2 Cerny R. and Filinchuk Y. Complex inorganic structures from powder diffraction: case of tetrahydroborates of light metals. *Z. Kristallographie* 226(2011)882-891, dx.doi.org/10.1524/zkri.2011.1409

3 Schouwink P., Smrcok L. and Cerny R. The role of the Li^+ node in the Li-BH_4 substructure of double-cation tetrahydroborates. *Acta Cryst. B*, 70 (2014) 871-878, dx.doi.org/10.1107/S2052520614017351

Keywords: powder diffraction, metal hydride

MS13-O2 Decomposing electron diffraction signals from multi-component microstructures

Alex Eggeman[1], Duncan Johnstone[1], Robert Krakow[1], Jing Hu[2], Sergio Lozano-Perez[2], Chris Grosvenor[2], Paul Midgley[1]

1. University of Cambridge
2. University of Oxford

email: ase25@cam.ac.uk

Recent development of spatially resolved (scanning) diffraction in the TEM offers the capacity to study phase and crystallographic orientation with nanometre spatial resolution [1]. However despite the relatively small sample thickness in TEM there is still the possibility of two or more distinct phases contributing to a diffraction pattern in the dataset. One solution is to use multivariate statistical analysis [2] approaches to separate out the unique diffraction signals (or components) from the different phases in the system. This can provide useful information about the general diffraction signal from a phase by removing the small variations in diffraction patterns arising from local variations in the sample thickness or bending, allowing a more robust pattern match for regions of the same structure and orientation. It can also provide a robust method for localising phases within a scanned area allowing completely embedded phases to be separated from within the scanned diffraction data.

This approach will be shown through a number of different studies, starting with the analysis of twinning and epitaxial growth in semiconductor nanowires and continuing through to the separation of phases in partially oxidised zirconium, leading to confirmation of the existence of a proposed intermediate oxide [3] structure found at the metal-metal oxide interface.

The onward development of this approach is to isolate and track individual phases through a tilt-series of measurements, allowing tomographic reconstruction of the individual phases combined with understanding of the complete 3-D orientation relationships within the microstructure. This will be shown through a study on a nickel superalloy sample highlighting the coherent interface between matrix and precipitates within the microstructure.

[1] E. F. Rauch, *et al.*, Microscopy and Analysis **22**, (2008), S5-S8.

[2] F. de la Peña. *et al*. Ultramicroscopy **111**, (2011), 169-176.

[3] J Hu et al. Micron **69,** (2015), 35–42

Keywords: Scanning electron diffraction, principle component analysis, orientation tomography