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Laue Multi-Grain Indexing with Neutrons

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Polycrystalline materials undergoing thermal or mechanical loading suffer deformations and damage which can modify their grain size, orientation and texture. To obtain multigrain information from crystalline samples, 3D grain mapping is performed using x-ray diffraction at synchrotron radiation sources. However, the scope of this technique is limited due to the lack of penetration power inside of bulky metallic samples. Neutrons have usually a higher penetration depth in comparison with x-rays, and some grain maps have already been reconstructed from neutron data. However these methods have so far been dependent on the use of energy-resolved neutron imaging techniques, either with a velocity selector or a time-of-flight approach.

We are developing a new method to obtain the position, orientation and shape of grains from polycrystalline samples without initial wavelength resolution needs. So far the technique has been validated for grain sizes in the range of hundreds of microns and samples up to 2 cm diameter. The novelty of the reconstruction approach, enabling white beam measurements, lies in the use of a forward model to predict diffraction patterns being fitted to the position of the experimental diffraction spots and hence revealing number, position and orientation of individual grains. This is very different from common energy resolved crystal diffraction where the wavelength is typically used to solve Bragg's law.

The approach utilizes the knowledge of the beamline setup and crystal composition to predict the geometry of the Laue pattern measured during the experiment on the diffractometer. The code compares and optimizes the predicted pattern with respect to the measured diffraction patterns concerning grain positions and orientations until the match is satisfactory. As a result the positions and orientations of contributing grains are retrieved. The process of search and optimization is first done for individual grains and repeated until no additional grains are found with statistically significant anymore.

Experiments were performed at the E11 thermal beamline of the BERII neutron source at the Helmholtz Zentrum Berlin in Germany. The detection system of the installed instrument FALCON is a scintillator-camera based neutron imaging set of two detectors with a field of view of 400x400 mm each and a pixel sizes of 100 µm. For our experiments we typically set one detector in forward diffraction direction and the other one in backward diffraction mode.

The current version of the code has already been proven capable of indexing 18 grains from an annealed α-Fe cylindrical sample with 5 mm diameter and 5 mm height. In addition 8 grains have been indexed from a YBaCuFeO5 multiferroic oligo-crystal using only forward diffraction data.

With the current version of our code white beam Laue neutron multi-grain indexing becomes possible. However, this is only the first step towards retrieving a full 3D grain map including the morphology. Our next steps are focused on advancing these capabilities, finding new applications and bringing the code to a user-friendly level.

Primary author(s) : Mr RAVENTOS, Marc (Paul Scherrer Institut)

Co-author(s) : Dr MEDARDE, Marisa (Paul Scherrer Institut); Dr TOVAR, Michael (Helmholtz Zentrum Berlin); Dr SHANG, Tian (Paul Scherrer institut); Dr STROBL, Markus; Dr GRÜNZWEIG, Christian; LEHMANN, Eberhard (Paul Scherrer Institut); Prof. SCHMIDT, Søren (Technical University of Denmark)

Presenter(s) : Mr RAVENTOS, Marc (Paul Scherrer Institut)

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