

Minutes for the diffraction workshop at DMSC, April 7<sup>th</sup> on data analysis from Sonja Holm

Mantid at MLZ

2D unit conversion software, is in development.

Users need graphical interface. Good experience at TOFTOF.

Basic GUI of Mantid is going to be redone. It is a known issue.

PDF measurements corrections is not core requirement but should be made. Background subtraction is essential.

We need 1D data sets. From STAP.

Data smoothing and interpolation. To make nice pictures. For vanadium normalization.

Is every detector treated by itself? Resolution, efficiency, ... Yes, it is in Mantid.

Amount of data is manageable at the moment? It will maybe not scale in a useful manner.

Data analysis software for powder and single crystal

The budget is limited; basic analysis will be available

Live analysis. Remote access.

Not covered; co-analysis, portability

Why use FULLPROF? It is free.

Jana will not be sustained

It is for the large-scale facilities should not let software die.

You should decide the Rietveld software for ESS.

Python interface for FULLPROF. It will be curated.

Jana is a must have. For single crystals Jana is best.

FULLPROF for powder diffraction.

The refinement process is very different for the two programs

You have many different opinions.

We have to curate the software and FULLPROF needs is urgently. Not all programs can be maintained at ESS, but they can be used.

A document for all the programs should be written; what can that do, where are they in five years, what is the user community...

Polarization analysis; we have no choice.

FULLPROF library is valuable.

All facilities need to come up with a strategy together. For EU funding in 2020.

User-friendliness

People from DMSC should be involved in experiments.

More types of users will need to be accommodated.

Virtual experiment for estimates of measuring times.

The instrument teams should maintain up to date McStas models of the instrument.

There will more more diffractometers than what can be checked manually.

The use of beamtime should be optimized so that sample changes can be done outside the cave.

Robot sample changer is an issue for software development.

New science needs new methods and software is essential. E.g. the development of diffraction tomography.

DMCS should coordinate development of software from partners. An approval of the software project from DMCS could help in funding process. The software should be in useful language that is maintainable.