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Unprecedented Accessibility



GrainMapper3D White Paper

with Lab-based DCT Advanced Acquisition







Projections geometry

 $L_{SS} < L_{SD}$



Working Principles of Lab-based DCT

A Lab-based DCT experiment consists of two scans:

- **Absorption CT**, where contrast is gained by the x-ray attenuation coefficients of materials, enabling a 3D reconstruction of phase differences, *i.e.* features like cracks, defects and inclusions. Projections are collected through a 360° rotation of the sample illuminated by the direct beam and used to define the sample outline.
- DCT, where contrast is gained by Bragg diffraction of individual grains inside the sample, enabling a 3D reconstruction of crystallographic orientations and shapes of individual grains, *i.e.* a 3D space-filling grain map. Projections are collected while the sample is rotated (and translated for advanced acquisition), to cover the sample region of interest (ROI) uniformly. For DCT the divergent, polychromatic x-ray beam is constrained by an aperture to illuminate a volume in the sample defined by the field of view (FOV). A beamstop after the sample blocks transmitted x-rays on the detector to increase sensitivity towards the substantially weaker diffraction signals.

The setup in Laue focusing geometry, exploits that for a divergent point source of x-rays, a grain diffracts such that the x-rays are focused one-dimensionally in the Laue focal plane at a sample-detector distance (L_{SD}) equal to the source-sample distance (L_{SS}) . The typical working distance is 12-20 mm. A high-resolution detector is placed at this distance, and the Laue focusing effect makes the diffracted signals appear as line-shaped spots optimizing the signal-to-noise ratio, minimizing spot overlap and allowing to record larger volumes or more grains.

The projection geometry setup, employs a flat panel detector at a typical working distance of 200 mm < L_{SD} < 550 mm while the source-sample distance is kept significantly shorter, typically 10 mm < L_{SS} < 100 mm. These working distances and the detector efficiency offer some potential advantages for larger samples. The projection geometry, $L_{SS} < L_{SD}$, means that the shape of the grains is projected into the shape of the diffractions spots as can be seen on the schematic.



advanced acquisition

Enabling Advanced DCT Acquisition

The recent GrainMapper3D v3.0 took lab-based DCT to the next level of throughput, versatility and representative volume mapping. This was done by introducing three advanced scanning schemes - Helical Phyllotaxis, Helical Phyllotaxis Raster and Helical Phyllotaxis HART, aimed towards much larger sample volumes and varied sample geometries, and by the release of CrystalCTTM, a dedicated microCT system for 3D grain mapping.

GrainMapper3D v3.1 released a major enhancement in the reconstruction algorithm and the introduction of reconstruction boosting. The benchmark testing results show a 3.4× speed up in reconstruction time compared to v3.0 and a $24 \times$ speed up compared to v2.0.

This basically means that the reconstruction times for conventional and advanced DCT scans should now be counted in hours and days, respectively, rather than in days and weeks.

Along the path of advanced data acquisition, the current GrainMapper3D v3.2 implementation features a further step in enhancing the users' capability to process large datasets. By advanced memory handling, more than 10,000 DCT projections can now be accommodated with the RAM freed up for 3D grain map reconstruction.

With significantly enhanced versatility built into each new version, the GrainMapper3D reconstruction engine for lab-based DCT continues to expand capabilities and enables addressing a widening range of scientific and engineering problems.





DCT Acquisition Wizard The dedicated advanced acquisition user interface

DCT Data Acquisition Overview

Conventional DCT data collection assumes that the sample ROI is fully illuminated by the aperture FOV for all rotation angles. This puts a major constraint on the types of samples that can be imaged, often requiring researchers to modify the sample to a smaller cylindrical or "matchstick" sized specimen. In order to accommodate analysis of more complex, real sample geometries with reduced sample preparation time, new advanced scanning modes have been introduced.

Advanced scanning of samples that do not fulfil the criteria for a conventional DCT scan can be performed with the DCT Acquisition Wizard. The advanced scanning schemes allow seamless collection of DCT data for larger, irregularly shaped sample volumes with a uniform sample illumination both angularly and spatially. This is done by combining complex rotational and translational sample stage movements to enable optimal and efficient collection of DCT data. Reconstruction of the corresponding data is equally seamless, simultaneously using all data to reconstruct the full illuminated volume without the need for stitching of data subsets or sample sub-volumes.

The three advanced scanning schemes offered by the DCT Acquisition Wizard are [5]:

- Helical Phyllotaxis This scan covers samples with a vertical extent larger than the illuminating x-ray beam height by means of a golden angle rotation of ~137.5° combined with a vertical translation on the order of \sim 1–5 µm between consecutive projections.
- Helical Phyllotaxis Raster This scan combines the sample rotation and vertical translation of the helical phyllotaxis scan with a fixed number of horizontal translation steps for all projection angles to cover samples wider than the FOV.
- Helical Phyllotaxis HART (high-aspect ratio tomography) - This scan mode is tailored to specimens with plate-like geometries. It is similar to the helical phyllotaxis raster scan, except the number of horizontal steps is adapted to tightly fit the ROI at every projection angle.

DCT Advanced Acquisition Implementation

The DCT acquisition wizard is the dedicated advanced acquisition user interface allowing seamless collection of DCT data from samples with a ROI that exceeds the aperture FOV. From GrainMapper3D v.3.2 it also allows the user to import and run absorption recipes from Scout-and-Scan. Hence, the entire DCT experiment, from the acquisition of both the DCT and absorption data to the automatic reconstruction of the latter, can be performed at once from within the wizard.

Acquisition Settings are the parameters determined to give the best diffraction patterns during the sample screening.

Region of Interest (ROI) can be defined either by dragging rectangles on top of the 0° and -90° absorption projections to cover the desired sample ROI, or by typing the ROI limits. The FOV coverage corresponding to the selected acquisition settings and strategy (displayed as partly overlapping red boxes) will update accordingly.

Acquisition Strategy allows the user to:

- Choose one the three advanced scanning schemes.
- Provide the number of projections depending on the detector working distance - a tooltip is available.
- Define whether the sample cross section is circular or rectangular as this affects the required number of horizontal steps in a Helical Phyllotaxis Raster scan.
- Reduce sample rotations to scan faster at the potential expense of poor illumination at the bottom of the ROI if the scan is aborted.

Reference Collection axes and intervals can be defined by the user. When performing scans exceeding 400 projections or lasting more than 12h, collecting multiple references may improve data quality.



Helical Phyllotaxis scanning scheme handles sample with width fitted in the aperture FOV. Large sample volume and grain statistic are achieved by covering extended sample height along the rotation axis.

Helical Phyllotaxis Raster





Cu coil, cubic , Ø~18×36 mm (Dr. J. Guo, Chongqing Univ.)



316L steel, cubic, 4.4×0.7×0.7 mm (Prof. G. Winther, DTU)

Helical Phyllotaxis Raster scanning scheme handles sample with width larger than the aperture FOV. Samples with irregular shapes and extended dimensions can be readily defined in the scanning ROI.



Helical Phyllotaxis HART





Electrical steel, cubic, 40×20×0.4 mm (Prof. P. Yang, USTB)



AA5657, cubic, 4×2×0.6 mm (Dr. R. Sanders, Novelis)

Helical Phyllotaxis HART scanning scheme is specialized for sample with a high aspect ratio geometry. The adaptive sample translation efficiently collects data accommodating varying sample dimensions.

