Introduction to Crystallography (Homework No. 4)

Due Date: December 3th, 2008

- 1. In class, we have dealt with various examples of 1D-diffraction. The main purpose of this procedure is to understand the general features of diffraction. The following is two notable messages we can conclude from one-dimensional calculations. By employing appropriate one-dimensional examples, explain how these statements can be concluded. You should include graphical representations in your explanation. (It is encouraged to utilize computer plotting programs.)
- (a) When we observe diffraction patterns produced by periodic scattering centers, the main peaks become sharper as the number of scattering centers increases. This tendency also accompanies the reduction of subsidiary peaks to a noise level.
- (b) The reciprocal feature of diffraction can be noticed when you consider the size effects. As the interacting obstacle becomes smaller, the resulting peak becomes broader. (Try changing the width of your slit.)
- 2. Considering the following diagram, the size effect discussed in the previous problem seems to be applicable to the first and third section. Firstly, consider the first section which corresponds to the information of the motif of the crystal. Since the actual motif function can be much more complex than the digital function indicated in the diagram, the resulting Fourier transform is likely to not give much information about the size of the motif. The third section is the so-called shape function which reflects the practical limiting factors such as grain size, beam size, etc. Assuming that you observe the diffraction pattern of crystalline grains with different shapes, extend your conclusion from 1D-results to explain how the shape of the grains (ex: rod or plate-like) would affect your diffraction patterns.



3. From one-dimensional demonstration, it has been concluded that three types of structural information could be derived from diffraction patterns: information concerning the lattice, motif and crystal shape. Explain, with reasons and in detail, which attributes of the diffraction pattern give the data of each structural information.