



POWTEX

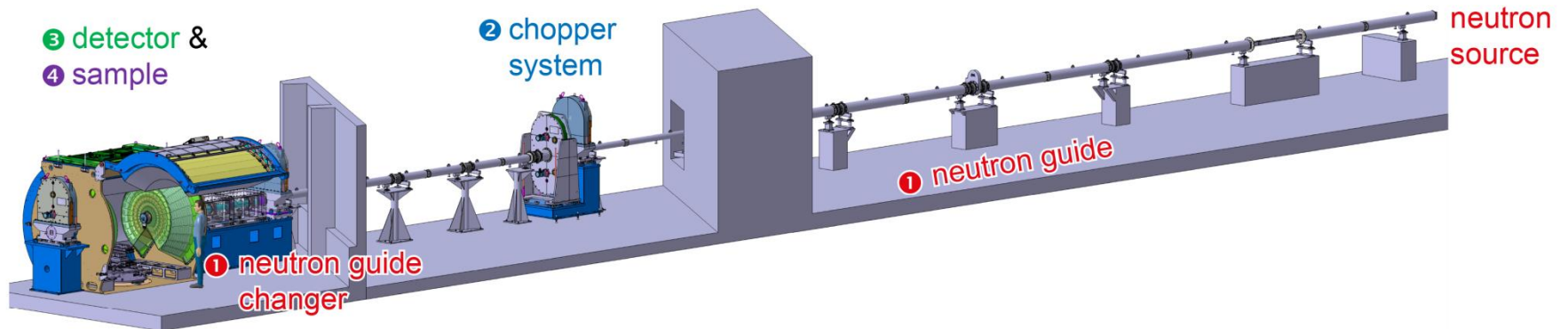
High-Intensity time-of-flight diffractometer

Data reduction for multidimensional Rietveld

Data reduction for multidimensional Rietveld
Andreas Houben, Philipp Jacobs, Werner Schweika, Marina Ganeva, Peter Harbott, Andreas Poqué, Christoph Tiemann, Anja Schwaab and many others



POWTEX beam line at SR5, FRM II



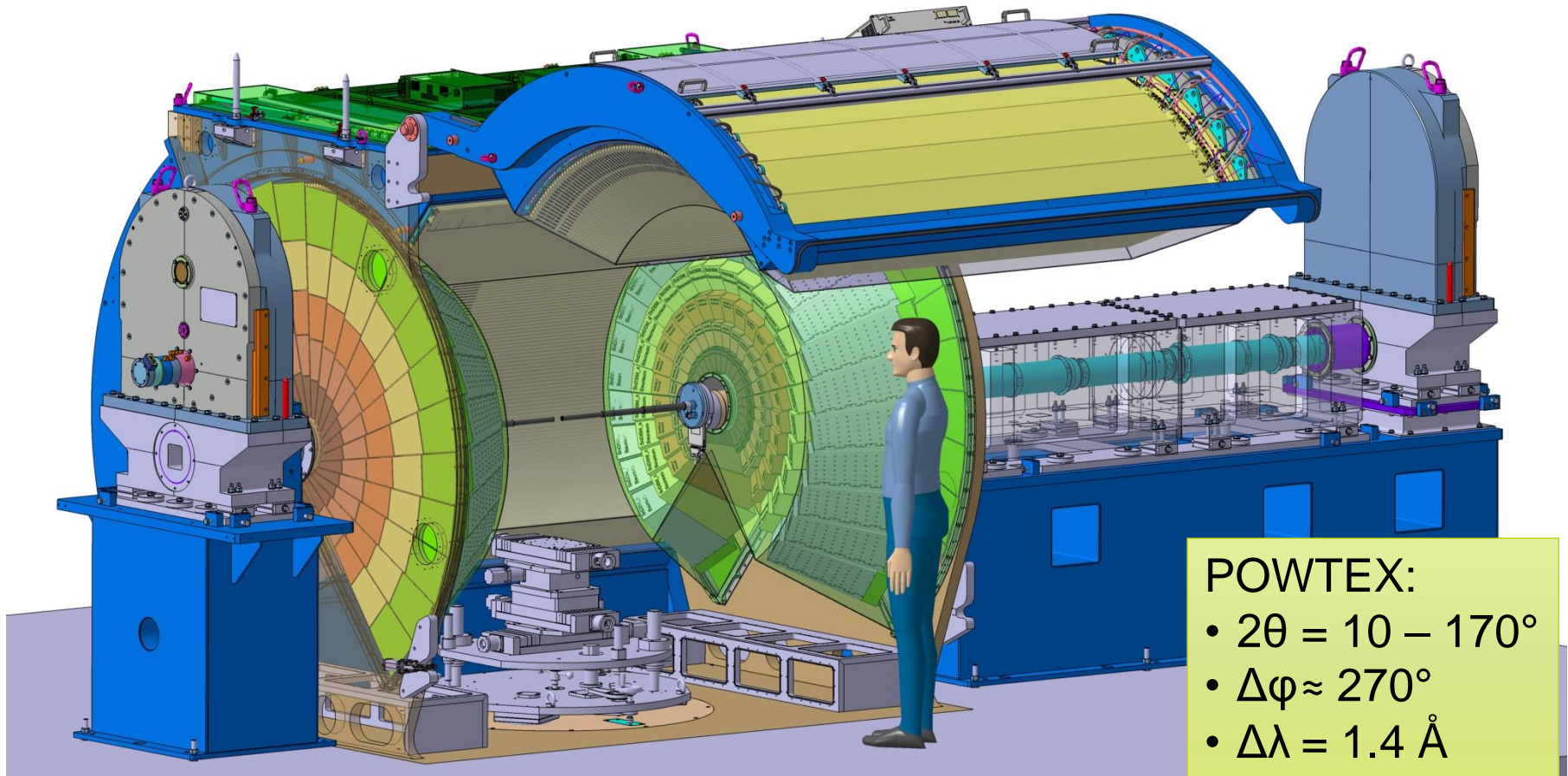
New concept

- TOF at a continuous source
- wavelength & angular dispersive
- high intensity, large detector coverage
- short measurements, small samples

Developments in

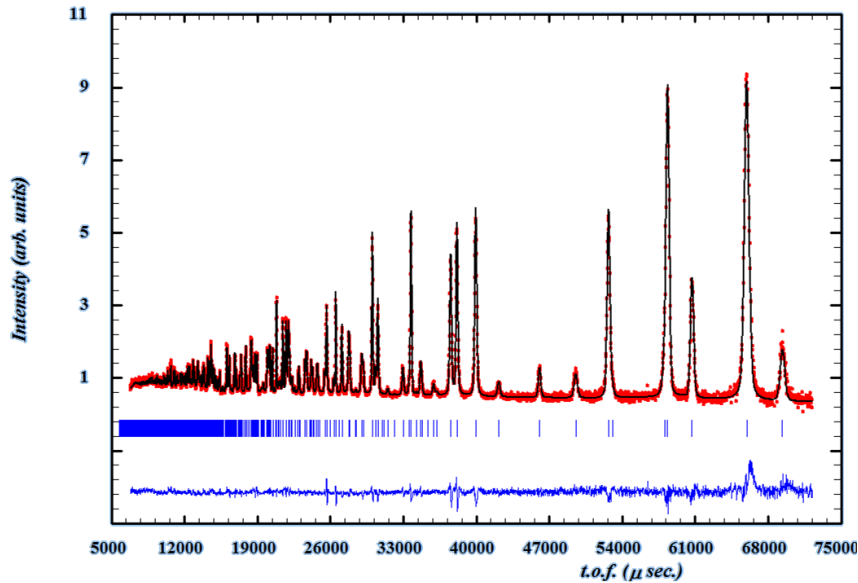
1. double elliptic guide
2. chopper system
3. detector development
4. 2D data analysis

POWTEX detector on a cylindrical surface

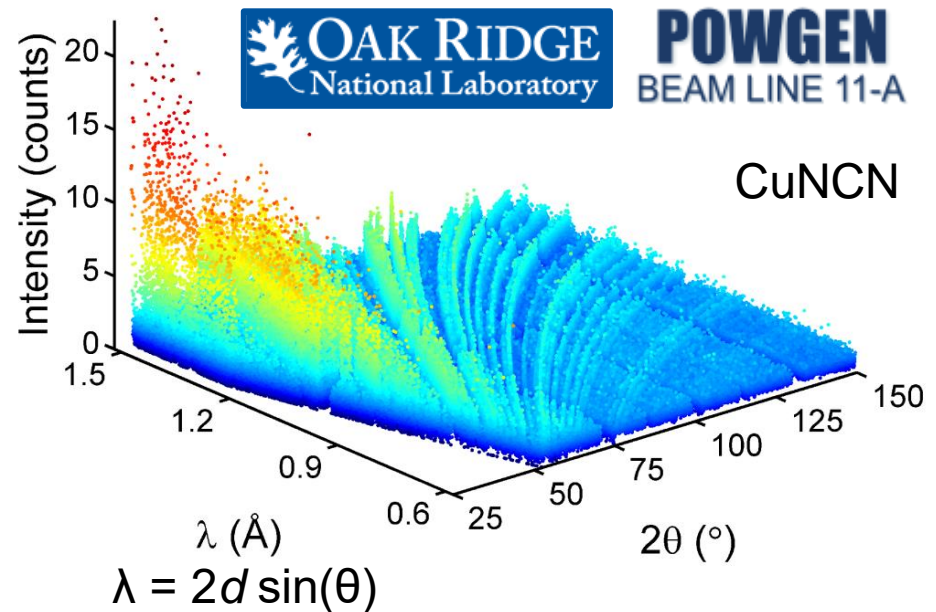


- POWTEX:
- $2\theta = 10 - 170^\circ$
 - $\Delta\varphi \approx 270^\circ$
 - $\Delta\lambda = 1.4 \text{ \AA}$

Data reduction to 1D



1D pattern



2D pattern

„Diffraction focusing“

Motivation for multidimensional data treatment

- mixing of resolutions (peak width) and peak shapes
- background treatment (e.g., Hydrogen)

Data reduction to 2D (or more)

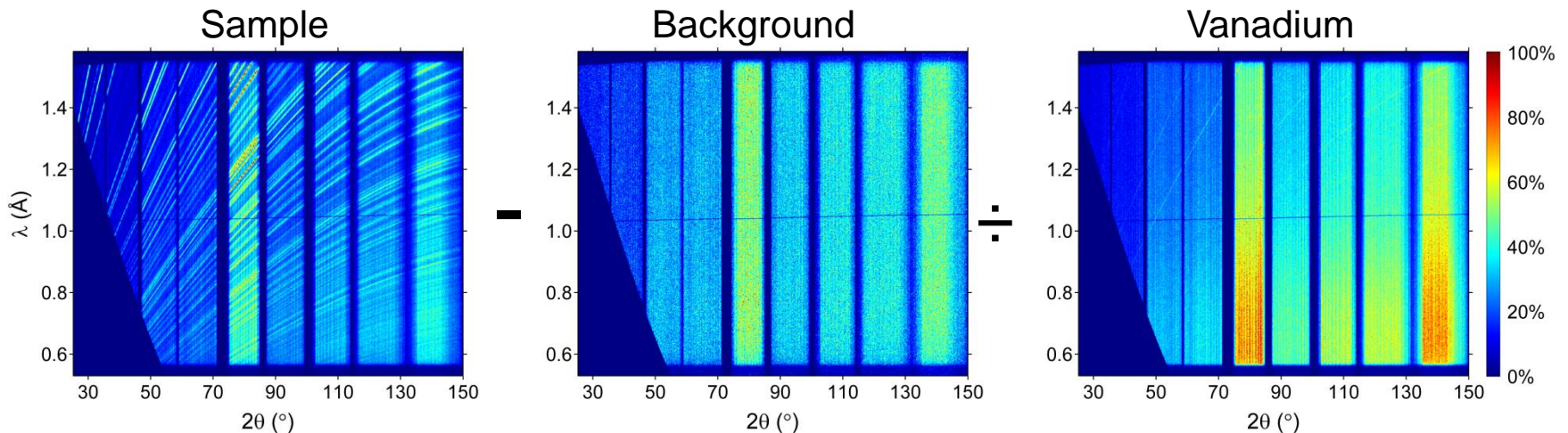
Planned procedure for POWTEX

- Main technique developed with MATLAB
- Transfer to productive systems, with following steps:
 - Detector library from CDT (raw events)
 - TANGO server, NICOS controller
 - Export detector events as raw data + meta data (Chopper, Clock, sample environment, ...)
 - Stored in Nexus format
 - Use Mantid for multidimensional data reduction (here for diffraction, 2D)
 - Multidimensional data treatment, e.g., Rietveld refinement
 - Test planned with POWTEX detector module at POWGEN, End of 2017

Multidimensional data reduction in principle using Mantid

Using POWGEN Nexus data, work in progress

- Usual steps using event data, like in 1D:
FilterBadPulses, RemovePromptPulse, MaskDetectors, AlignDetectors
- Rebin data in 2θ , λ or other and generate 2D matrix
- For Sample and also for background and Vanadium correction

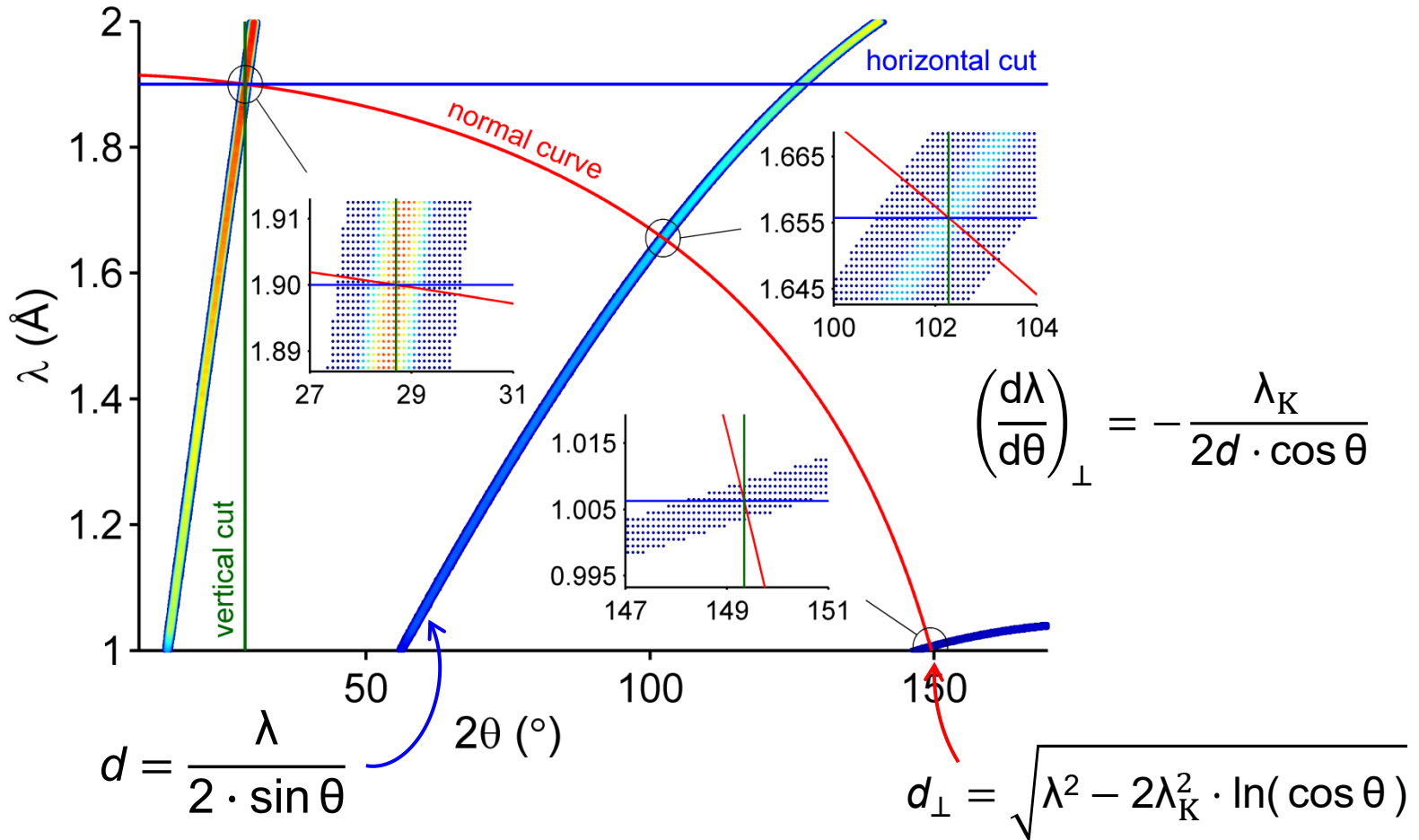


- Export data files, provide instrument parametrization (IRF or instprm files)

Instrument parametrization in the d, d_{\perp} coordinate system

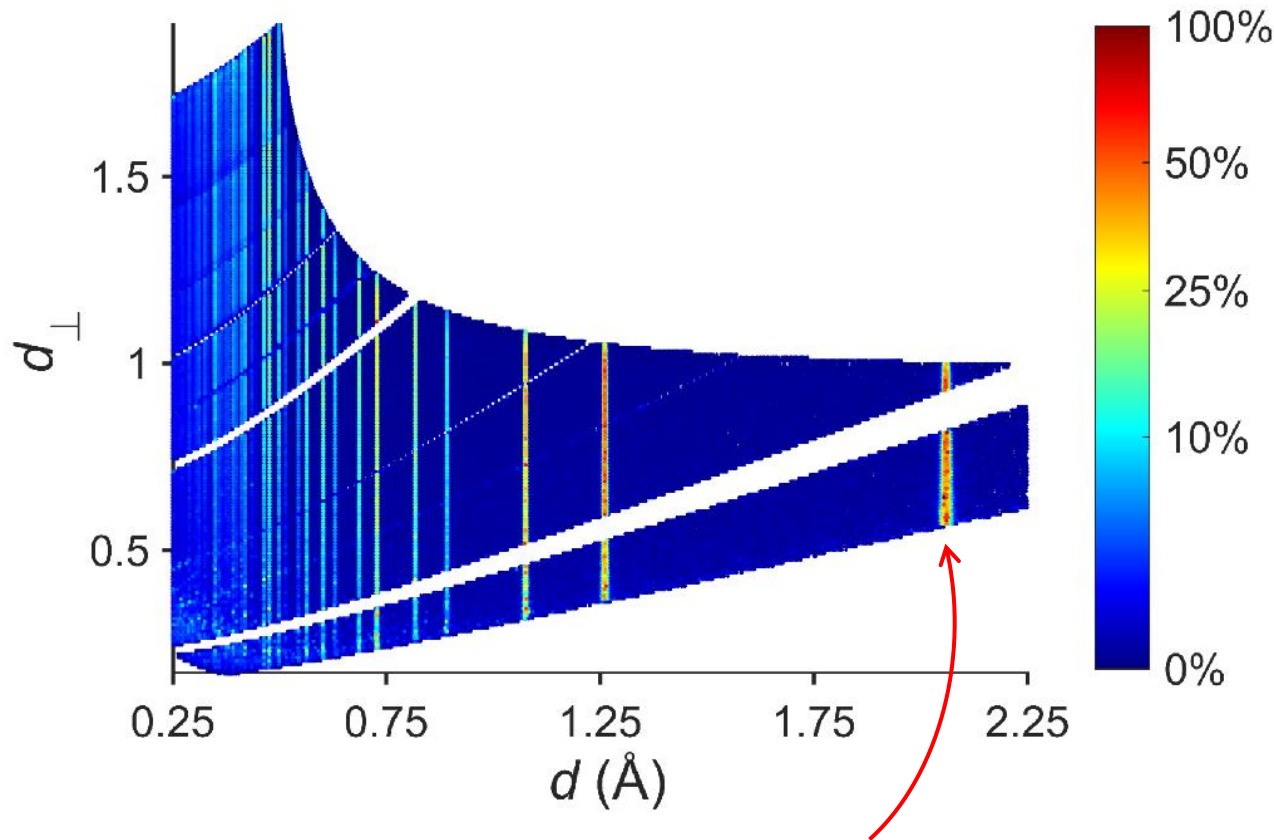
P. Jacobs, et al., *J. Appl. Crystallogr.* **2015**, 48, 1627.

P. Jacobs, et al., *J. Appl. Crystallogr.* **2017**, accepted.



Instrument parametrization in the d , d_{\perp} coordinate system

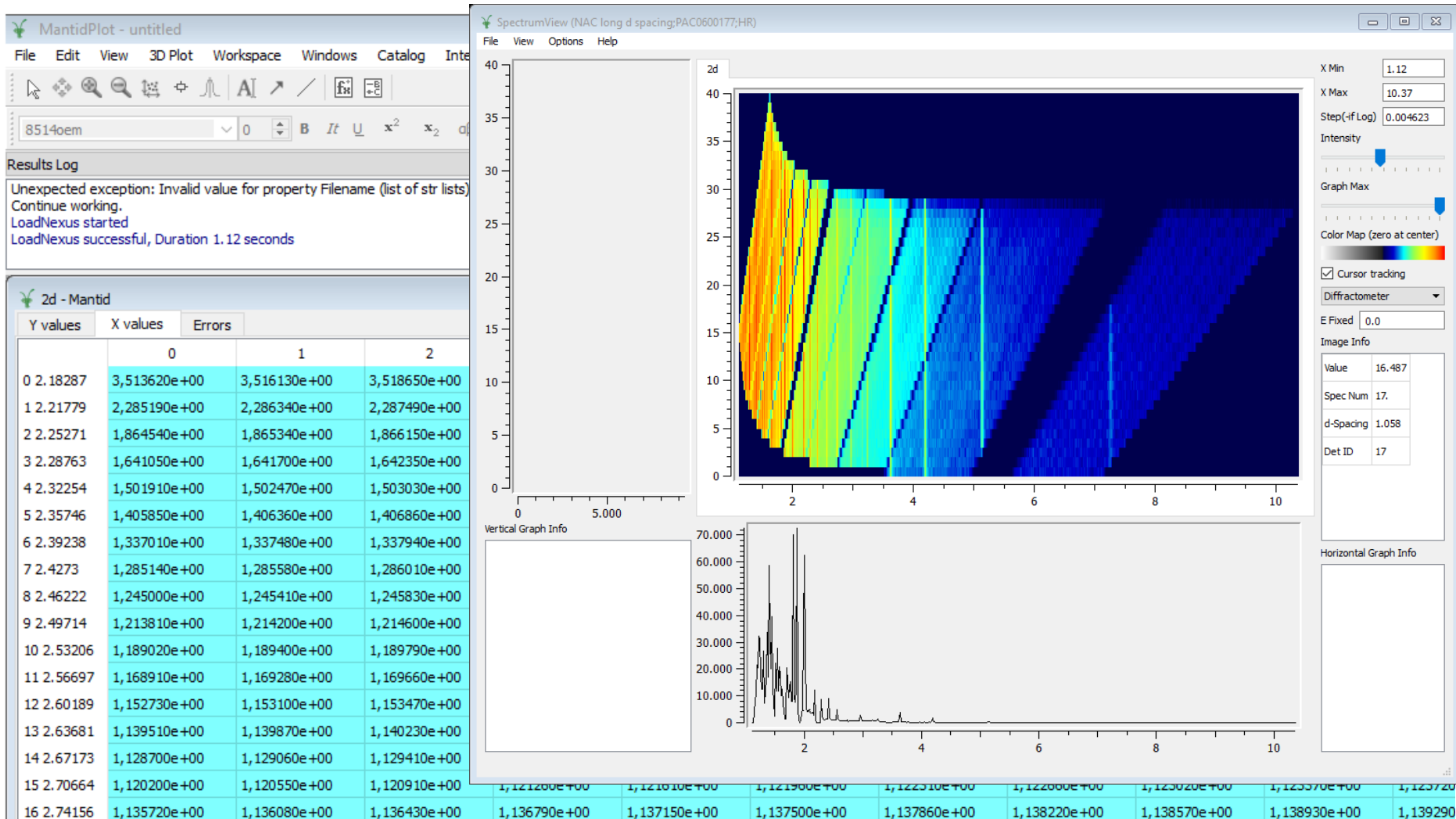
Pattern in d , d_{\perp} coordinates



POWGEN: almost no change in peak width

POWTEX/DREAM: strong change in peak width and peak shape (detector shape)

Screenshot of Mantid (forge from Marina Ganeva, JCNS)



Refinement of Diamond@POWGEN using GSAS II (forge Jan. 2016)

The screenshot displays the GSAS II software interface. On the left, a terminal window shows the execution of the GSAS II binary and the loading of various Python modules. The main window shows a powder pattern plot for 'P2DD Diamond -0.0008_0.0218.p2d'. The plot shows intensity versus 2θ (°) and λ (Å). A color scale on the right indicates intensity from 0 to 72. On the right side, a data tree shows the loaded data structure, including the loaded data file and the phase 'Diamond'. Below the plot, a 'Phase Data for Diamond' window is open, showing a table with the following data:

Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso	U11
0	C(1)	C	F	0.12500	0.12500	0.12500	1.0000	mm2d001	48	I	0.01000

Data and phase information loaded

POWTEX