# DS 4 Thin film analysis II

Time: Monday 11:15–12:45 Room: GER 38

DS 4.1 Mon 11:15 GER 38

**Determination of Mn valency using ELNES in the (S)TEM** — •Thomas Riedl, Thomas Gemming, and Klaus Wetzig — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The analysis of electron energy-loss near-edge structures (ELNES) in the (S)TEM provides a tool to probe the symmetry-projected density of unoccupied states near the Fermi level at high spatial resolution. In particular, the Mn-$L_{2,3}$ and O-K edges undergo characteristic changes with Mn valency. With increasing Mn valency the white-line intensity ratio $I(L_3)/I(L_2)$ decreases and the energy separations between (a) Mn-$L_3$ and O-$K_a$ and (b) O-$K_b$ and O-$K_a$ increase [1]. Our ELNES measurements of $La_{1-x}Sr_xMnO_3$ ($x$=0.2, 0.4) manganites indicate that the Mn valence sensitivity of both energy separations exceeds that of $I(L_3)/I(L_2)$ by a factor of ≈2. With respect to the impact of oxidation states on the performance of magnetoelectronic devices based on manganite thin films the mentioned Mn valence-sensitive ELNES quantities have been investigated at the $La_{1-x}Sr_xMnO_3$ /$SrTiO_3$ interface. Preliminary results point to a reduction of the Mn valency close to the interface [2].

[1] J. H. Rask et al.: Ultramicr. 21 (1987) 321

[2] We acknowledge the DFG for financial support via FOR 520, project GE 1037/8.

DS 4.2 Mon 11:30 GER 38

**Epitaxial anatase (012) and (001) films grown on (110) and (100) $SrTiO_3$** — •Andriy Lotnyk, Stephan Senz, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

Rutile, anatase and brookite are well known polymorphs of $TiO_2$. The rutile structure is the thermodynamically most stable structure of $TiO_2$ at high temperatures and is the most widely studied. The anatase phase is a low temperature phase. This modification cannot be easily obtained with good crystallinity and its fundamental properties are not well understood. We report on the growth of epitaxial films of $TiO_2$ on (110) and (100) $SrTiO_3$ (STO). A $TiO_2$ target was electron beam evaporated in a high vacuum system with $P_{O2}$=1 × $10^{-2}$ Pa. The substrates were heated at temperatures between 500°C and 1100°C during deposition. The grown films were investigated by XRD, AFM and TEM. The films are predominantly of anatase (A) structure at substrate temperatures between 500°C and 600°C. Texture measurements revealed the following orientation relationships: (012)/[100]A ∥ (110)/[001]STO and (001)/[100]A ∥ (100)/[001]STO. The orientation relationship of anatase films on (110) STO is reported first. With increasing temperature the average grain size of the thin films is increasing, as indicated by AFM investigations. (HR)TEM observations revealed grain boundaries in the films.

DS 4.3 Mon 11:45 GER 38

**Aberration correction used for interface characterisation with atomic resolution** — •Meiken Falke[1], Andrew Bleloch[2], Uwe Falke[2], Gunter Beddies[1], and Steffen Teichert[1] — [1]Institut f. Physik, TU-Chemnitz, 09107 Chemnitz, Germany — [2]superSTEM, Daresbury Laboratory, Daresbury, WA44AD, UK

Recently aberration corrected dedicated scanning transmission electron microscopy with a probe size of 0.1 nm became available . The high angle annular darkfield signal acquired with this spatial resolution allows to distinguish between atomic columns of different composition in a crystal. Thus $C_s$-corrected dedicated STEM provides a powerful tool for studying metal silicon compounds (silicides) and their interfaces to the silicon substrate. Epitaxial cobalt- and nickel-disilicide silicon (001) junctions of buried thin films were studied by dedicated aberration-corrected STEM. Two different interface structures were unequivocally identified, one of which represents a (2×1) reconstruction found experimentally for the first time. The results are consistent with predictions from total energy calculations. Due to the cubic crystal symmetry of both, the silicide and the Si substrate, the interface consists of a patchwork of different domains. In addition to the usual misfit dislocations at a relaxed commensurate interface, here dislocations are required at the boundaries of those domains. A complex defect structure, was found to solve both crystallographic constraints. The Burgers vector for each type of interface domain junction could be derived from the identified atomic arrangement in the two interface structures and from crystallographic considerations.

DS 4.4 Mon 12:00 GER 38

**Texture Characterization of Pyrolytic Carbon Layers: A Quantitative Study by Polarized Light Microscopy and Selected Area Electron Diffraction** — •Andreas Pfrang[1], David Bach[2], Dagmar Gerthsen[2], and Thomas Schimmel[1,3] — [1]Institute of Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — [2]Laboratory for Electron Microscopy, University of Karlsruhe, D-76128 Karlsruhe, Germany — [3]Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

Many properties of pyrolytic carbon strongly depend on the degree of texture which is frequently analyzed by polarized light microscopy (PLM) and selected area electron diffraction (SAED). PLM allows the fast determination of the extinction angle Ae. SAED exhibits a higher spatial resolution and allows the determination of the orientation angle.

A quantitative model for the relationship between extinction angle determined by PLM and orientation angle determined by SAED is presented and applied to our experimental data. The distribution of the orientation of coherent domains is derived from SAED data and the reflection coefficients of pyrolytic carbon are calculated as the sum of the reflection coefficients of the coherent domains. The only fit parameters in our model are the ratio of the reflection coefficients of the coherent domains for extraordinary and ordinary rays, and the relative phase shift. Good agreement between calculation and experiment is achieved.

[1] A. Pfrang, D. Bach, D. Gerthsen, Th. Schimmel. Texture analysis of pyrolytic carbon by polarized light microscopy and selected area electron diffraction. Carbon 2005, Gyeongju, Korea (2005)

DS 4.5 Mon 12:15 GER 38

**Local density profiles in thin films and multilayers from diffuse x-ray and neutron scattering** — •Markus Rauscher[1,2], Harald Reichert[1], Simon Engemann[1], and Helmut Dosch[1,2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70469 Stuttgart, Germany

We develop a technique to determine local density profiles in rough thin films and multilayers for which conventional reflectometry does not work. The main idea is to integrate the total scattered intensity for a given vertical momentum transfer over the parallel momentum transfer. Probing Fourier space globally results in a local probe in real space and the integrated intensity is proportional to the local reflectivity of the surface. We also discuss the influence of a finite range of integration as well as sample inhomogeneities. This technique is limited to situations where the kinematic Born approximation is sufficient to describe the scattering process. However, in certain cases the technique can be used in the vicinity of the critical angle of total external reflection as well.

DS 4.6 Mon 12:30 GER 38

**Coherence experiments with white synchrotron radiation** — •Gudrun Gleber, Tobias Panzner, and Ullrich Pietsch — Universität Siegen, Siegen, Germany

3rd generation storage rings provide partly coherent radiation allowing a new kind of x-ray experiments, so called x-ray photon correlation spectroscopy (XPSC) experiments. XPSC experiments gives access to static or dynamic properties of a sample on a nanometer length scale.

Usually XPCS-experiments are performed by use of monochromatic radiation. To record the whole reciprocal space information by this way, one has to change stepwise the angle of incidence, which also will change the illuminated sample area and subsequently the diffraction pattern. Using a polychromatic beam provided at the energy dispersive reflectometry beamline (EDR-beamline) at the BESSY II and an energy dispersive detector, we are able to measure the same information without changing the incident angle which keeps the illuminated sample area constant. This is a big advantage for the surface reconstruction from the measured diffraction pattern. Due to the fact, that one energy spectrum gives access to different regions of the sample we are using this technique to observe slow processes in polymers.

In this talk we will report on the present status of the static and dynamic measurements in an energy dispersive regime.