3D Neutron Diffraction

Cereser, Alberto; Strobl, M.; Hall, S.; Steuwer, A.; Tremsin, A.; Bergbäck Knudsen, Erik; Willendrup, Peter Kjær; Kiyanagi, R.; Shinohara, T.; Schmidt, Søren

Publication date:
2015

Document Version
Publisher's PDF, also known as Version of record

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A Cereser[1,2], M Strobl[2], S Hall[2,3], A Steuwer[4], A Tremsin[5], EB Knudsen[1], P Willendrup[1], R Kiyanagi[6], T Shinohara[6] and S Schmidt[1]

[1]Technical University of Denmark - [2]ESS-AB - [3]Lund University - [4]Business Region Skåne - [5]University of California at Berkeley - [6]J-PARC

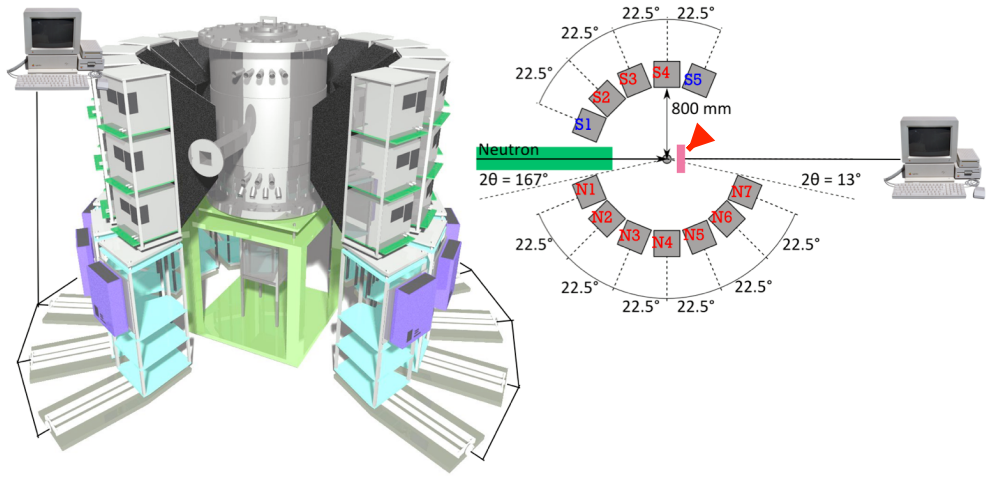
3D Neutron Diffraction (3DND) is a new technique to study shape and orientation of the individual grains composing polycrystalline samples. 3DND enables non-destructive 3D grain mapping of mm- to cm-sized samples that is not possible using other techniques.

Technique	Sample size
TEM	<100nm
X-ray techniques like 3D X-ray Diff. [1]	100nm to 1mm
3DND	1mm to 1cm

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].

Time-of-flight 3DND

In June 2014 at BL18 we analysed an Armco Iron sample (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.

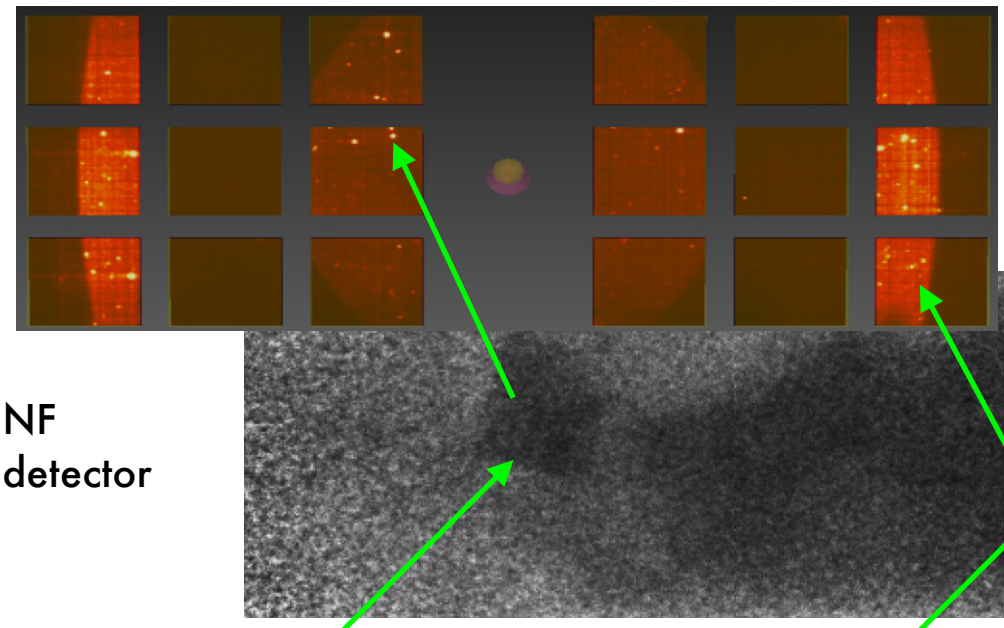
Near- field detector	MCP detector, 28x28mm^2 1200 fr/s, pixel size 55μm Use: shape of the grains
Far-field detectors	36 det, each 256x256mm^2 Pixel size 4 mm, Q: 0.6-30.7 Use: orientation of the grains

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



FF detector

NF detector

Extinction spot

Small grains, powder-like structure

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

Alberto Cereser - PhD student at the Technical University of Denmark.
alcer@fysik.dtu.dk