3D Neutron Diffraction

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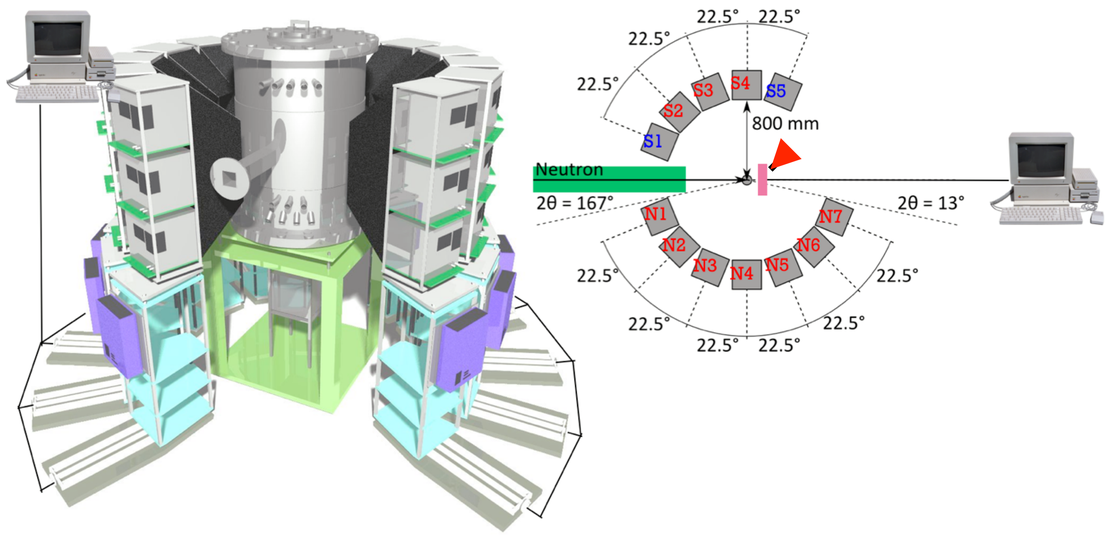
3D Neutron Diffraction (3DND) is a new technique to study shape and orientation of the individual grains composing polycrystalline samples. 3DND enables non-destructive 3D grain mapping of mm- to cm-sized samples, covering larger sample volumes than existing X-ray methods like 3D X-Ray Diffraction (3DXRD) [1]. 3DND would complement 3DXRD, providing information on mechanical evolution, stress/strain states, recrystallization and allowing in-situ studies under extreme conditions.
We are developing the algorithms for the 3D reconstruction based on datasets collected at BL18 (J-PARC), ENGIN-X (ISIS), ICON (PSI), and virtual experiments done using McStas [2].
These are the approaches we used:

1. Laue diffraction, with wide bandwidth and a near-field diffraction detector in backscattering mode.
2. Time-of-flight diffraction, with transmission data collected by a near-field detector and diffraction data collected by far-field ones.

Time-of-flight 3DND

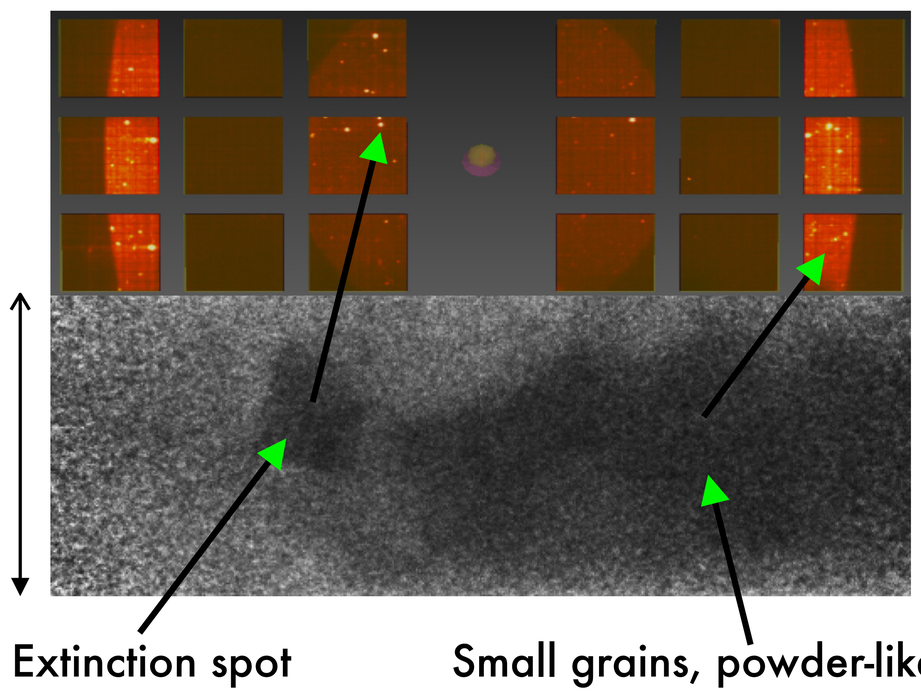
In June 2014 at BL18 we analysed an Armco Iron sample (length: 5 cm, diameter: 1 cm, 99.8% purity), prepared to contain mm-sized grains. The sample was scanned over 180deg in 3deg steps, acquisition time per projection ~1h.



Setup used at BL18. Data were acquired simultaneously by near- (indicated by red arrow) and far-field detectors.

Near- field (NF) detector	MCP detector, 28x28mm^2 1200 fr/s, pixel size 55μm Use: shape of the grains
Far-field (FF) detectors	36 det, each 256x256mm^2 Pixel size 4 mm, Q: 0.6-30.7 Use: orientation of the grains

Data collected by near- and far-field detectors at BL18, Fe sample



Data analysis

Data acquired simultaneously by NF and FF detectors

FF
- CM of diff spots [3]
- $\vec{G}_i^r \longrightarrow \{\vec{G}_i^r\}_j, U_j$ [4]
- FF covers 2.3 st $\{\vec{G}^r_{meas,i}\}_j \subset \{\vec{G}^r_{calc,i}\}_j$

NF
- Binarise, locate [5] extinction spots

Sync diff, ext spots via ToF (λ)

U_j + 3D grain shape = 3D map

3DND is a nondestructive technique to investigate, in a reasonable time frame, the 3D structure of mm- to cm-sized polycrystalline samples. It completes existing X-ray techniques, enabling to use complex sample environments. Combined with a time-of-flight beam, 3DND can be used to study samples composed by a large number of grains. Once the reconstruction algorithm is fully implemented, we will apply 3DND to study shape memory alloys.

[1] HF Poulsen el al. (2001). [2] K Lefmann and K Nielsen (1999). [3] T Ohhara et al (2009). [4] S Schmidt (2014). [5] W Ludwig et al (2008)

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