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Synchrotron Diffraction

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Synchrotron Applications

What?

Diffraction data are collected on diffractometer beam lines at the world's synchrotron sources. Most synchrotrons have one or more user facilities or ports that perform diffraction experiments.

The extreme X-ray photon flux rate of a synchrotron allows users to much latitude to vary instrumental conditions. Diffractometer lines often use custom optics and detectors designed to improve resolution, sensitivity or capture data quickly.

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Synchrotron Applications

Why?

Materials can be studied dynamically while under stress, strain, heating or cooling. The high flux rate allows users to rapidly collect many data scans as a function of conditions.

High resolution, combined with high signal to noise, provides improved accuracy in structure solution, phase identification and quantitative analysis.

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Synchrotron Applications
How?

To best use the PDF databases for synchrotron applications, users need to adjust applicable parameters in the database.
This includes:

1) Using integrated intensity options for all entries.

2) Changing the input wavelength for all data simulations.

3) Adjusting both the optical geometry and peak width for simulations.

4) Using calculated patterns where possible. Calculated patterns have intensities calculated from 1-1000, experimental patterns have intensities from 1-100.

5) Adjusting background and peak finding algorithms in SIeve+ for higher sensitivity.

(Note: The enhanced signal to noise in most synchrotron experiments means that low intensity peaks are often observed.)

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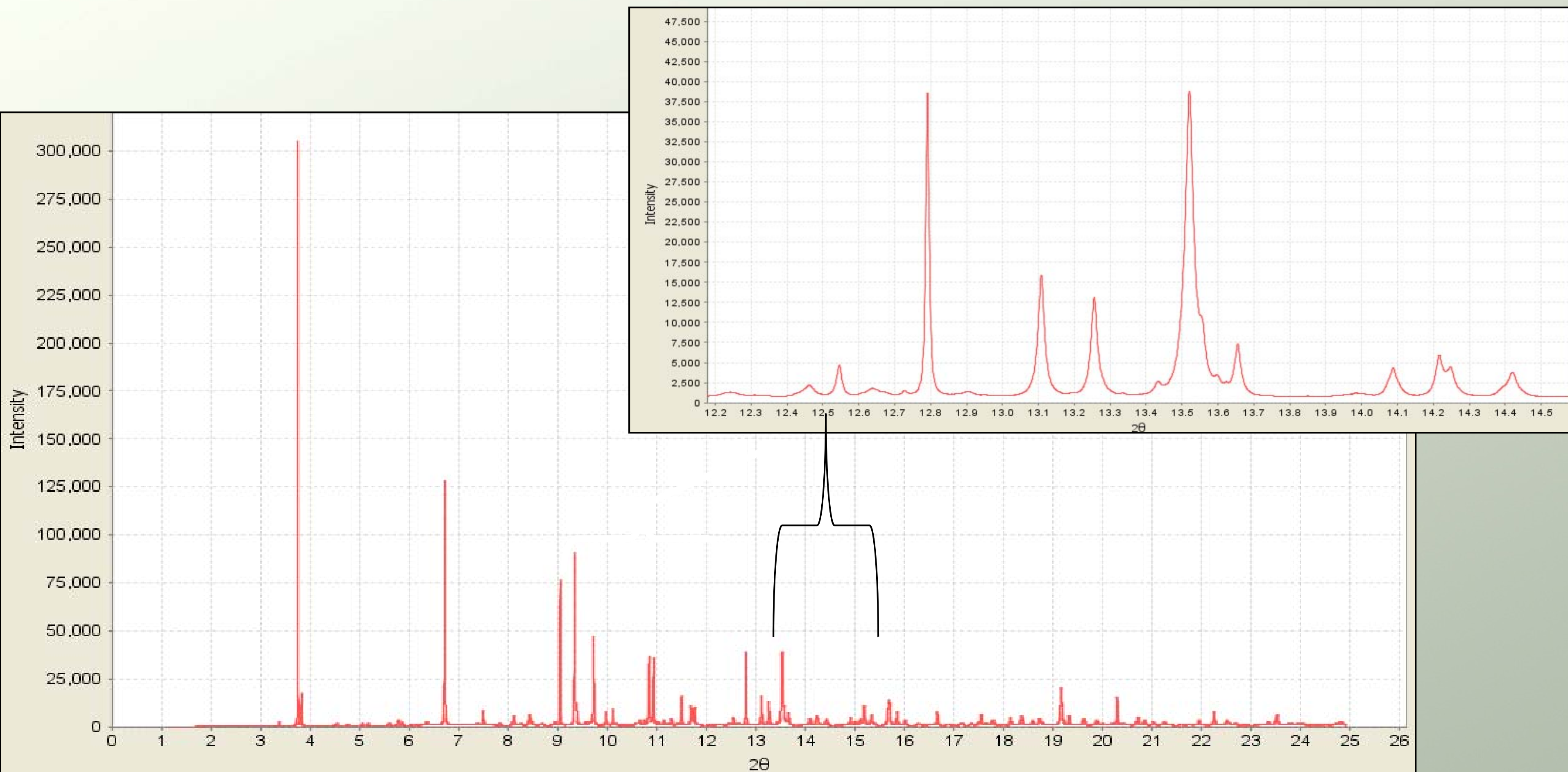
Synchrotron Data versus Laboratory Data

- Wavelengths are variable.
- Incident beam is often monochromatic and/or parallel.
- Peak resolution is high for crystalline materials (i.e., very small instrumental contributions to the peak profiles, 0.01 FWHM or less).
- High count rates and signal to noise ratio are expected for synchrotron data.

Synchrotron Data



Clearly resolved low intensity peaks and high signal to noise.

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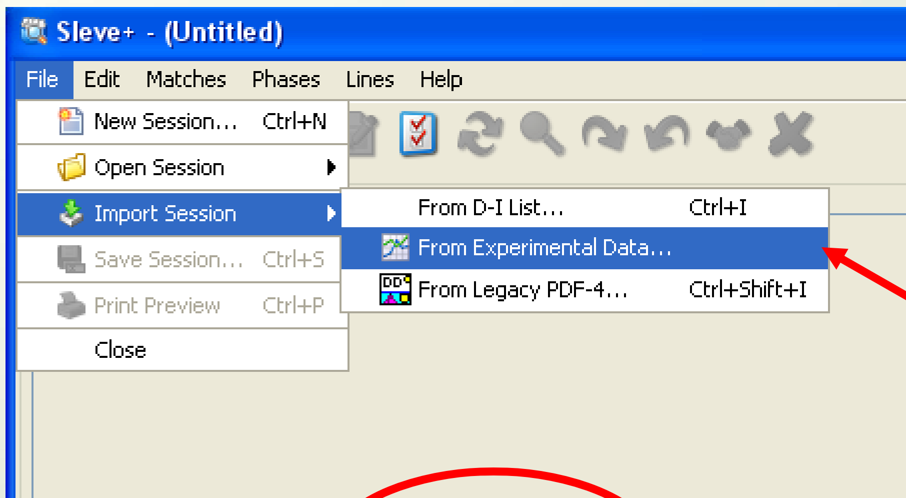
Changing Display Options Using DDView+

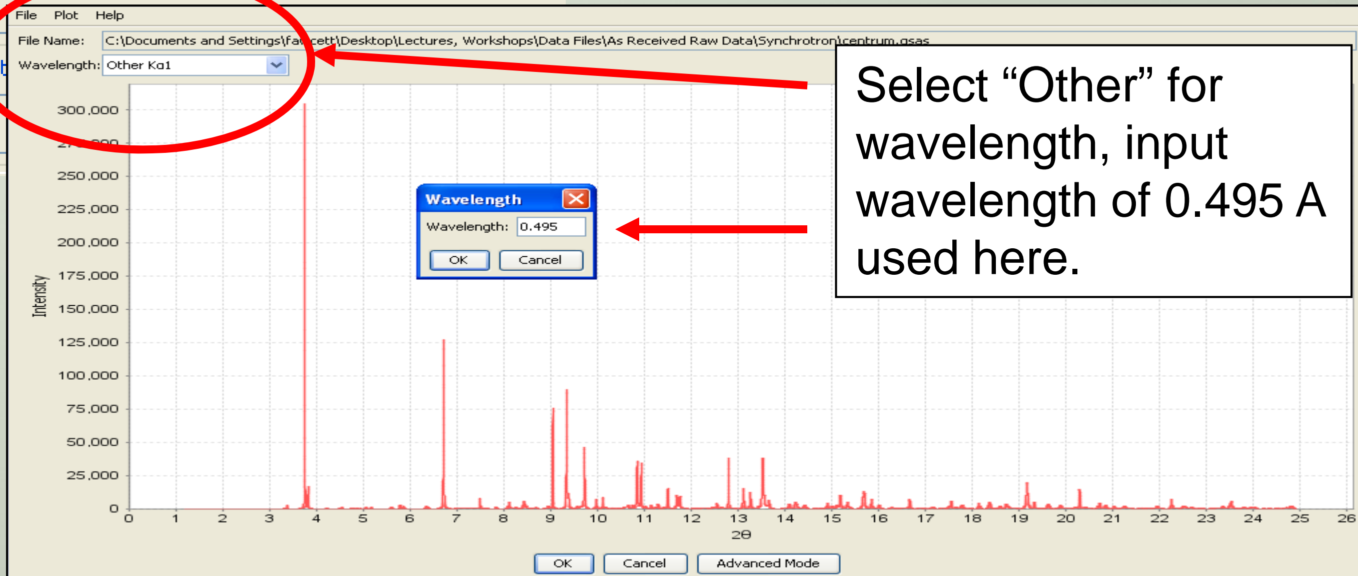
Custom Displays

Importing Data



Import data using the drop down menus. The importer supports GSAS formats.

This selection will display a browser to find data files.



Select "Other" for wavelength, input wavelength of 0.495 A used here.

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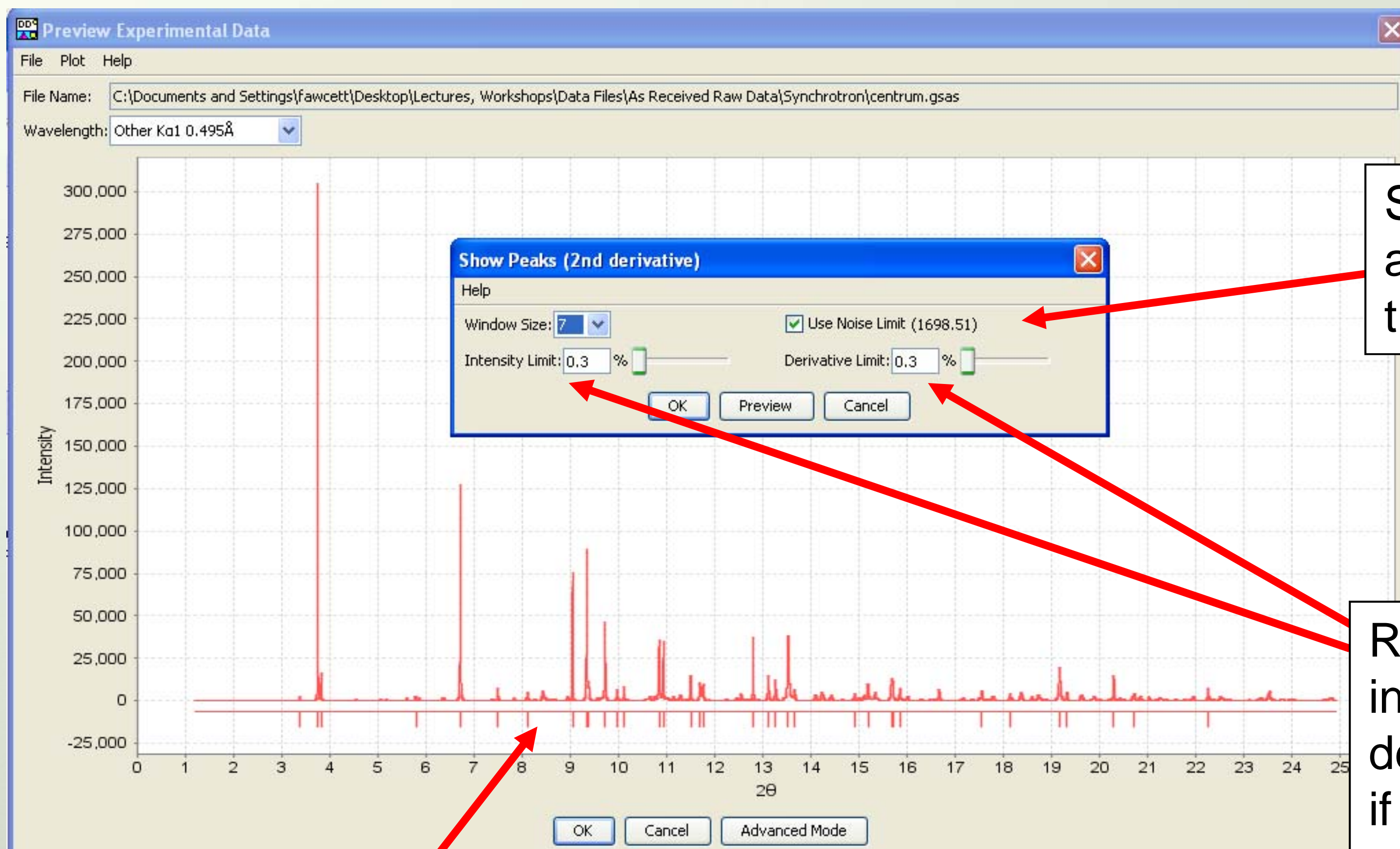
Change Sensitivity Scale and Calculation Limits

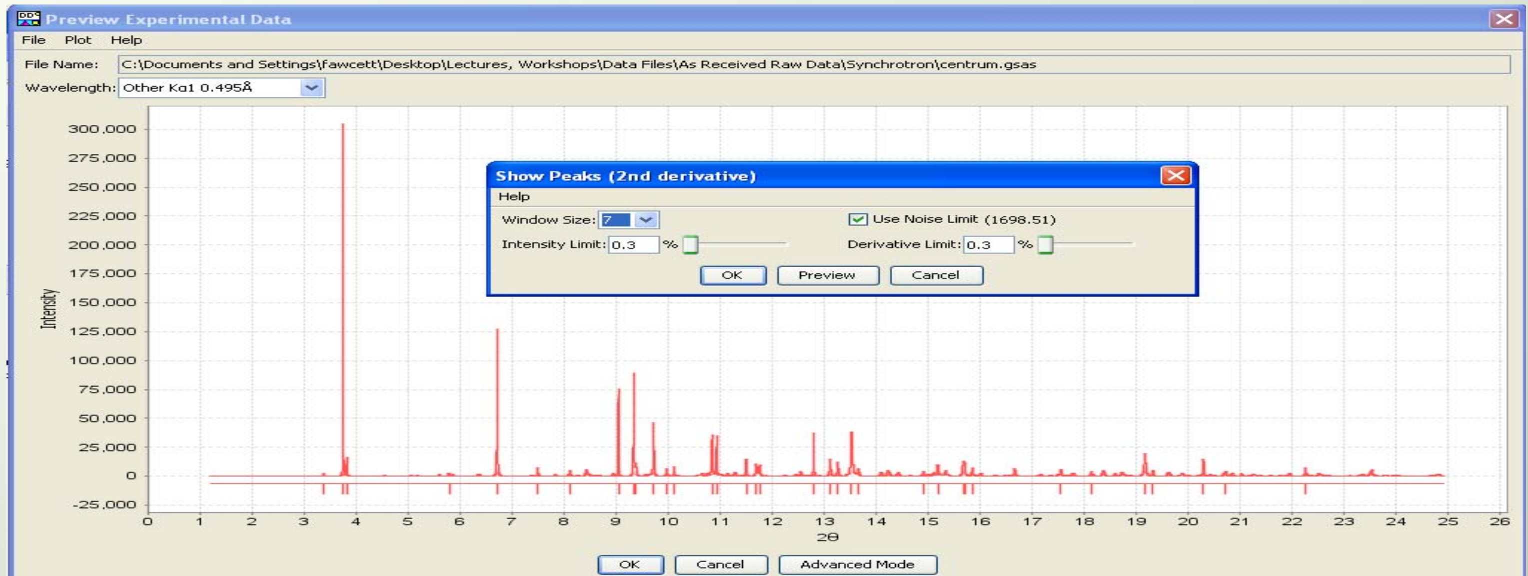


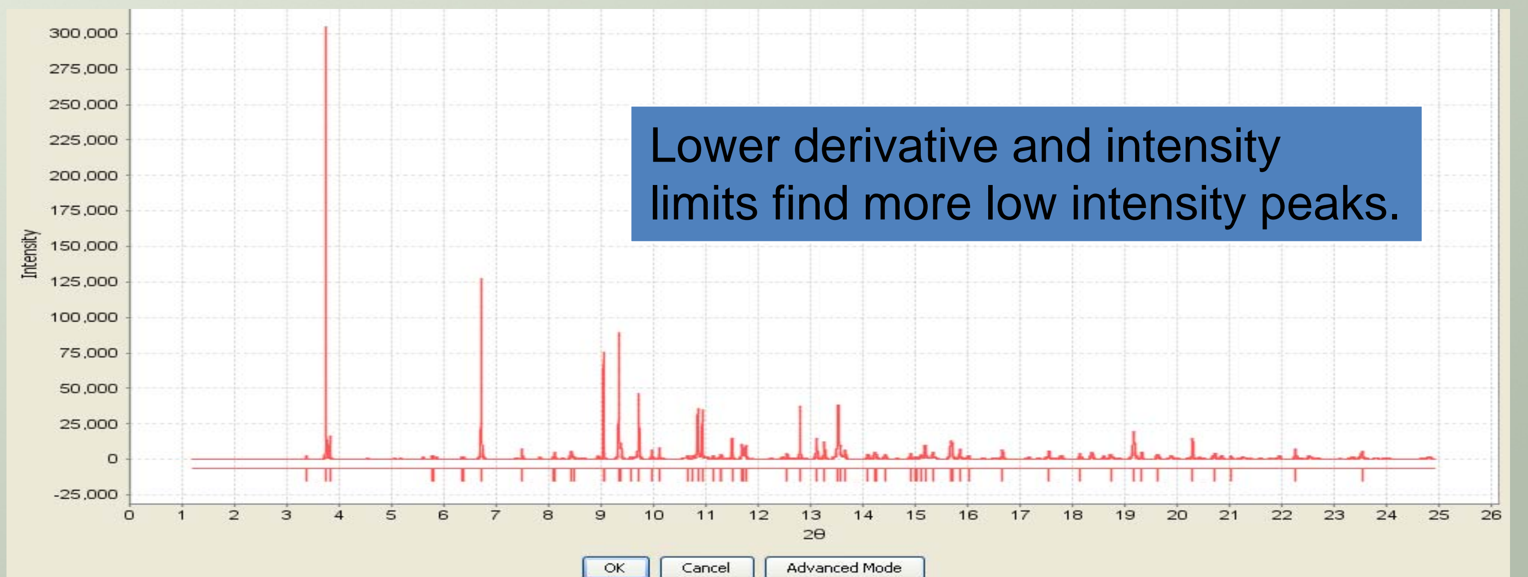
SIeve calculates a noise limit from the data file.

Reduce the intensity and derivative limits, if warranted, to values below the 1.0 default.

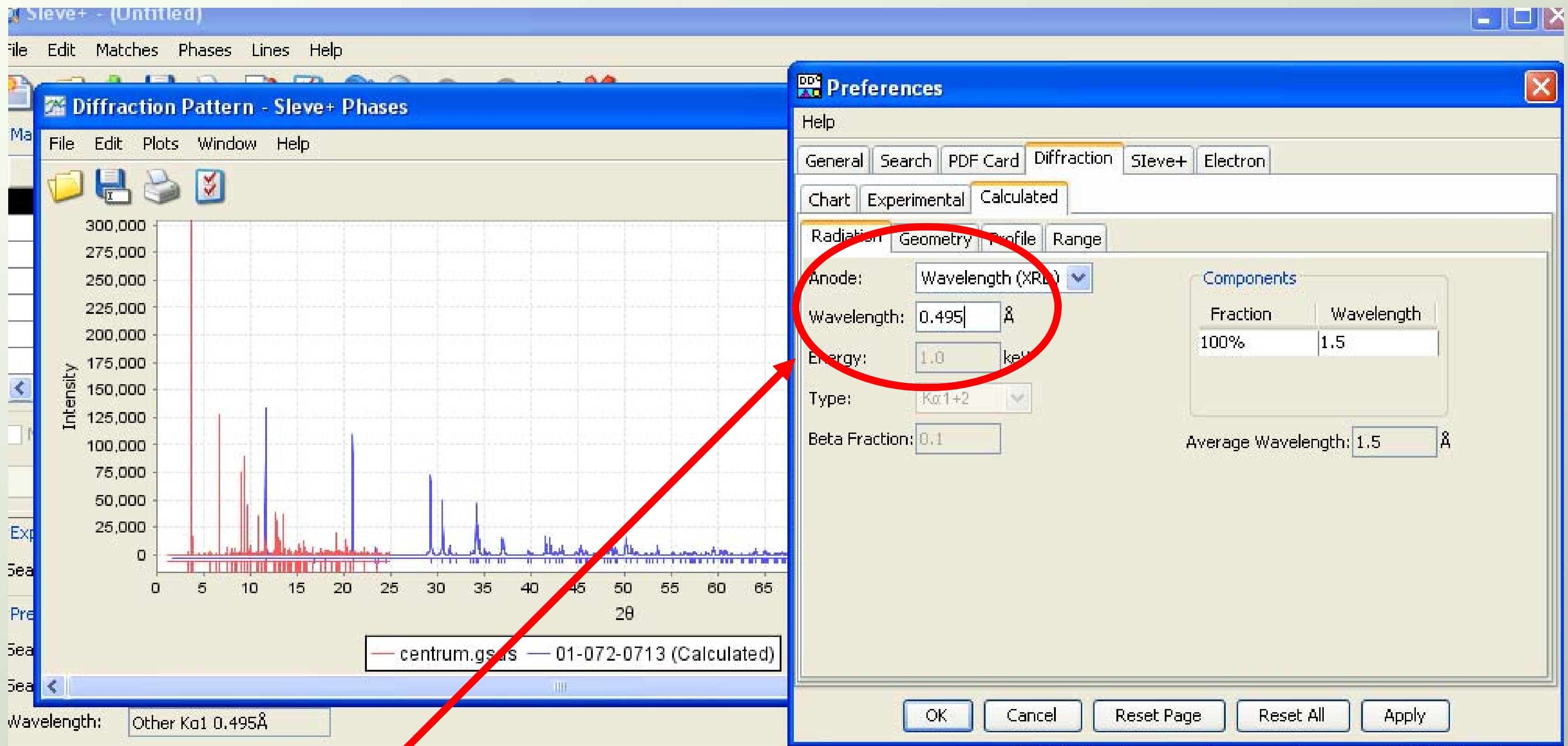
"Preview" will show the peaks determined with the input limits - use interactively, press "OK" when done.

Data Processing



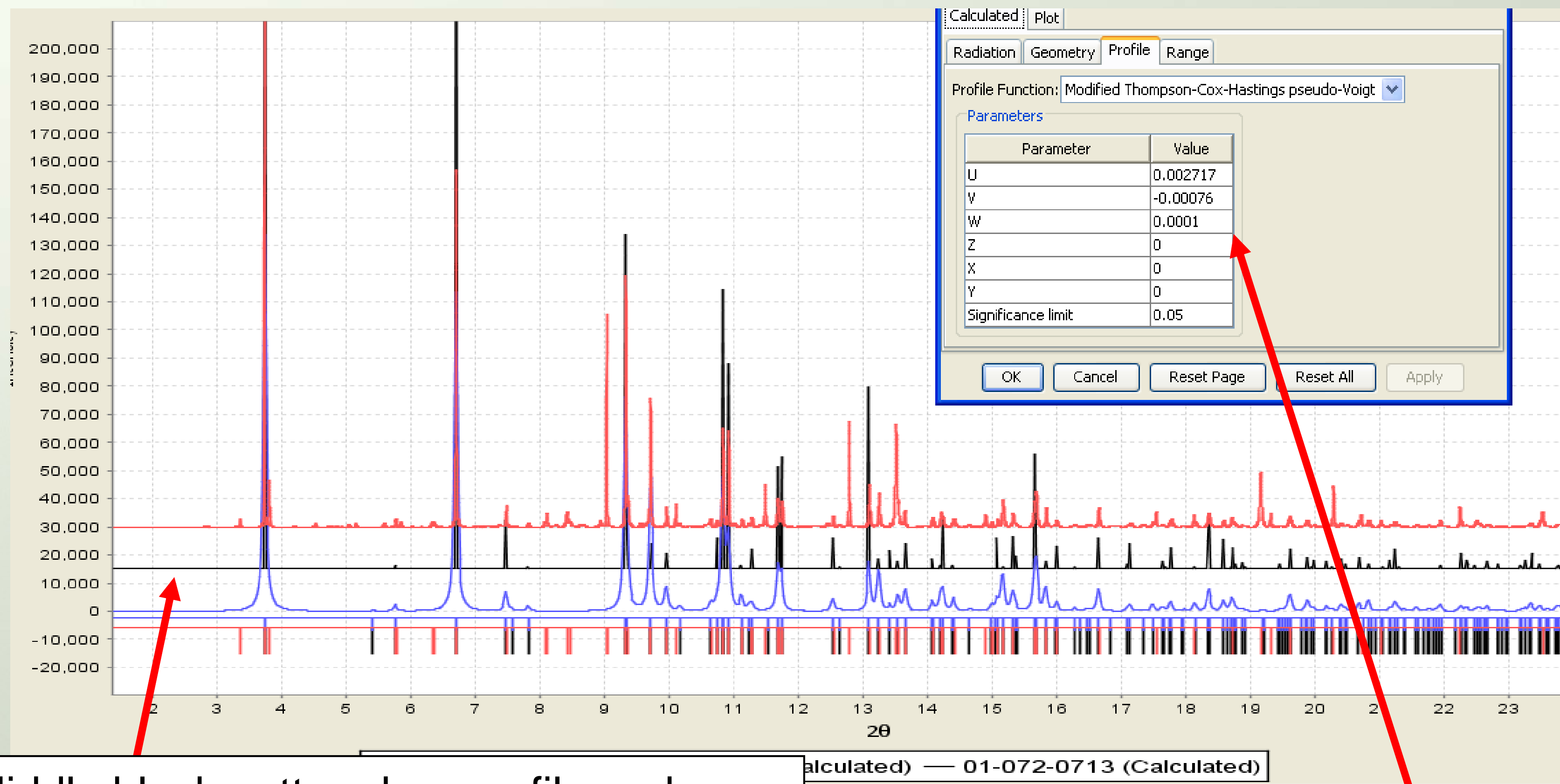


Adjust for Wavelength



All digital pattern simulations require a wavelength adjustment. This can be done through the Preferences Module and inputting 0.495 (or any other wavelength) under XRD wavelength.

Adjust for Peak Profile



Middle black pattern has profile and wavelength adjusted, bottom pattern only has the wavelength adjusted.

Narrow the peak profile to simulate higher resolution.

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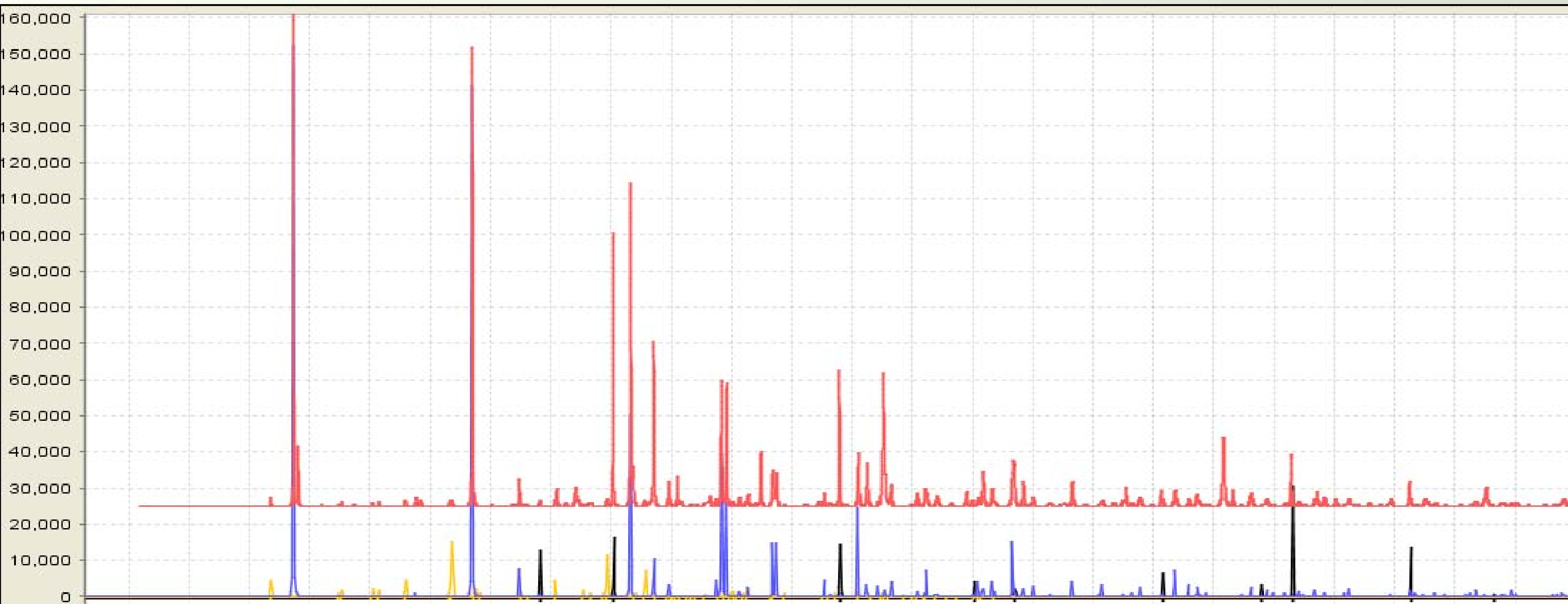
Reiterate



Above (red) – Experimental data taken on a vitamin pill. Bottom – Three phase pattern simulation with adjusted wavelength and profile resolution. In the simulation, each phase is a different color.

More Information

For more information on how to perform complex multi-phase simulations, see the Digital Pattern Simulations tutorial.

Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD website
(www.icdd.com).

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