

FA5-MS39-P02**Depth resolved lattice constant determination in bended samples using Cu, Mo & Ag K α radiation**Thomas Holz^a, Reiner Dietsch^a, Markus Krämer^a,^aAXO DRESDEN GmbH, Heidenau, GermanyE-mail: thomas.holz@axo-dresden.de

When a work-piece is bended or deformed, internal stress in the piece leads to a change of its lattice constants. Consequently, stress gradients in the sample lead to lattice constant gradients. In order to determine these gradients as a function of depth below the sample surface the standard Twin-Mirror Arrangement was modified. Small slits were used both at the primary beam side and at the diffracted beam side to define a small sample volume on the omega axis of the diffractometer. A sample movement through this volume delivers one-dimensional depth information which is needed for stress gradient analysis.

In order to take advantage of deeper penetration depths we used, in addition to the common Cu K α radiation, the Mo K α and Ag K α lines. A bended aluminium test sample was characterized in depth by XRD with different photon energies. It is shown that the presented technique is capable of measuring relative lattice constant changes ε (in the range of 0.1% - 0.3%) in depth. The advantages of using different photon energies are discussed as well.

Keywords: deformation, lattice properties, X-ray instrumentation

FA5-MS39-P03**Beyond Simple SAXS: Beating Ambiguity by**

Integration. Peter Laggner^{a,b}, Heinz Amenitsch^a, Maria Schmuck^a, Benedetta Marmiroli^a, M. Weygand^b and Manfred Kriechbaum^{a,b}, ^aInstitute of Biophysics and Nanosystems Research, Austrian Academy of Sciences, Graz, Austria, ^bHecus X-Ray Systems GmbH, Graz, Austria

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The ambiguity of SAXS results can be overcome by using its fundamental strength, the ability for integrating *in-situ* chemical and physical experiments. Many ways have been explored by synchrotron radiation techniques, such as time-, temperature-, pressure-, composition-resolving experiments, including also microfluidics and gas-phase techniques [1-3]. The additional chemical and/or physical information allows SAXS to reach far beyond the static information conventionally obtained. Transfer of the technologies explored at synchrotrons to home laboratory routine is an imperative issue in X-ray analytical system development.

With modern, point- or line-focussing laboratory microsources and optics, and their extreme brilliance, the integration of SAXS/WAXS with other physical techniques, such as scanning calorimetry, pressure scanning, gas sorption techniques, has been realized and incorporated in industry-standard systems (e.g. Hecus S3-MICRO). DSC/SAXS provides real-time information on the structural events during enthalpic transitions, a topic essential e.g. in food- and drug analytics. Especially in pharma-development, where metastable, amorphous formulations are in the focus of interest, the question of 'polyamorphicity' becomes tractable.

Gas-sorption SAXS, as e.g. the study of CO₂ – effects on coal under different pressures provides essential information needed for terrestrial CO₂-sequestration strategies. With detectors suitable for direct absolute-scale measurements, the technique becomes even superior to conventional gas sorption (e.g. BET) methods, as it is faster and applicable to original samples without baking. Finally, in-situ GISAXS/XRR measurements on solid surfaces under controlled condition, previously possible only at synchrotrons in reasonable times, have been turned into laboratory routine, as e.g. in the study of triglyceride phase structure in 'surface blooming' of chocolate.

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FA5-MS39-P04**Low-energy Electron Diffraction Structure Analysis**

of the Al₁₃Co₄(100) Surface. Heekun Shin^a, Renee D. Diehl^a, Katariina Pussi^b, Julian Ledieu^c, Emilie Gaudry^c, Peter Gille^d, ^aDepartment of Physics, Penn State University, University Park, PA, USA, ^bDepartment of Mathematics and Physics, Lappeenranta University of Technology, Finland, ^cDepartment CP2S, Institut Jean Lamour, Ecole des Mines, Parc de Saurupt, Nancy, France, ^dDepartment of Earth and Environmental Sciences, Crystallography Section, LMU, München, Germany

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Low-energy electron diffraction (LEED) has been used to determine the surface structure of the Al₁₃Co₄(100) surface, which is a periodic approximant of the 10-fold surface of the Al-Co-Ni quasicrystal. The surface studied is the T1 termination [1] of this crystal, and the terminating surface was found to correspond to a puckered bulk layer. The surface comprises a 50:50 mix of two orientations, which correspond to terraces from two different types of bulk planes. The sample surface was prepared by Ar ion bombardment followed by heating to 1173 K for several hours, and the LEED data were measured at 80 K. The LEED analysis used a modified version of the SATLEED package. The surface structure determined in this study is similar to truncation structures of the bulk planes, but with no Co atoms present at the surface. Thus, the surface layer consists entirely of Al atoms. This structure was found to be one of the most stable structures of several considered in a related density functional theory study. This represents the most complex surface structure ever determined by LEED, with an analysis that includes 71 unique diffraction beams having a total energy range of > 20,000 eV.

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