DF 14: Poster III – 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, CPP, DF, GP, MA, MI, MM)

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

DF 14.1 Wed 15:00 Poster E

Clip - The Cologne Laue Indexation Program — •Olaf J. Schumann — Fraunhofer-Institut für Naturwissenschaftlich-Technische Trendanalysen, Euskirchen, Deutschland — II. Physikalisches Institut, Universität zu Köln, Germany

The Cologne Laue Indexation Program is a software for the analysis and simulation of Laue images.

Clip features a modern graphical user interface, could read a large variety of image formats and allows to mark spots *and* zones in a recorded image. These could be used for automatic indexation of the image for arbitrary crystal symmetries and refinement of lattice constants and projection plane parameters. Clip helps with the alignment of the crystal to a desired orientation. It is an open source software (GPL) written in C++ and the cross platform toolkit Qt and runs on Windows, Linux and Mac OS X.

DF 14.2 Wed 15:00 Poster E

A new access to extinction corrections — •Anne K. Hüsecken and Ullrich Pietsch — Naturwissenschaftlich Technische Fakultät, Fachbereich Physik, Universität Siegen, D-57068 Siegen, Germany

In x-ray crystal structure analysis a problem, called extinction, occurs due to multiple scattering in crystals. Over the years several extinction correction theorems have been formulated, but the used parameters have never been proved to be valid for a certain crystal under investigation. Perfect crystals scatter according to the dynamical theory (I~|F|) and imperfect crystals or ideal mosaic crystals due to the kinematical theory (I~|F|*). In most cases, the measured intensities of real crystals are in between both cases and an extinction correction is needed to fulfil the kinematic approach. Present theories dealing with extinction corrections are based on the approach of a mosaic crystal and describe x-ray scattering in terms of the kinematic approach using certain "correction terms" to implement the structure of a real crystal. The mosaic blocs within a real crystal are misorientated to each other and are affected by lattice strain. In addition both 3D shape and size of the blocs are not known. All these parameters can be determined by high-resolution x-ray diffraction techniques performing ω- and ω-2θ-scans through certain reciprocal lattice points. The measured parameters can be used to determine extinction. Our aim for crystallography is to perform these scans only for a few reflections, make a short analysis, to get the size, misorientation and lattice strain of the mosaic blocs. With these parameters it should then be possible to decide which one is the best extinction correction to use.

DF 14.3 Wed 15:00 Poster E

Evaluation of interfacial orientation information from 3D X-Ray diffraction contrast tomography in and its application in a mesoscale grain coasening model — •Melanie Syha, Fabian Sehn, Andreas Trenkle, and Daniel Weygand — Karlsruher Institut für Technologie, IAM

The orientation information from 3D X-Ray diffraction contrast tomography investigations in polycrystalline $SrTiO_3$ ceramics was evaluated before and after annealing. Special emphasis was put on local interface orientations, showing a preference for <100> orientated interfaces that increases during microstructural evolution. Moreover the data was used to investigate orientation dependent relative interface mobilities. The results are discussed in the context of the abnormal growth behavior found in $SrTiO_3$ and used to adapt a mesoscale grain coarsening model to more realistic simulations of microstructure evolution in this material.

DF 14.4 Wed 15:00 Poster E

Inter-layer disorder in sodium cobaltate — •David Jonathan Pryce Morris[1], Alan Tennant[1,2], Klaus Seiffert[1,3], Esther Dudzik[1], Dharmalingam Prabhakaran[4], Jon Goff[5], Michel Roger[6], and Jon Wright[7] — [1]Helmholtz-Zentrum Berlin, Germany — [2]TU-Berlin, Germany — [3]Kiel University, Germany — [4]Oxford University, UK — [5]Royal Holloway, University of London, UK — [6]CEA-Saclay, France — [7]ESRF, France

Sodium Cobaltate is a layered material which has been studied as a potential battery material, has shown good thermoelectric properties and becomes superconducting when hydrated. The physical properties are dependent on sodium content and the ordering of sodium ions. Sodium ordering in NaxCoO2 has previously been observed to have long-range order. Using x-ray diffraction we have observed a phase with long-range in-plane order and inter-layer disorder. Here we will present the data giving a possible structural interpretation.