg — [2]HZB, Albert-Einstein-Str. 15, 12489 Berlin — [3]MPI for CPfS, Nöthnizer Straße 40, 01187 Dresden

NiO has been serving as the model system to study electronic correlations and antiferromagnetism of transition-metal oxides, mostly because of its appealing properties like large bandgap and high Néel temperature. Nevertheless, it is still a challenge to describe NiO theoretically as common methods such as DFT and LDA+U are known to fail. We use Resonant X-Ray Reflectivity (RXR) in combination with cluster calculations to study the optical properties of NiO. RXR is a non-destructive technique with a probing depth >100 nm and sub-nm spatial resolution. Thus RXR provides an excellent opportunity to extract layer-resolved optical constants, which are directly related to physical properties like crystal field effects and spin-orbit interactions. However, because of the screening effects it is hard to determine these parameters theoretically. This results in uncertainties in the calculations. We perform RXR measurements on *in situ* grown NiO thin films of different thicknesses and on cleaved NiO bulk crystals to overcome these problems and to tune unknown variables in the state of the art cluster calculation. The analysis combines theory and experiment in order to give remarkable insight into the physical properties of correlated electron systems.