

X-Ray Diffraction Data – Readme

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The x-ray powder diffraction data included on this CD-ROM provide a fair representation of the diffraction patterns of elements, metals, and common inorganic phases. For example, there are patterns for simple bcc, fcc, and hexagonal structures, plus a diamond cubic structure, which is based on the fcc structure. There are also patterns for more complicated structures, such as quartz (a form of SiO_2) and corundum (a form of Al_2O_3). There is even a diffraction pattern for a non-crystalline material, glassy carbon.

I hope you find these data interesting and useful. Suggested exercises and activities are:

1. Import and plot the data to see what real x-ray diffraction patterns look like. Plots should be 2θ versus intensity (counts per second) or 2θ versus relative intensity ($I_{\text{Max}}=100\%$ relative intensity).
2. Note the differences in intensities in the different patterns.
3. Note how all of the peaks seem to come in pairs, and that as 2θ increases the distance between these peaks increases. Using only Bragg's law and the appropriate wavelengths, you should be able to explain this behavior.
4. Compare the positions of the peaks in these patterns to those listed in the sample PDF files that are in the *Articles* page of this CD-ROM.

All of the data was collected on the x-ray diffractometer shown in figure 1. This instrument is a Scintag XDS 2000, built in 1993. It features complete computer control, a solid-state intrinsic germanium detector coupled with a single channel analyzer to provide excellent filtering of



Figure 1 The Scintag x-ray diffractometer.

unwanted x-rays (continuous and other characteristic x-rays) with little loss in intensity. A beam collimator, scatter, divergence and receiving slits direct the x-ray beam towards the sample and a nickel filter provides additional filtering of unwanted x-rays. (See figure 2.) The x-ray source uses a line-focus tube to help produce sharply defined peaks. The target in the tube is copper, so the primary characteristic x-ray produced has a wavelength $\lambda_{k,1}=0.1540562$ nm while the secondary characteristic radiation (about half as strong as the primary) has a wavelength $\lambda_{k,2}=0.1544390$ nm. (In some of the patterns you may see tiny peaks just to the left of the larger peaks. These were produced by Cu- k_{β} (0.1392218 nm) and W-L. ($\lambda=0.147639$ nm) characteristic x-rays.)

The data files themselves are in the form of ASCII text files that can be easily imported into a spreadsheet or other plotting programs, divided into columns, and plotted. The data are organized either as:

Header	Name, date, comments, and selected data collection parameters
Column 1	2 θ position in degrees
Column 2	Measured intensity in counts
Column 3	Counting time in milliseconds
Column 4	ESD, standard deviation, a measure of the certainty associated with each data point. A lower value relative to the intensity indicates greater certainty.

or for files from an older version of the system's software:

Header	Name, date, comments, and selected data collection parameters
Column 1	2 θ position in degrees
Column 2	Measured intensity in counts per second
Column 3	ESD, standard deviation, a measure of the certainty associated with each data point. A lower value relative to the intensity indicates greater certainty.

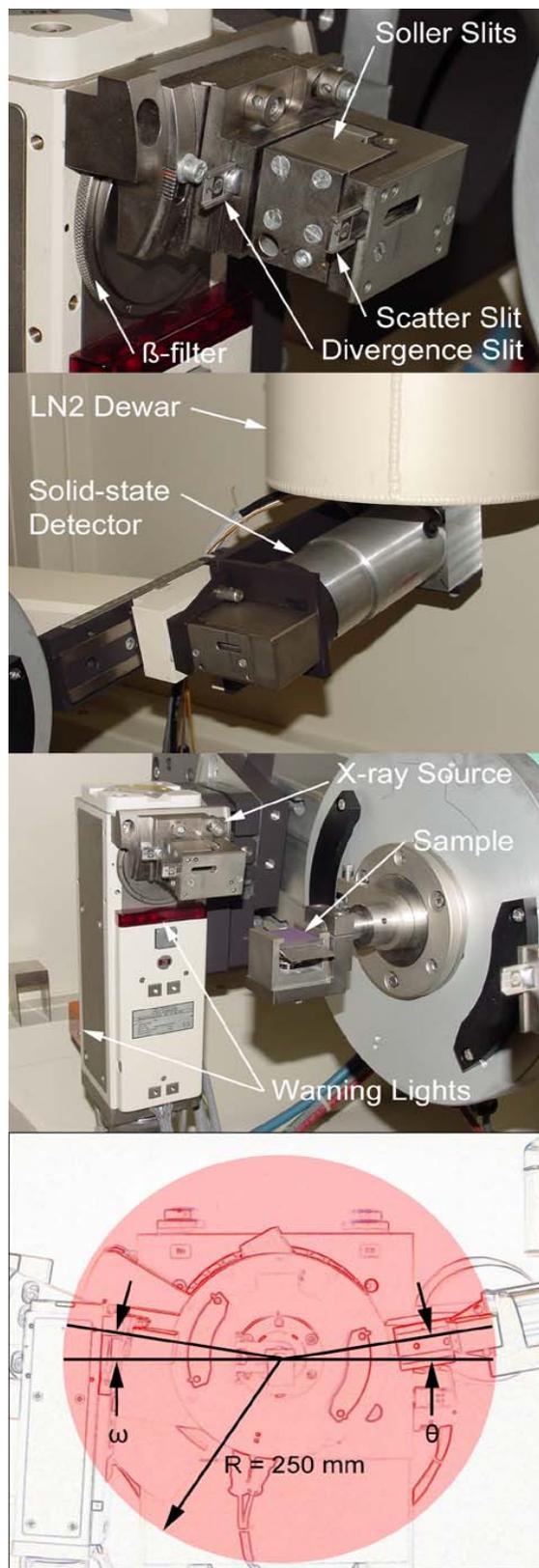


Figure 2 Tops: source, Second: detector, Third: source and sample, Bottom: angles and goniometer radius.

All of the data are raw data. Normally x-ray diffraction data undergoes some basic processing to remove artifacts such as:

- Background Characterized by a baseline intensity greater than 0.
- $K_{\alpha 2}$ -stripping Removing the peaks produced by the $K_{\alpha 2}$ x-rays.
- Peak finding Note the positions and intensities of the remaining peaks.

Further processing may be done to correct for instrumental errors and sample-dependent errors such as the transparency of the sample to x-rays (Low-Z elements tend to be more transparent than high-Z elements.) If you look closely you will be able to see these artifacts and evidence for these errors in the data.