Software requirements for diffraction (DREAM, MAGIC, BEER, HEIMDAL)

# Data Reduction and Visualization

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **DREAM** | | | **HEIMDAL** | | | **MAGIC** | | | **BEER** | | |
| M = Must, S = Should, N = Nice | M | S | N | M | S | N | M | S | N | M | S | N |
| **Reduction algorithms** |  |  |  |  |  |  | X |  |  |  |  |  |
| Normalize for detector efficiency | X |  |  | X |  |  | X |  |  |  |  |  |
| Normalize for incident beam spectrum | X |  |  | X |  |  | X |  |  |  |  |  |
| Correct for the Lorentz factor |  |  |  |  |  |  | X |  |  |  |  |  |
| Convert each event to Q-space, intensity, weight | X |  |  | X |  |  | X |  |  |  |  |  |
| *Find peaks* |  |  | X |  |  | X\* | X |  |  |  |  |  |
| *Find the best orientation matrices* |  |  | X |  |  | X\* | X |  |  |  |  |  |
| *Find possible propagation vectors (user input required to constrain lattice parameters)* |  |  | X |  |  |  | X |  |  |  |  |  |
| *Predict position of all relevant peaks* |  |  | X |  |  | X\* | X |  |  |  |  |  |
| *Integrate intensity (spherical, ellipse, cylindrical) for each polarization channels (up to 6)* |  |  | X |  |  |  | X |  |  |  |  |  |
| *Export to hkl, intensity, error, ASCII file* |  |  | X |  |  |  | X |  |  |  |  |  |
| Automatic reduction to 1D Rietveld in GSAS, TOPAS and FULLPROF formats | X |  |  | X |  |  |  |  |  |  |  |  |
| Reduction to PDF format | X |  |  | X |  |  |  |  |  |  |  |  |
| **CLI & GUI Interfaces** |  |  |  |  |  |  |  |  |  |  |  |  |
| Fully python scriptable, including SE | X |  |  | X |  |  | X |  |  |  |  |  |
| Advanced user GUI with all parameters available |  | X |  |  | X |  | X |  |  |  |  |  |
| Simple GUI with minimal input from users (execute full reduction and ask for user's confirmation about orientation and propagation vector) | X |  |  | X |  |  | X |  |  |  |  |  |
| Online logbook with report of machine status (unexpected shutdown) including a summary of the instrument configuration | X |  |  |  | X |  |  |  |  |  |  |  |
| **Data visualization** |  |  |  |  |  |  |  |  |  |  |  |  |
| Live Laue pattern visualization |  | X |  |  |  |  | X |  |  |  |  |  |
| 3D hkl space display |  |  | X |  |  |  | X |  |  |  |  |  |
| 2D hkl slice display |  | X |  |  |  |  | X |  |  |  |  |  |
| 1D hkl line display |  | X |  |  |  |  | X |  |  |  |  |  |
| ROI integrated intensity vs temp/field/pressure | X |  |  | X |  |  | X |  |  |  |  |  |
| 3D/2D/1D polarization channels sum/difference/ratio |  |  |  |  |  |  | X |  |  |  |  |  |
| Manipulation of raw 1D and 2D powder data: subtraction, multiplication, summation |  | X |  | X |  |  |  |  |  |  |  |  |
| Live plotting of 1D powder data as a function of temperature, field, pressure for in-situ measurements | X |  |  | X |  |  |  |  |  |  |  |  |
| Incident beam spectrum | X |  |  |  | X |  |  |  |  |  |  |  |
| Display of the reduced data on the instrument website, for remote monitoring | X |  |  |  | X |  |  |  |  |  |  |  |
| Visualization of full detector data (n-dimensional (nD) : 2theta, Phi, E, d) projected in flexible and “clever” ways for detector testing and calibration, background assessment, environment, shielding | X |  |  | X |  |  |  |  |  |  |  |  |

\* The need for hkl indexing is related to moving diffraction spots from sample environment e.g. diamond or sapphire cells.