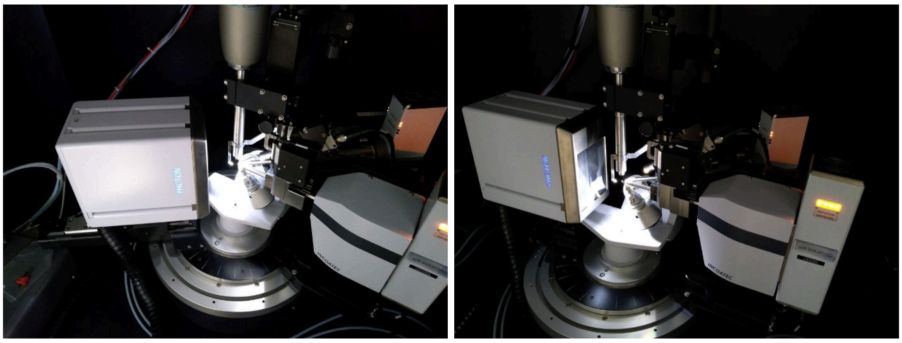
1 Experimental setup



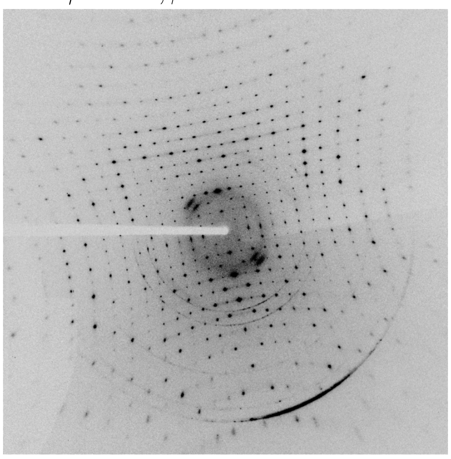
Above are two images of the D8 diffractometer at the X-ray Centre.

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?

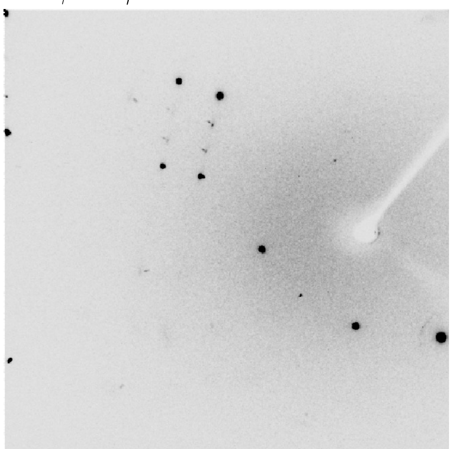
2 Diffraction images

The following two diffraction images were shown during the lectures:

$14.2 \times 16.2 \times 27.9$ Å^3
$\alpha = \gamma = 90°, \beta = 87.9°$

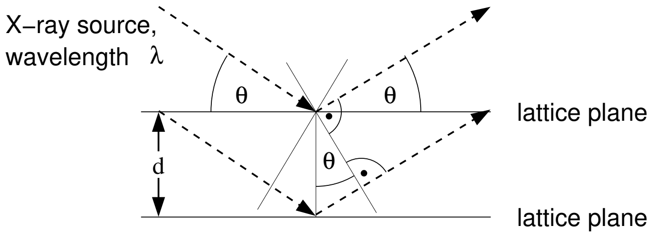


$10.56 \times 11.64 \times 16.14$ Å^3
$\alpha = \beta = \gamma = 90°$



The unit cells have quite similar dimensions, yet the left images shows many, many more spots. What could be the reasons? (Hint: two different possibilities)

3 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.

4 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:

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



In crystallography, the Fourier transform transforms electron density into 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 piano has the same resolution.)

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

5 Unit cell

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