SLS Special Symposium on

Grain Mapping

Tuesday, January 30, 2018

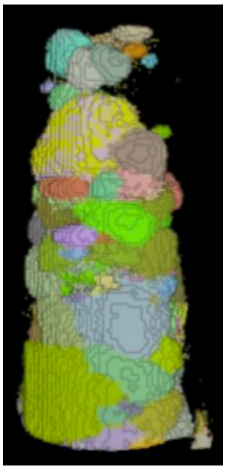
10:00 to 11:45, WBGB/019

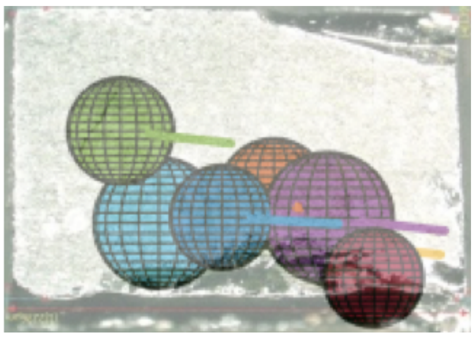
10:00 Invited Guest: Søren Schmidt *Dep. of Physics, Technical University of Denmark*

Examples from diffraction based imaging at a Synchrotron and at a Neutron Spallation Source as well as Multicrystal indexing at a X-ray Free Electron Laser

11:00 Coffee

11:15 Forward model algorithm for multigrain indexing in Laue mode
Marc Raventos, E. Lehmann, C. Grünzweig, M. Tovar, M. Medarde, T. Shang and S. Schmidt





Examples from diffraction based imaging at a Synchrotron and at a Neutron Spallation Source as well as Multicrystal indexing at a X-ray Free Electron Laser

Søren Schmidt
Department of Physics, Technical University of Denmark 2800 Kgs. Lyngby, Denmark

Polycrystalline materials are found anywhere in Nature (rocks, sand, ice, bones) and form the basis of much of modern industry (metals, ceramics, some semiconductors). The physical and mechanical properties of these materials are strongly dependent on the local structure, both on the scale of the individual crystallites and averaged over all the crystals within a small sub-volume of the entire specimen. In this presentation a few examples of non-destructive characterization of the microstructure through X-ray and Neutron diffraction based imaging will be given along with an overview of the reconstruction algorithms used in the data analysis. As an example of a technique for structure determination of crystals, a method for indexing individual crystals in a single shot diffraction image recorded at a X-ray Free Electron Laser will be presented.

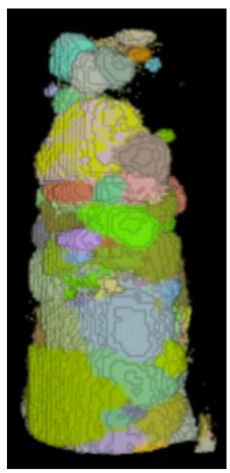


Figure 1: Example of imaging individual crystals (grains) in a iron sample using time-of-flight neutron diffraction imaging.

Forward model algorithm for multigrain indexing in Laue mode

M. Raventos,[1,2] E. Lehmann,[1] C. Grünzweig[1], M. Tovar[3], M. Medarde[1], T. Shang[1] and S. Schmidt[4]
[1] *Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland; E-mail: marc.raventos@psi.ch*
[2] *DQMP, University of Geneva, CH-1211 Geneva, Switzerland*
[3] *Helmholtz-Zentrum, 14109 Berlin, Germany*
[4] *Department of Physics, Technical University of Denmark 2800 Kgs. Lyngby, Denmark*

Growing high quality single crystals is necessary for the study of different material properties at the atomic level. However the process of crystal growth is complex, and sometimes the formation of multiple grains with different orientation cannot be avoided. These defects can make the identification of crystal orientations very difficult.

We propose a new method for grain indexing. By comparing experimental Laue diffraction data with simulations from a forward model, we can obtain the orientation and position of every grain in a polycrystalline sample. The model is originally designed to handle neutron data.

We tested the code with data from the FALCON Laue diffractometer of HZB for two different samples: an annealed αFe sample and a $YBaCuFeO_5$ sample. The measurements took 3 hours per sample under full illumination using forward and backward detectors simultaneously. The indexing time for the algorithm depends on the symmetry of the crystal and the amount of grains, for our experiments it ranges between 1 and 5 hours. We have been able to retrieve 16 grain orientations and positions from the Fe sample and 7 from the $YBaCuFeO_5$.

The strength of this method lies in the use of the full white beam spectrum of a continuous source to perform multi-grain indexing with a faster data acquisition than before. This method shows promising results for the determination of twinned and multiple grain crystals orientations and for coarse grain metallurgy samples.

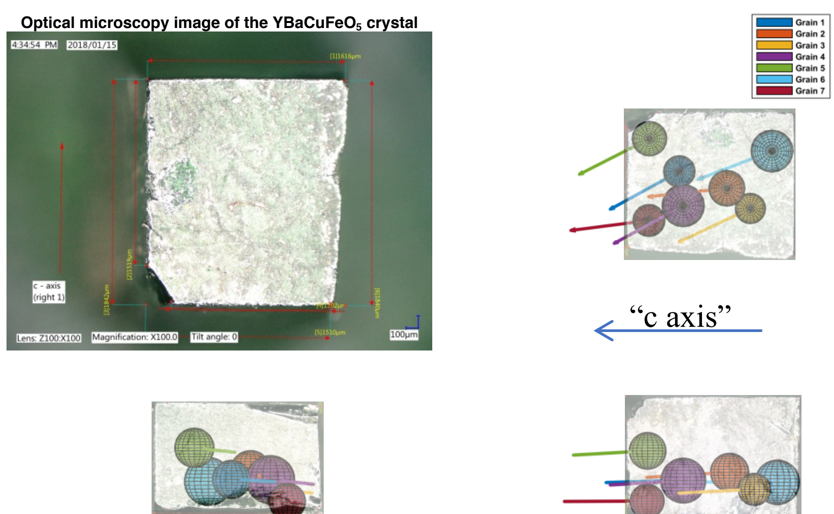


Figure 1: Orientation and relative size of the $YBaCuFeO_5$ crystallites vs optical microscopy.