KR 5: Poster - Crystallography

Time: Wednesday 15:00–17:30 Location: Poster B2

KR 5.1 Wed 15:00 Poster B2

Determination and correction of distortions and systematic errors in low-energy electron diffraction — •Falko Sojka[1], Matthias Meissner[1], Christian Zwick[1], Roman Forker[1], Claudius Klein[2], Michael Horn-von Hoegen[2], and Torsten Fritz[1] — [1]University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany — [2]University of Duisburg-Essen, AG Horn-von Hoegen, Lotharstr. 1-21, 47048 Duisburg, Germany

LEED on epitaxial layers is a powerful tool to examine long-range ordering at the interface. However, due to limitations like distortions of the LEED images, additional efforts have to be made in order to derive precise epitaxial relations from the measured LEED patterns.

We developed and implemented an algorithm to determine and correct systematic distortions in LEED images. The procedure is independent of the design of the device (conventional LEED, MCP-LEED, SPA-LEED). Therefore, only a calibration sample with a well-known structure and a suitably high number of diffraction spots is required. The algorithm provides a correction matrix which can be used to rectify all further measurements generated with the same device. Additionally, we found an axial distortion which occurs due to a tilted sample surface. This axial distortion can be described theoretically, and thus it is possible to correct those measurements, too.

Only corrected LEED images represent an unaffected view of the reciprocal space. So we can use them for the determination of the lattice parameters or epitaxial relations by numerical optimization achieving a very high accuracy.

KR 5.2 Wed 15:00 Poster B2

Digital electron diffraction: a new approach for determining crystal symmetry at the nanometre scale — Richard Beanland[1], Paul J Thomas[2], David I Woodward[1], Pam A Thomas[1], and •Rudolf A Römer[1,3] — [1]Department of Physics, The University of Warwick, Coventry CV4 7AL, UK — [2]Gatan UK Ltd, 25 Nuffield Way, Abingdon, Oxon, OX14 1RL, UK — [3]Centre for Scientific Computing, The University of Warwick, Coventry CV4 7AL, UK

The functional properties of materials are normally determined by their symmetry. This is equally true on the nano-scale as it is at the macro-scale. Whilst for bulk material the structure and symmetry can routinely be solved by X-ray diffraction, there is no comparable technique for nanostructured materials. Electron diffraction has the required nano-scale resolution and sensitivity, but overlapping data from different diffracted beams has limited its use to date. Here, we demonstrate that computer control of beam tilt and image capture in a conventional transmission electron microscope can be used to overcome this problem, quickly providing very rich diffraction datasets. The technique requires no new hardware, no more expertise than conventional electron diffraction and takes less than two minutes to acquire and process a complete data set. We apply the new technique to the question of a centrosymmetry phase of VO2 and show large differences between theory and experiment for every oxide so far examined.

KR 5.3 Wed 15:00 Poster B2

Structure, mechanical, and tribological properties of C:Ni nanocomposite films grown by IBAD — •S. Gemming[1,2], M. Krause[1,3], T. Kunze[1,3], A. Mücklich[1], M. Fritzsche[1], R. Wenisch[1], M. Posselt[1], A. Schneider[1], and G. Abrasonis[1] — [1]HZ Dresden-Rossendorf, D-01314 Dresden — [2]TU Chemnitz, D-09107 Chemnitz — [3]TU Dresden, D-01062 Dresden

The mechanical and tribological properties of nanostructured carbon:nickel films on silicon substrates are investigated by a multi-scale experimental and theoretical approach. The C:Ni nanostructures comprising either tilted columns or three-dimensionally self-organized nanopatterns are grown by ion-beam assisted deposition (IBAD). Complex layer architectures were obtained by sequential deposition by rotating the substrate in relation to the assisting ion beam after each deposition step. Atomic composition of the films was determined by ion beam analysis. The phase structure of carbon was analyzed by Raman spectroscopy, that of nickel by X-ray diffraction. The microstructure of the films was determined by high resolution transmission electron microscopy. The films show good adhesion as probed by scratch tests. The film hardness is about 20 GPa, and the elastic modulus 200 GPa.

Friction coefficients on the order of 0.1 are found for oscillating wear conditions under ambient conditions. Atomistic computer simulations assist the experimental findings for dry and liquid contacts. The simulation shows a complex behaviour for the carbon-carbon interaction, e.g. resulting in the formation of a tribo-layer. Support by the ECEMP excellence cluster is acknowledged.

KR 5.4 Wed 15:00 Poster B2

Modelling the growth of ZnO nanocombs synthesized by vapor-liquid-solid method — •Farzaneh Fattahi Comjani[1], Ulrike Willer[2], Stefan Kontermann[1], and Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, Goslar, Germany — [2]Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Am Stollen 19B, Goslar, Germany

Generally, ZnO nanocombs are synthesized by the carbothermal reduction process between graphite and ZnO powder. Mechanisms for the growth of ZnO nanocombs have been proposed, which relate the formation of nanocombs with a self catalytic effect related to the Zn cluster at the defective site on the polar +(0001) surface of the ZnO nanobelt or the enrichment of Zn at the growth front +(0001). However, these mechanisms cannot explain why the ZnO nanowires grow equally spaced on the polar +(0001) surface of the backbone nanobelt. This work reports on the synthesis of ZnO nanocombs by the vapor-liquid-solid (VLS) method. For this, we use the molar ratio ZnO:C (2:3) instead of the standard molar ratio (1:1). Additional emphasis is laid on the development of a model for the growth of nanocombs based on the piezoelectric character of ZnO. Applying the perturbation and elasticity theory and using the Fourier expansion, the induced mechanical strain and piezoelectric potential distribution in the backbone nanobelt are approximated. The coupling of the mechanical strain to the piezoelectric field across the nanobelt thickness explains the equidistant growth of nanowires on the polar +(0001) surface of the nanobelt as a consequence of a self catalytic growth process.

KR 5.5 Wed 15:00 Poster B2

BL 10 at DELTA, an interesting new beamline for crystallographers — •Anne Kathrin Hüsecken[1], Konstantin Istomin[1], Ralph Wagner[2], Stefan Balk[2], Dirk Lützenkirchen-Hecht[2], Ronald Frahm[2], and Ullrich Pietsch[1] — [1]Universität Siegen — [2]Bergische Universität Wuppertal

DELTA is a small synchrotron in Dortmund performing at 1.5 Gev and a maximum current of 130 mA. After the commissioning of the beamline BL 10 was finished in August 2012 it is now open for all users. The beamline is devoted to materials science research with the focus on X-ray diffraction and absorption spectroscopy measurements. Possible experiments are precise single crystal diffraction, charge density studies and also fatigue studies in metals, transmission and fluorescence EXAFS measurements and reflection mode EXAFS. The beamline is working at an energy range of 4.5 to 16 keV with an energy resolution of $dE/E \propto 1.6 \cdot 10^{-4}$. Depending on the aperture it is possible to measure with a beamsize between $3 \cdot 10\text{mm}^2$ and $0.5 \cdot 0.1\text{mm}^2$. The photon flux is with a focusing mirror expected to be $5 \cdot 10^9 \text{Photons/s mm}^2$. The user can decide between several detectors, a Pilatus 100K 2D, a Scintilation Counter, an Avalanche Photodiode or Ionization Chambers. First diffraction measurements with Quartz powder obtained with the 2D and point detectors show that high-quality powder diffraction measurements are possible at the beamline. And the diffraction of a BSO single crystal shows that the intensity is comparable to the now closed beamline D3 at Doris. So we close a gap for all users who do not get beamtime at big synchrotrons.

KR 5.6 Wed 15:00 Poster B2

Optical characterization of the protonation and deprotonation of pyroelectric single crystals — •Thomas Köhler, Erik Mehner, Juliane Hanzig, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, D-09596 Freiberg, Germany

Pyroelectric crystals are used in many optical devices, therefore, understanding of structural defects is essential. It is easy to incorporate hydrogen in air-grown LiNbO3 and LiTaO3, however, the exact processes are only partially understood. Hence, the incorporation of hydrogen in both materials was investigated via FT-IR and UV/VIS absorp-

tion spectroscopy. Specifically the hydrogen in the congruent crystals leads to OH absorption bands with two components at $3468\,\mathrm{cm}^{-1}$, $3485\,\mathrm{cm}^{-1}$ in LiNbO$_3$ and at $3463\,\mathrm{cm}^{-1}$, $3481\,\mathrm{cm}^{-1}$ in LiTaO$_3$, respectively.

It is observed that the OH bands decrease in reduced and increase in protonated and reprotonated crystals. A third component at about $3500\,\mathrm{cm}^{-1}$ is discernible in the protonated LiNbO$_3$. Reduced crystals show no reprotonation – only in LiNbO$_3$ crystals deprotonated above $900\,^{\circ}\mathrm{C}$ the return of the OH band was observed. Furthermore, the varying degree of reduction of the samples has influence on the absorption in the visible range. A broad band is observed in heavily reduced crystals, which is assigned to the formation of polarons [1]. The formation of polarons is different in the two material systems and shows influence on their optical behavior and their defect structure.

[1] A. Dhar, A. Mansingh. J. Appl. Phys. 1990, 68 (11), 5804-5809.