*Mantid Roadmap for Single Crystal Diffraction*

* Is development progressing as you would like?
* What are your short, mid and long-term requirements in Single Crystal Diffraction?

**Short, mid-term requirements**

Live data reduction capability with User Interface and interactive 3D graphics display for indexing and integrating single crystal diffraction data while measuring [Functionality available in ISAW, See details in [2017 meeting report](https://github.com/mantidproject/documents/blob/master/Presentations/DevMeetings/2017-06/DiffractionReport_2017.pptx?raw=true)].

3D Graphic User Interface for indexing modulated structures.

Need tools for visualization and subtraction for reducing diffuse scattering data.

Consistent UB for different orientations.

Peak integration of twinned single crystal samples.

3D peak profile fitting and resolution deconvolution. High quality plot of MD volume.

Data normalization and absorption correction for different shape crystals.

Better calibration algorithms in mantid for single crystal TOF instruments.

Listed by SNS Instruments:

CORELLI: Need a user-friendly interface for peak integration and need to get it CORRECT. This is a very manual process now. Need tools for visualization and subtraction for reducing diffuse scattering data, no mature analysis options. Both Mantid and Nexpy provide interfaces for visualization with limited functions. Improve 3D PDF for publishable reduced data. Complete Javeline for defect structure simulation and optimization. SCD order parameters Python scripts calling mantid algorithms. There is a python notebook interface but needs improvement.

TOPAZ: Need live data reduction capability with User Interface and interactive 3D graphics display for indexing and integrating single crystal diffraction data while measuring [Functionality available in ISAW EventViewer, but it has yet to be implemented in mantid]; Advanced software tools for reducing multi-dimensional single crystal data, including diffuse scattering in 3D Q space and Bragg peaks from quasicrystal as well as incommensurately modulated single crystal samples

ManDi: Lauenorm is an old program not optimized for multi detector arrays it should be replaced with a Mantid module. Input for autoreduction needs to be made easier (This is under active development)

IMAGINE: Lauegen is a legacy program and un-supported. Requires user friendly auto-indexing software. Strategy software is under development. Priority: 1) Auto-indexing, 2) Data reduction; 3) Absorption/wavelength/other corrections.

DEMAND: Data reduction from the large area detector is critical and in development. Auto-reduction function needs to be developed; User friendly output for order parameter and polarization measurements. 3D peak fitting and resolution deconvolution. High quality plot of MD volume.

**Mid, long-term requirements**: Auto reduction program like that in the commercial single crystal X-ray diffraction. Diffuse scattering modelling for the single crystal instrument suite at ORNL.

* Considering these requirements and likely staff effort available, prioritise your requirements. There will be a Mantid release late March (just before this Workshop), a subsequent releases spaced at roughly four monthly intervals.

*Mantid in General*

* What do you like about Mantid and what don’t you like?
* What works well and what doesn’t? What needs to be improved?
* What’s missing from Mantid?

Live data viewer User Interface with **interactive** 3D graphics display for indexing and integrating single crystal diffraction data while measuring

* Does Mantid have too much functionality … if so what would you remove?
* Are you happy with the model for interaction with the Mantid Development team? Is there sufficient support available?

We are happy with the model for interaction with the Mantid Development team. But we need more support for single crystal diffraction. Single crystal software work is done primary at ORNL. Vickie Lynch is retiring in June this year. No other site is actively working on single crystal software. Sam Jackson who has worked with Pascal at WISH has another job and is not in the project.

*New Mantid Workbench*

* What do you like about the new Workbench?
* What problems have you encountered with it?
* What are the obstacles that would prevent adoption by your group?
* What functionality needs to be added?

Workbench **need** SCD interface and sliceviewer for single crystal.

*Mantid and your User Community*

* What fraction of your users are making use of Mantid?
* How are your users making use of Mantid (e.g. reduction and/or analysis)?

Mostly reduction. Need Analysis tools for Bragg peak profile and diffuse scattering data

* What is limiting the take-up of Mantid in your science area and what needs to be done to develop its use?

*Other comments/feedback*

* Anything else?