

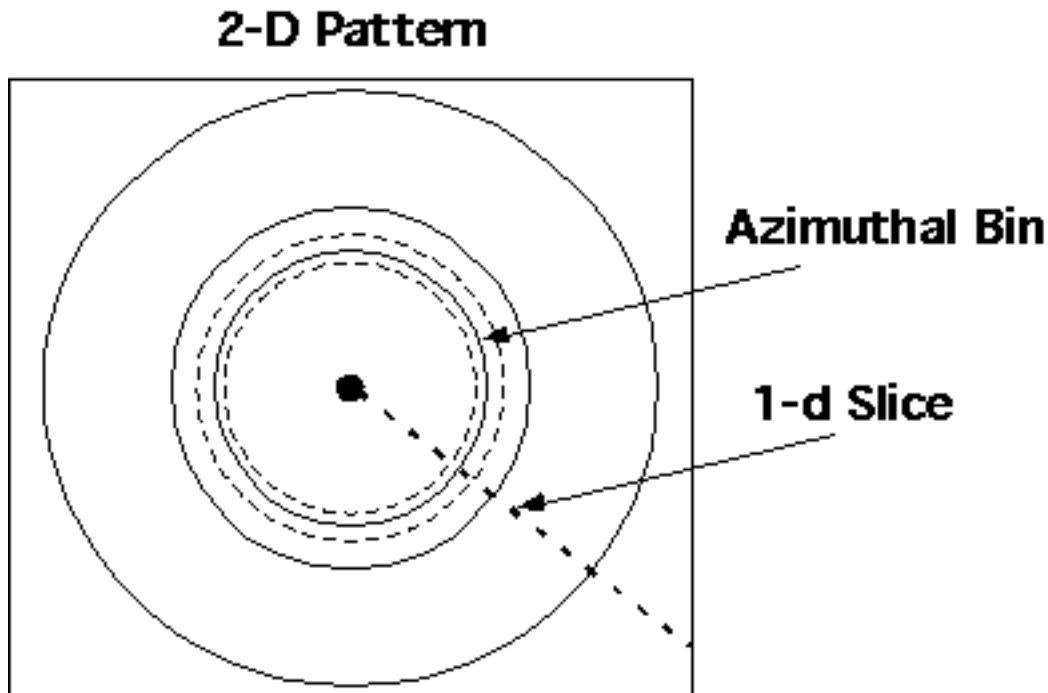
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[=Down Load 2-d Data \(.zip of a text file\).](#)

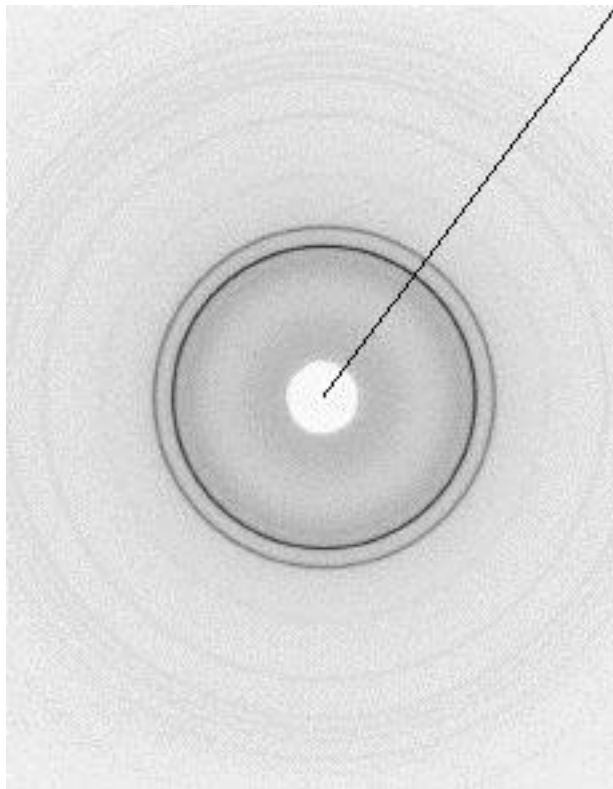
Computer Program

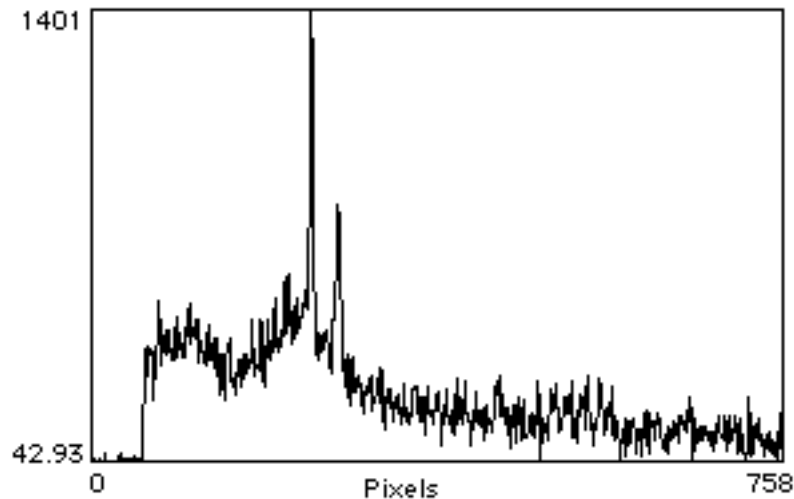
In many analytic measurements 2-dimensional CCD detectors have replaced step-scanner and 1-dimensional detectors. This is the case for IR/Raman spectroscopy, XRD, and SAXS for instance. Manipulation of large 2-d data sets, then becomes an important application of computer programming for analytic techniques. A typical manipulation of [a large 2-d data set](#) would be to azimuthally average a radially isotropic data set about a center point to produce the equivalent of a 1-d step scan. For example, in a powder-pattern for XRD, a diffractometer step-scans across 2θ generating an intensity versus 2θ plot (Bold Dashed Line Below). Such a 1-d step scan might take 2 to 3 hours. If the diffraction pattern is isotropic, the same accuracy can be achieved in minutes using a 2-d detector. The 2-d pattern in this case is averaged about the beam center by binning the data into rings as shown below.



Cartoon of a 2-d pattern that would result by insertion of a 2-d detector perpendicular to the transmitted beam for a diffraction experiment. Solid circles are Debye-Scherrer lines, bold dashed line is data that would be collected from a step-scanner diffractometer, dashed circles delineate one of many "bins" that would be used to average a certain value of 2θ , distance from the center. Dark spot in middle is the transmitted beam location.

*[A large 2-d data set](#) from a diffraction measurement on a semi-crystalline polymer will be provided as a "zip" compressed tab delimited text file. **The file contains 1226 rows and 962 columns with integers that range from 22 to 1566.** An image made from this 2-d table is given below with the slice indicated by the line in the following plot:*





Your computer program will perform the following sequence of operations on this 2-d tab delimited text file:

- 1. Read the 2-d text file*
- 2. Generate a 1-d slice of the 2-d data set similar to the dashed line in the figure above. Convert the 1-d slice to a 3 column tab-delimited text file of 2 Intensity and Standard Deviation that will be plotted.*
- 3. Generate a similar 3 column tab-delimited file by Azimuthally averaging the data using an azimuthal binning routine.*

You should assume that the input data is in counts.

The report must include:

- 1. A text printout of your program.*
 - 2. A plot of the two 1-d data sets with the error bars you have calculated.*
 - 3. A text printout of the two tab delimited text files.*
 - 4. A comparison of the two data sets and a discussion of the advantage of a 2-d detector over a 1-d detector or a step-scanning detector.*
 - 5. A brief discussion of the features evident in the final diffraction pattern.*
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