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# 3D Mapping Grain Morphology and Grain Orientations by Laboratory Diffraction Contrast Tomography

Leah Lavery[1], Nicolas Gueninchault[2], Hrishikesh Bale[1], Christian Holzner[1], Florian Bachmann[2] and Erik Lauridsen[2]

[1.] Carl Zeiss X-ray Microscopy, Pleasanton, CA, United States
[2.] Xnovo Technology, Køge, Denmark

Determining crystallographic microstructure of a given material in 2D can be challenging. Further extending such an investigation to 3D on meaningful volumes (and without sample sectioning) can be even more so. Yet reaching this insight holds tremendous value for 3D materials science since the properties and performance of materials are intricately linked to microstructural morphology including crystal orientation. Achieving direct visualization of 3D crystallographic structure is possible by diffraction contrast tomography (DCT), albeit only available at a limited number of synchrotron X-ray facilities around the world. Recent developments, however, have made DCT possible on a 3D X-ray microscope with a laboratory source.

The introduction of diffraction contrast tomography as an additional imaging modality on the ZEISS Xradia 520 Versa laboratory 3D X-ray microscope has opened up a whole new range of possibilities for studies of the effect of 3D crystallography on materials performance. The capability to link directly the crystallographic and grain microstructure information with that obtained via conventional absorption or phase contrast imaging, non-destructively in three-dimensions and all in the laboratory, creates a powerful and easy to access tool [1-2]. Using a polychromatic X-ray source, laboratory diffraction contrast tomography technique (LabDCT) takes advantage of the Laue focusing effect, improving diffraction signal detection and allows handling of many and closely spaced reflections.

Additionally, LabDCT opens the way for routine, non-destructive and time-evolution studies of grain structure to complement electron backscatter diffraction (EBSD). Crystallographic imaging is performed routinely by EBSD for metallurgy, functional ceramics, semi-conductors, geology etc. However, EBSD is an end-point characterization technique and prevents any investigation of microstructure evolution when subject to either mechanical, thermal or other environmental conditions.

Combination of grain information with microstructural features such as cracks, porosity, and inclusions all derived non-destructively in 3D presents new insights for materials characterization of damage, deformation and growth mechanisms. Furthermore, 3D grain orientation data is a valuable input into multi-scale, multi-layered modeling platforms that can virtually evaluate mechanical properties to produce high fidelity simulation results.

Recent developments of the LabDCT technique have extended its capabilities to include full reconstruction of the 3D grain structure including both grain morphology and crystallographic orientation, thereby making the LabDCT more comparable to conventional 3D-EBSD data – while still supporting 4D time dependent studies. We will present a selection of results of LabDCT with particularly emphasis on its non-destructive operation, demonstrated through 4D evolutionary studies obtained by repeating the imaging procedure numerous times on the same sample. We will discuss the

boundary conditions of the current implementation, point to the future of the technique and discuss ways in which this can be correlatively coupled to related techniques for a better understanding of materials structure evolution in 3D.

References:

[1] SA McDonald et al. Scientific Reports **5**, (2015) 14665.
[2] C Holzner et al., Micros. Today, **24**, **4**, (2016) p. 34..

**Figure 1.** Schematic of the laboratory diffraction contrast tomography (LabDCT) implementation on the ZEISS Xradia 520 Versa X-ray microscope.

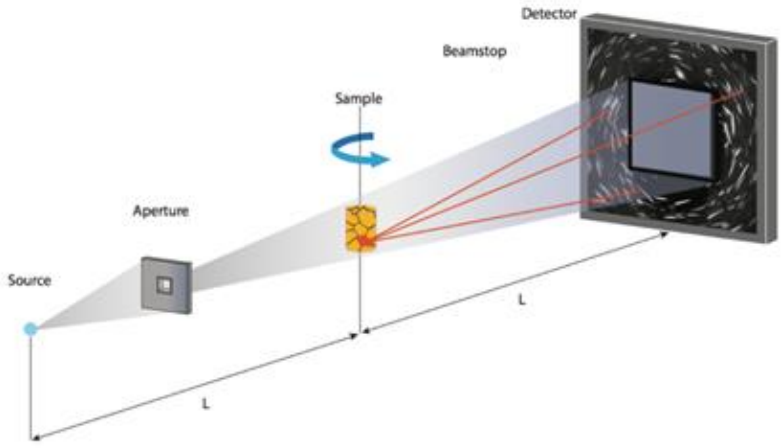
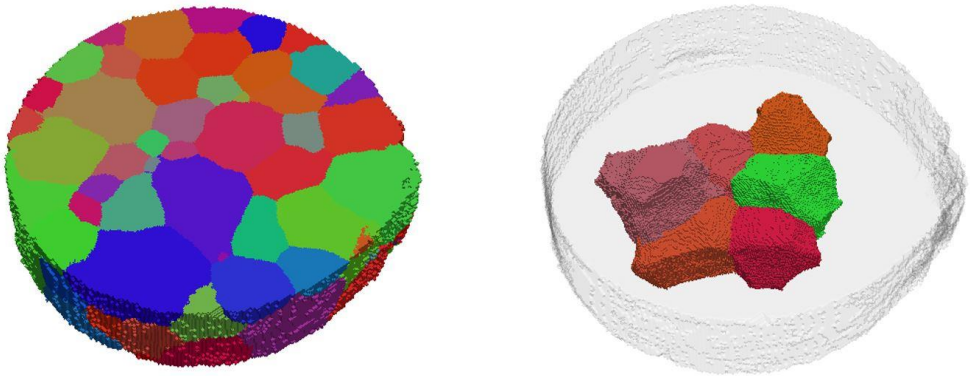



**Figure 2.** Figure 2 (a) 3D reconstruction of an AlCu polycrystalline sample. Grains colors are function of their orientation (IPF coloring). (b) Visualization of a cluster of 6 grains embedded in the bulk of the sample (same color code)



(a) (b)

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