POWTEX

High-Intensity time-of-flight diffractometer

Data reduction for multidimensional Rietveld

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Andreas Houben, Philipp Jacobs, Werner Schweika, Marina Ganeva, Peter Harbott, Andreas Poqué, Christoph Tiemann, Anja Schwaab and many others

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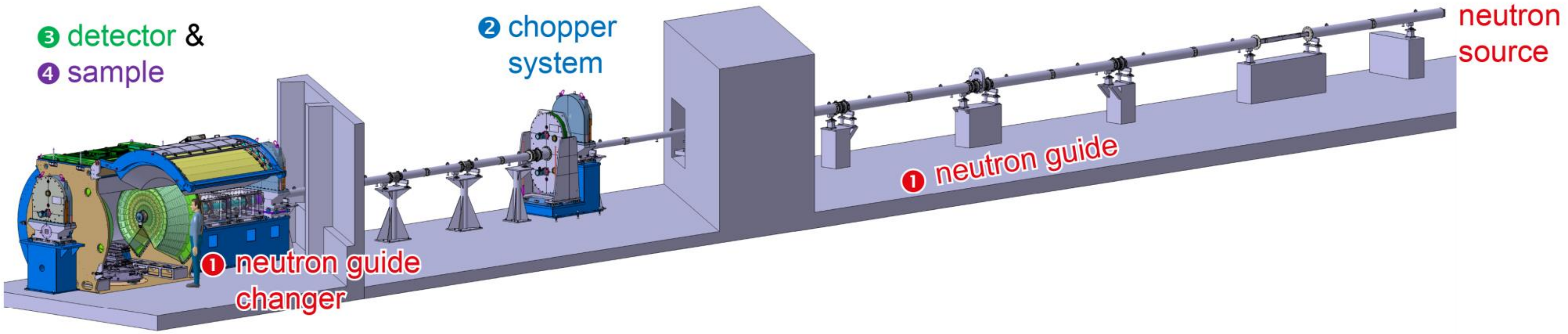
RWTH AACHEN UNIVERSITY

POWTEX beam line at SR5, FRM II



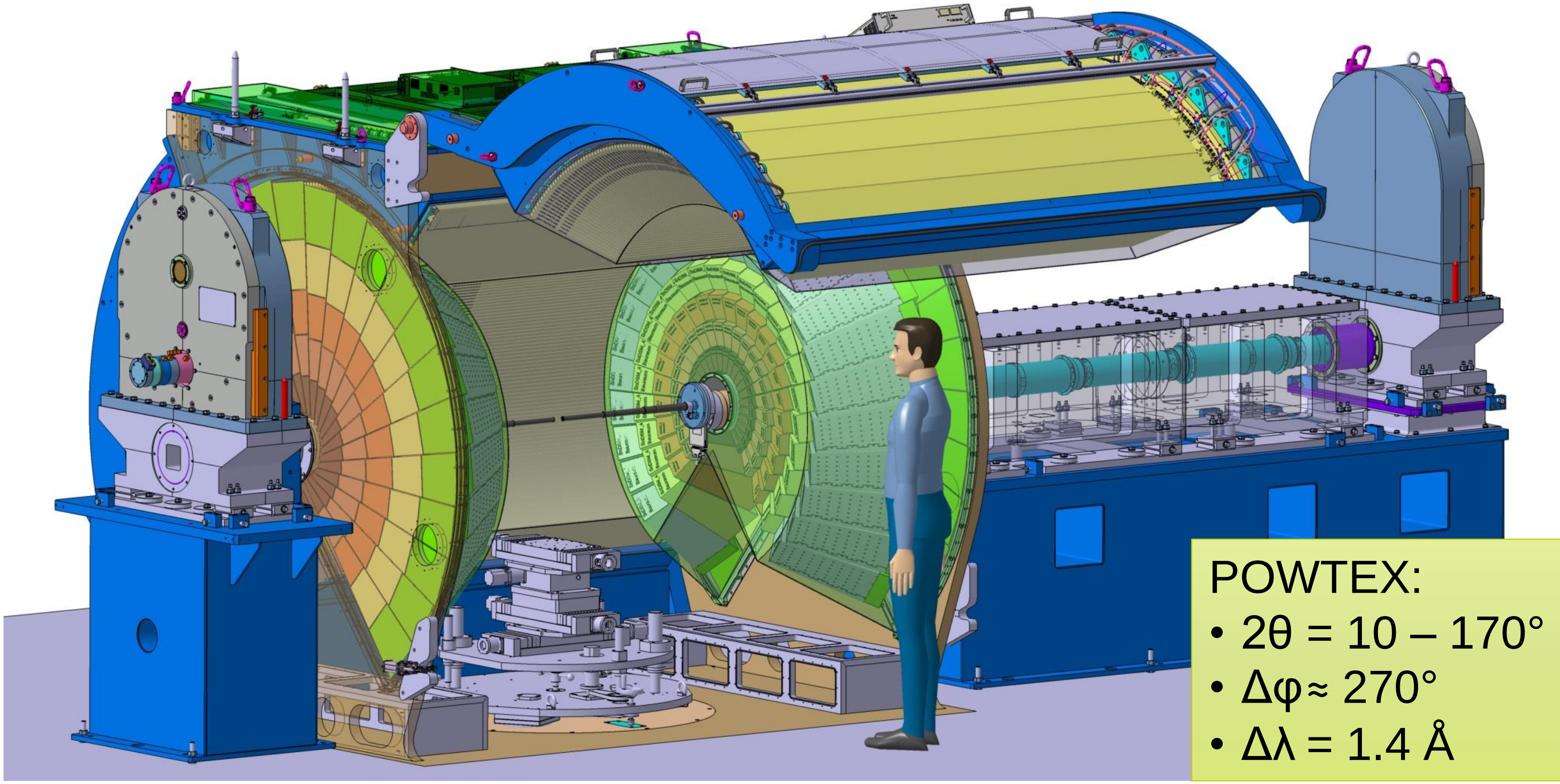
New concept

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

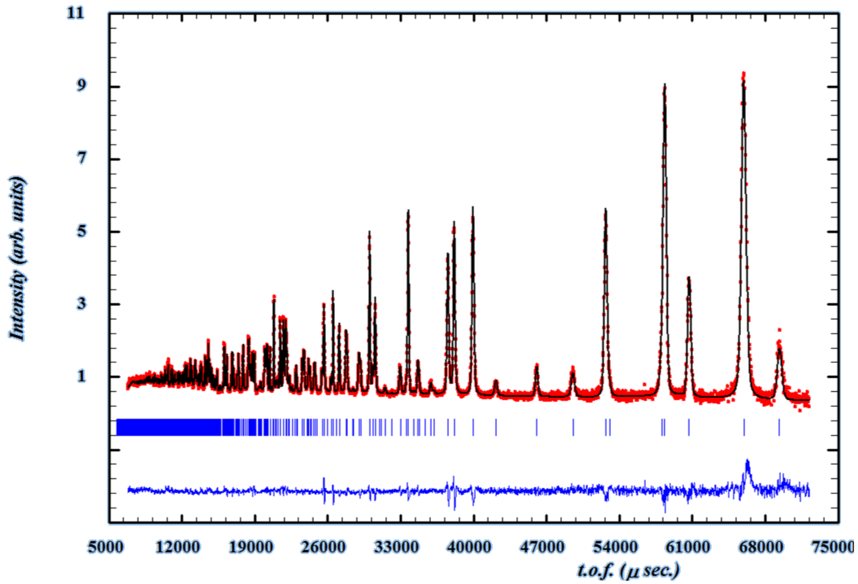
Developments in

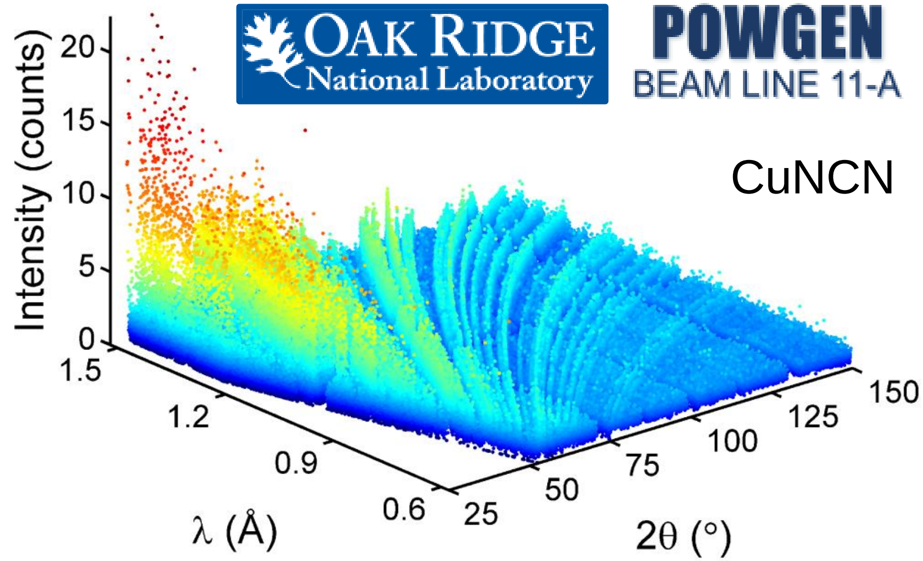
1. double elliptic guide
2. chopper system
3. detector development
4. 2D data analysis

POWTEX detector on a cylindrical surface



Data reduction to 1D





$\lambda = 2d \sin(\theta)$

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)

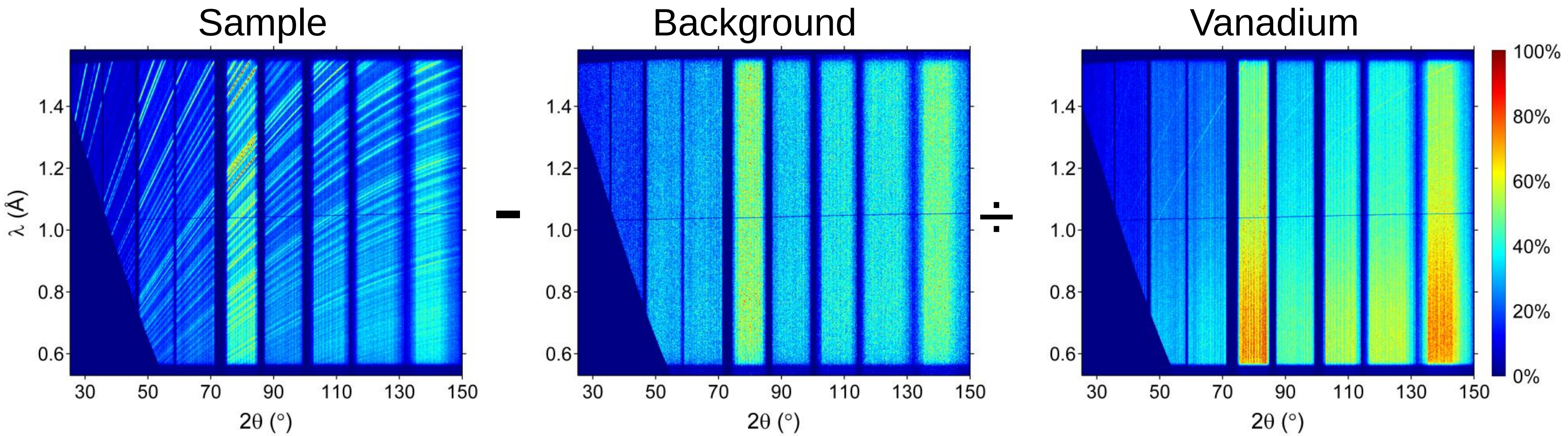
Planned procedure for POWTEX

- 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)

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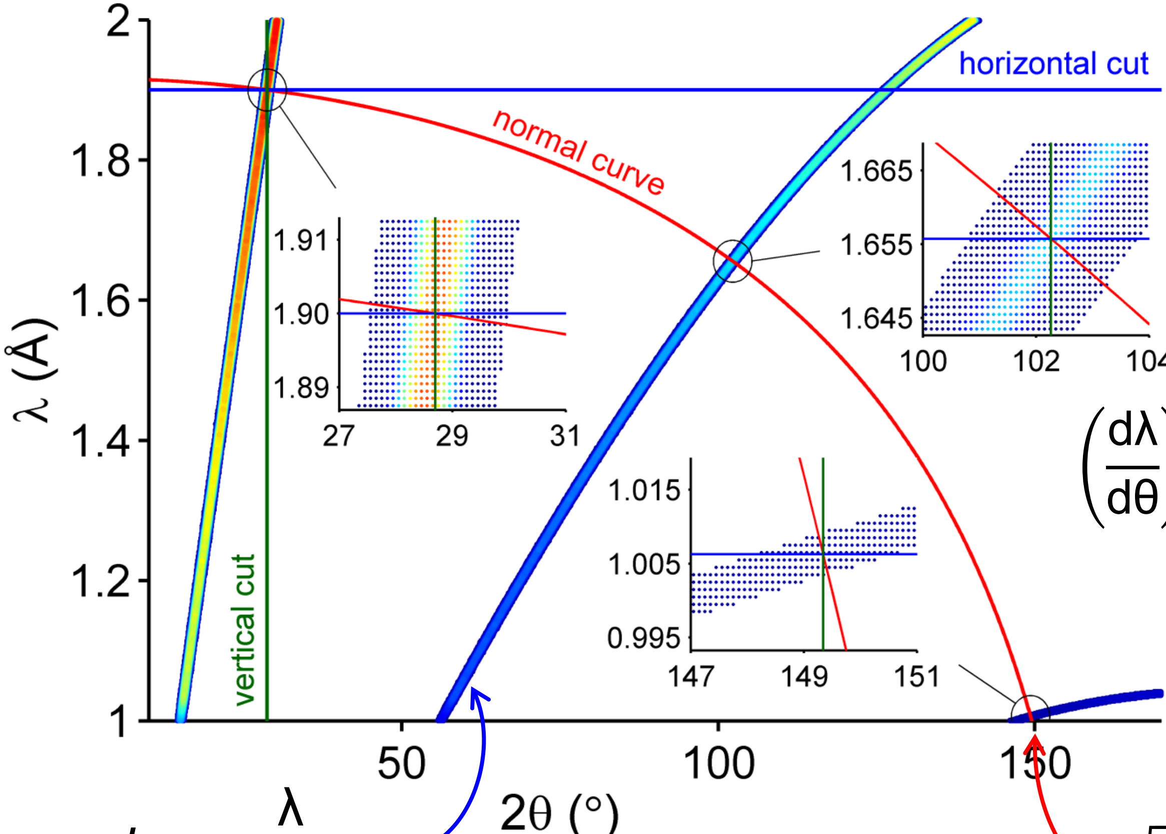
Instrument parametrization in the d, $d_\perp$ coordinate system

P. Jacobs, et al., *J. Appl. Crystallogr.* **2015**, *48*, 1627.
P. Jacobs, et al., *J. Appl. Crystallogr.* **2017**, *accepted*.



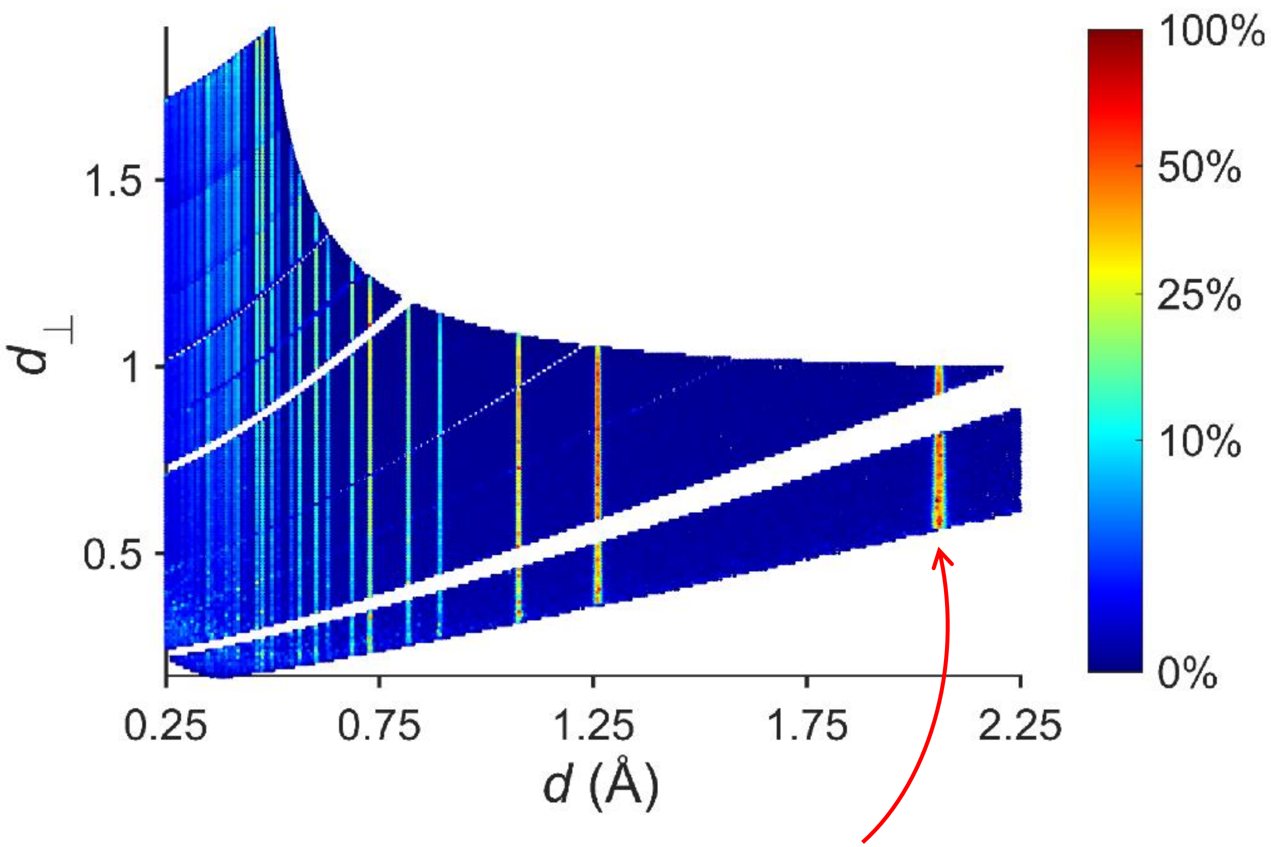
$$\left(\frac{d\lambda}{d\theta}\right)_\perp = -\frac{\lambda_K}{2d \cdot \cos\theta}$$

$$d = \frac{\lambda}{2 \cdot \sin\theta}$$

$$d_\perp = \sqrt{\lambda^2 - 2\lambda_K^2 \cdot \ln(\cos\theta)}$$

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)

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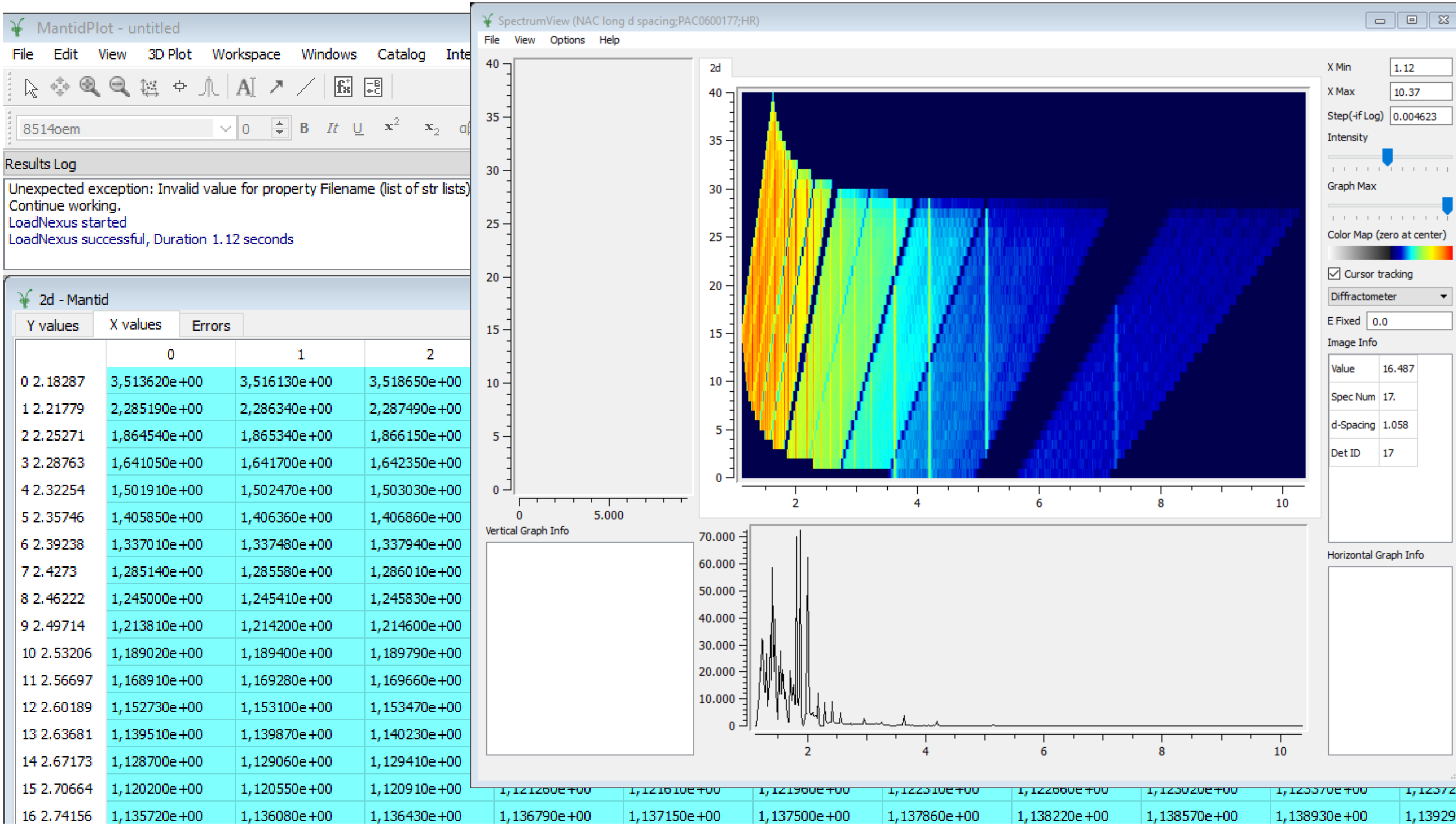
Screenshot of Mantid (forge from Marina Ganeva, JCNS)



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