## Technical University of Denmark



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# 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.

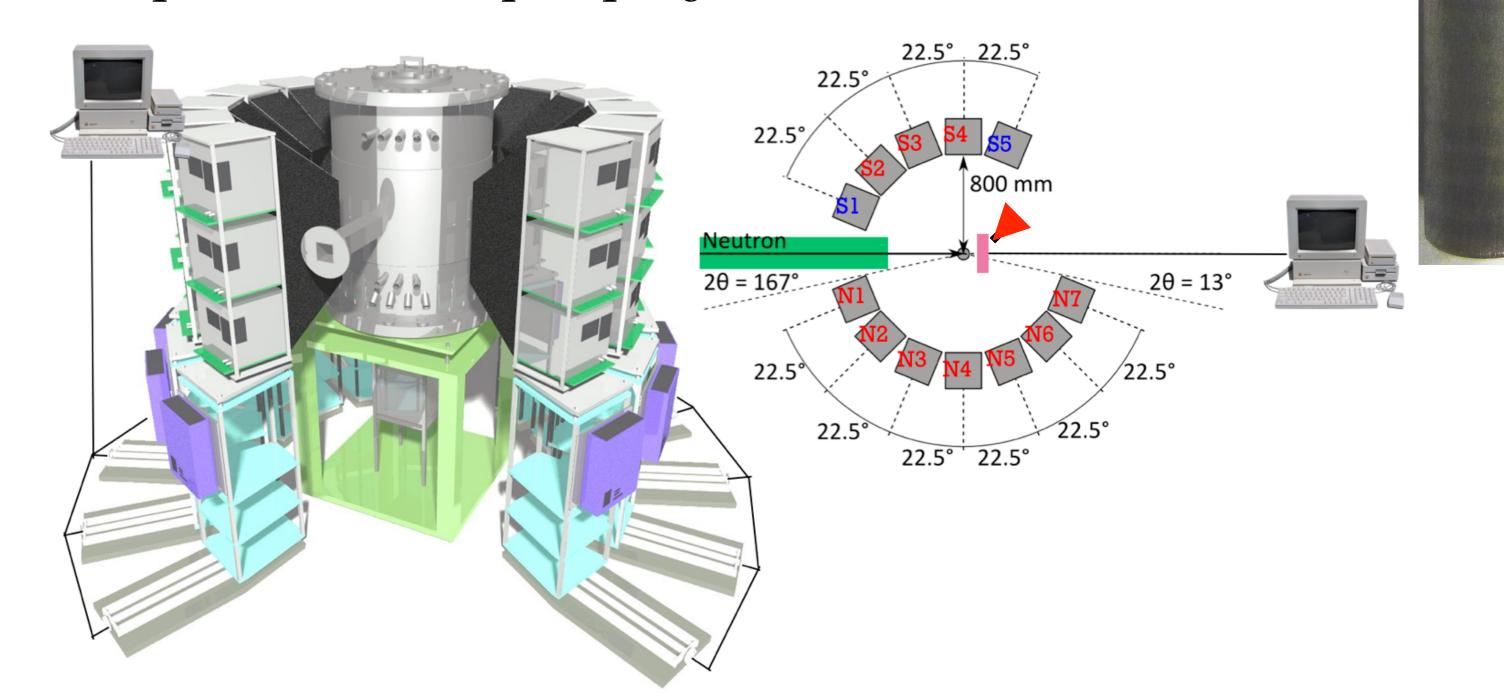
We are developing the algorithms for the 3D reconstruction based on datasets collected at BL18 (J-PARC), ENGIN-X (ISIS), ICON (PSI), and virtual experiments done using McStas [2].

These are the approaches we used:

- 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

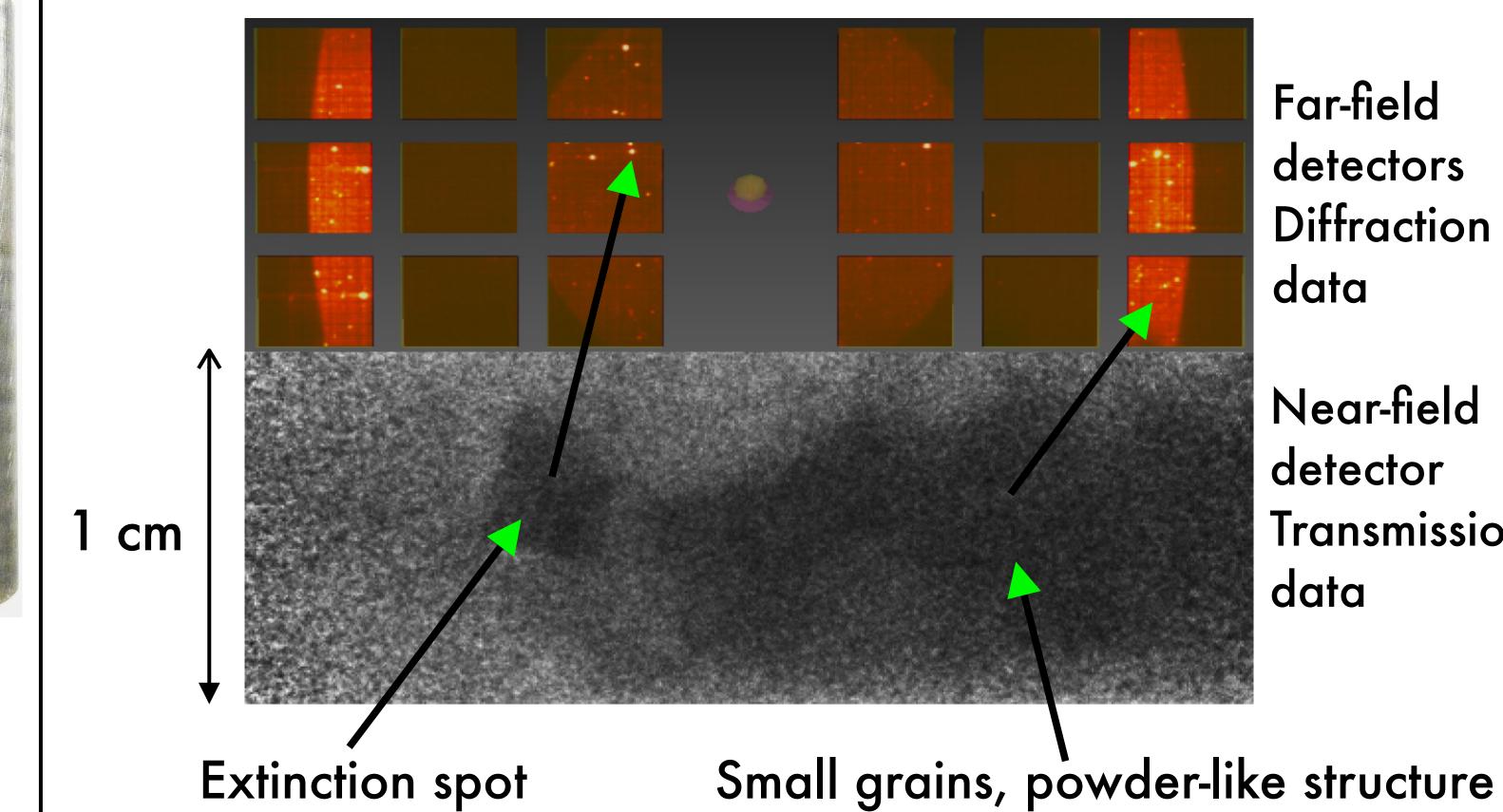
In June 2014 at BL18 we analysed an Armco Iron sample (length: 5 cm, diameter: 1 cm, 99.8%) purity), prepared to contain mm-sized grains. The sample was scanned over 180deg in 3deg steps, acquisition time per projection ~1h.



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

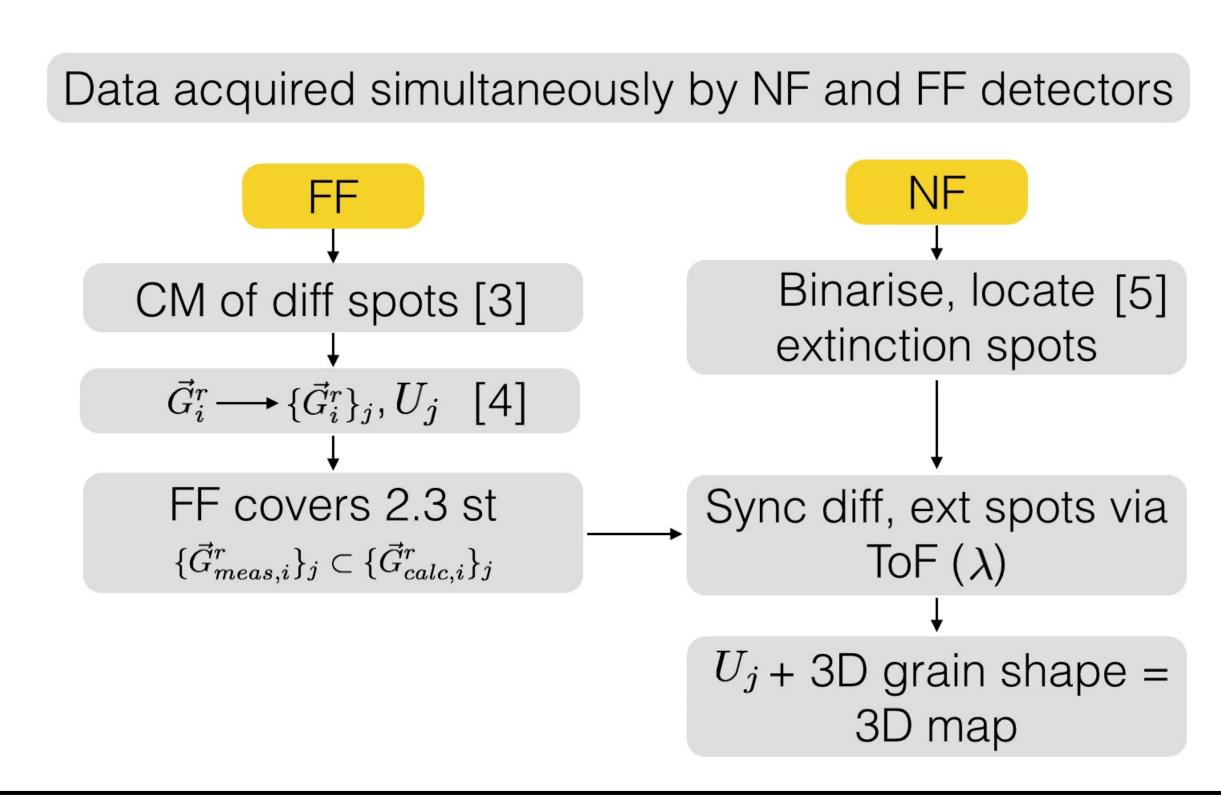
Near- field (NF) detector	MCP detector, $28 \times 28 mm^2$ 1200 fr/s, pixel size $55 \mu m$ Use: shape of the grains
Far-field (FF) detectors	36 det, each $256 \times 256 mm^2$ Pixel size 4 mm, Q: 0.6-30.7 Use: orientation of the grains

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



Transmission

## Data analysis



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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