The ternary instrument: data analysis and software development, issues for DMSC

In the previous sections of the proposal, we presented full simulations of the instrument up to data acquisition. There is a series of challenges to assure that the high counting performance of MAGiC will also be transformed into successful publication output. Following acquisition, a complex data treatment has to be carried out in order to extract the physics from the experimental data. We present here a list of data manipulation and/or correction to execute. Most of this work has been presented[1] and incorporated in MANTID by the joint effort of IPNS, ISIS and SNS IT groups.

Data integration:

- The experiment can be made as a classical Laue-TOF mode or preferably, in a continuous rotation mode. In the latter case the instrument will operate as a multi-monochromatic instrument.
- The first operation is to convert the event data into the instrument Q-space. An adaptative mesh refinement is then performed, sorting density voxels and allowing fast and efficient peak search.
- A fast Fourier Transform algorithm is applied on the detected peaks in order to refine the orientation matrix (UB matrix). A list of matching unit cells is proposed to the scientist to convert the event data into the sample Q-space.
- Each of the detected peaks is integrated. Various algorithms, like spherical, ellipsoidal, cylindrical or 1D shape refinement, have been developed and recently incorporated in MANTID (ref 67). All of them are equally performing, the simplest one, spherical integration, being one of the fastest.
- A list of hkl is then generated with the corresponding structure factors, wavelength, and parameters necessary for extinction correction.

Data correction and analysis:

- Absorption routine is already integrated into MANTID and is well performing.
- Extinction and incident spectrum inhomogeneity: Bragg extinction effects from various materials in the incident beam path may affect the incident spectrum and need to be taken into account for the refinement based on (hkl, F, wavelength) sets. The wavelength dependence of extinction correction has been recently introduced in JANA2006 to deal with Laue-TOF data. Extinction is a known problem from the Laue-instruments (Vivaldi and Cyclops). The continuous rotation combined with the TOF-Laue mode of MAGiC will allow spotting any irregularities by too weak reflectivities in a λ-dependent Bragg-profile. Indeed, each Bragg-profile has to match the defined flux curve and each dip irregularity can be rejected.

Expected R-factors: Actual R-factors on TOPAZ at SNS are as low as 3 to 4% and comparable to best monochromatic instruments at reactor facilities. Based on the contributions of both SNS and ISIS to MANTiD and the strong involvement of DMSC at ESS, further prospects are very good. We are confident that such R-factor will be obtained on MAGiC.

There has been a lot of progress within the development of MANTiD. For Laue refinements, it still needs adaption to studies of incommensurate structures, which are particularly prominent in magnetism, and one may expect to see further efforts to make it faster and more user-friendly.

Software for fast 3D visualization is developing. One example[2] becoming available creates a 3D transparent picture, which can be rotated in (user) real-time, providing the desirable fast view and possible first judgment of the data and its quality. The crystal orientation (UB-matrix) can be determined by superimposing Bragg peaks sensitively by the user's eye. The code will be open source and compatible with MANTID for further analysis

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[1] **Arthur J. Schultz *et al*, Journal of Applied Crystallography** 47, **915-921 (2014)**

[2] Florian Rhiem, Master thesis, FH Aachen, http://iffwww.iff.kfa-juelich.de/pub/doc/Masterarbeit_FlorianRhiem.pdf