MS30-P02 | Absolute structure assignment through interplay of X-ray diffraction and EBSD

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Various classes of compounds have gained strong interest in solid state sciences with respect to particular properties which are linked to the absence of a center of symmetry in the crystal structure. A prominent case are compounds adopting the B20 or FeSi type structure, respectively. Reliable characterisation of particular physical properties requires single crystals of adequate size and quality. However, it is of utmost importance to assure that crystals under investigation are single domain, i.e. twins by inversion have to be excluded rigorously. The universal approach introduced by the late Howard Flack is well established though has its weaknesses in cases of very simple but highly symmetric structures. For larger single crystals there exists no reliable method to obtain a proper set of Bragg intensities.

This contribution presents an approach in confirming the absolute structure of a larger single crystal via a combination of X-ray diffraction and Electron Backscatter Diffraction (EBSD) methods. A small but representative piece is extracted from the large crystal using Xe-ions in a Focused Ion Beam (FIB) micromachining setup. This particular crystallite allows for an entire structure determination including the assignment of the absolute structure. Finally, this structural model is used to map the entire crystal applying EBSD methods at high spatial resolution.