Chemical Crystallography: Exercise No. 2

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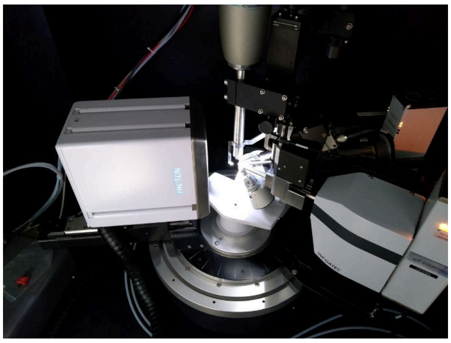
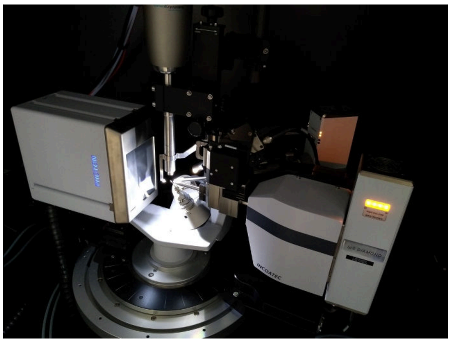
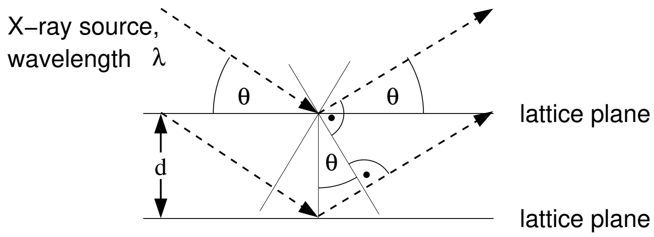
1 Experimental setup

Above are two images of the D8 diffractometer at the X-ray Centre.

1. Where is the crystal located?
2. Where is the detector?
3. The instrument has two X-ray sources. Where are they?
4. What are the two possible types of movements of the detector?
5. What are the effects of these two types of movement of the detector for the diffraction image?
6. What are the possible movements of the crystal?

2 Resolution



The resolution d in Bragg's law ($\lambda = 2d \sin \theta$) is **low**, when the planes are far apart, i.e., when d is large. The resolution is **high**, when the planes are close to each other, i.e., when d is a small number.

1. What is the resolution of an optical instrument like a microscope, or a telescope? Describe in simple words!
2. Discuss why a crystal is of "high quality", when it diffracts far, i.e., when the diffraction pattern reaches high resolution. **Hint:** Do not think in terms of Bragg's law, but consider what the crystal is composed of.

3 Fourier transform

The electron density $\rho(x, y, z)$ within the unit cell can be computed via the structure factors $F(hkl)$ by Fourier transform:

$$\rho(x, y, z) = const \cdot \sum_{h,k,l} F(hkl) e^{2\pi i(hx+ky+lz)}$$

The reverse equation is called "back transform:

$$F(hkl) = const' \cdot \int_{\text{unit cell}} \rho(x, y, z) e^{-2\pi i(hx+ky+lz)} dxdydz \quad (1)$$

In crystallography, the Fourier transform transforms the continuous electron density into discrete structure factors, and the other way round.

1. A piano can be considered a Fourier transform instrument. What does the piano transform?

   (**Hint**: Both in optics, as well as in acoustics, physicists work with "waves".)

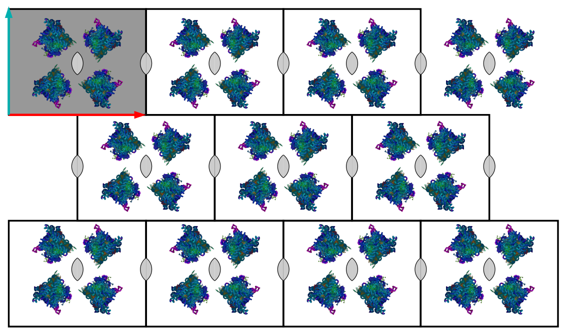
2. What does the electron density correspond to, and what do the structure factors correspond to?

3. What could you consider the resolution of the piano? (**Hint**: every (normal) piano has the same resolution.)

4. Would you consider a trombone a Fourier transform instrument, too?

4 Unit cell

You are familiar with the following figure from the lecture. The greyed area is not a unit cell for this crystal. Why?



5 Powder diffraction

You are given the wavelength λ for ein X-ray diffraction experiment, and the resolution d for some reflection $(h_{\text{Ex. 5}} \quad k_{\text{Ex. 5}} \quad l_{\text{Ex. 5}})$. The detector place at $2\theta = 0°$, i.e. the direct beam points at the centre of the detector.

1. How much does this information tell you about the position of the reflection on the detector?

2. How much do you know about the position of all of the symmetry equivalent reflections of $(h_{\text{Ex. 5}} \quad k_{\text{Ex. 5}} \quad l_{\text{Ex. 5}})$?

3. Try to figure out (qualitatively), what the diffraction pattern for a microcrystalline powder looks like (e.g. finely ground sugar, or finely ground salt)!

6 Symmetry

This exercise needs the game of skill. For each piece, figure out in how many ways it can be fit into its frame! What are the respective symmetry elements?