（ ※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。 ）

CROSS TOKAI **Experimental Report** J-PARC	承認日 Date of Approval 2016/05/09 承認者 Approver Takashi Ohhara 提出日 Date of Report 2016/05/09
課題番号 Project No. 2014B0132 実験課題名 Title of experiment Time-of-flight 3D neutron diffraction for multigrain crystallography 実験責任者名 Name of principal investigator Soeren Schmidt 所属 Affiliation Technical University of Denmark	装置責任者 Name of Instrument scientist Takashi Ohhara 装置名 Name of Instrument/（BL No.） SENJU (BL18) 実施日 Date of Experiment Feb 23 2015 – March 1 2016

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）

Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

These are the samples investigated during the experiment:

1. Iron rod (100% Fe) with a diameter 10 mm and 50 mm height;
2. Iron based Meteorite, round shape with roughly 10 mm diameter.
3. Co-Ga-Ni shape memory alloy, rectangular shape, 4x4x8 mm^3

2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）

Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

3D neutron Diffraction (3DND) is a novel diffraction based imaging technique for non-destructive characterization of the individual grains in polycrystalline materials. Project 2014B0132 was divided into two periods: Feb-March 2015 and Feb 2016. In the first period the Iron rod was measured both SENJU and the MCP imaging detector. With the 3DND reconstruction method starting out by processing the MCP data, 119 grains where located in the sample, see Figure 1.

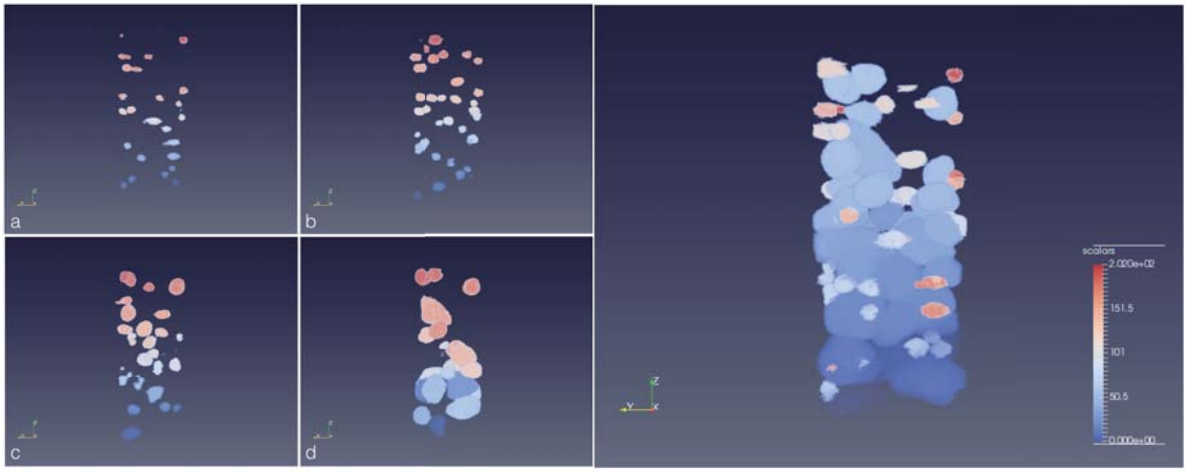

Figure 1: Reconstructed position and shape of the 119 grains in the Iron rod. *Left*: in a), b), c) and d) divided into 4 groups according to volume. *Right*: all grains are shown.

The reconstruction procedure is shown in Figure 2. The individual extinction spots are located on the MCP detector, grouped and reconstructed into a 3D grain shape using back-projection methods.

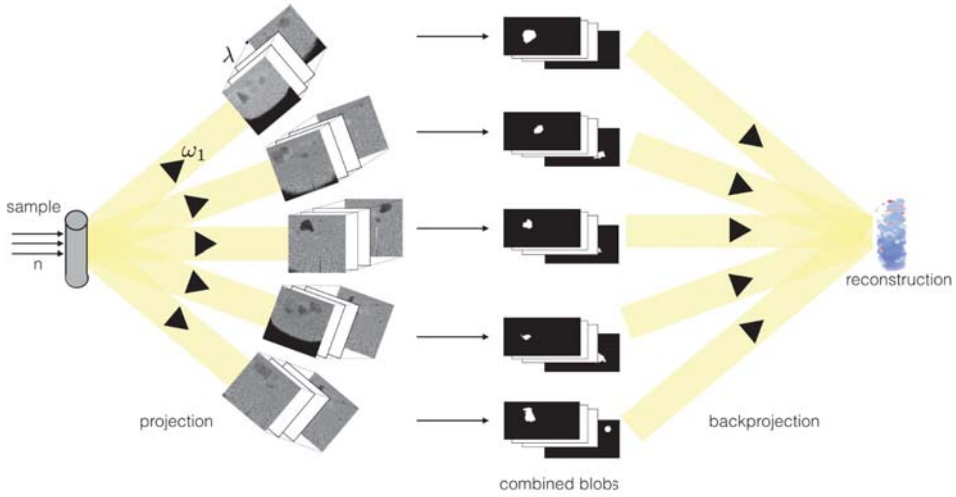

Figure 2: Reconstruction procedure for MCP data.

With 3DND two indexing procedures are available, working with SENJU and MCP data, respectively. As an example from the MCP data, the sample rotations ω and wavelengths λ of the grouped extinction spots from one grain is shown in Figure 3, *left*. The superimposed lines correspond to the predicted orientation from the indexing procedure. Each line in the plot represents an indexed atomic plane, hkl. For the SENJU data, the StarGazer software produces scatter vectors, which can be indexed by the GrainSpotter program [1]. In the Iron rod data, 205 grains where indexed, see Figure 3, *right*. It has been verified that the two indexing procedures agrees, although additional orientations can be retrieved from the SENJU data. The second route where the SENJU grains seed the MCP reconstruction is currently being investigated and should lead to additional grains being reconstructed. With this work 3DND feasibility studies will be completed.

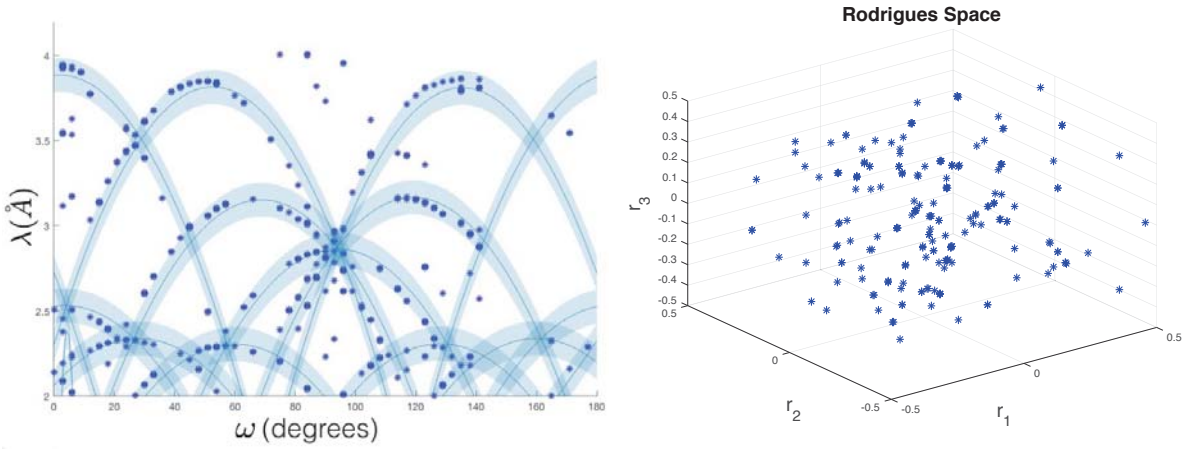

Figure 3: *Left*: Indexing of MCP data (ω, λ) for a single grain. *Right*: Multi-crystal indexing using StarGazer and GrainSpotter. The 205 crystallographic orientations are represented in the Rodrigues space.

In the second period (Feb 2016) the following samples where measured: Shape Memory Alloy (SMA) Co-Ni-Ga and an Iron based Meteorite. Preliminary studies show that the Meteorite has large mosaicity. An example of a transmission image is shown in Figure 4. A Full 3D reconstruction of the complex microstructure is being perused using next generation 3DND software. For the Co-Ni-Ga sample the Austenite to Martensite transformation was studied through tensile deformation.

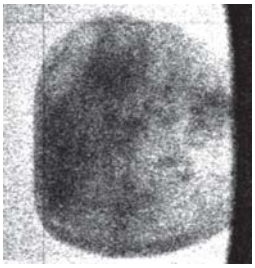

Figure 4: Meteorite

References

[1] Schmidt, S. (2014). J. Appl. Cryst (2014), **47**, 276-284.