

## The equations: (Good-Parts version: what you really need to remember)

Bragg's law (as used to track each individual scattered ray):

$$\lambda = 2d_{h,k,l} \sin(\theta_{h,k,l}) \quad \frac{1}{d_{h,k,l}} = \frac{2 \sin(\theta_{h,k,l})}{\lambda} \quad \text{between } d_{h,k,l} \text{ and } \theta_{h,k,l}$$

Remember this equation!

Note the reciprocal relationship

d: distance, but direction only implied!

$d_{h,k,l}$  is a particular indexed distance in the crystal, and is the “resolution” of the  $h,k,l$  diffracted ray. The smaller the  $d$ , the better the resolution, thus the best resolution data is from diffracted rays with the largest angles. The index carries a lot of the “direction” information.

These “ $d$ ”s are distances between “Bragg Planes”. Bragg Planes are simply ways of dividing the unit-cells of the crystal into equally spaced intervals (the “ $d$ ” spacing). So Bragg Planes are oriented families of parallel planes with a particular separation. The  $h,k,l$  indices, along with the unit cell dimensions and shape, define both the orientation and the  $d$ -spacing of a particular set of Bragg Planes.

(The unit cell is the basic repeating unit of the crystal: the repeat is done entirely by translations, and the unit cells “tile” (completely fill) the volume of the crystal.)

The “ $\theta$ ” is the angle the ray makes to the Bragg Plane, and in the defining construction the angle of the incident ray is equal to the angle of the diffracted ray, just like a classical reflection, so the diffracted rays are often called “reflections”.

### CAVEAT:

When discussing crystallography, many people remember Bragg's law this way:

$$n\lambda = 2d \sin(\theta) \quad \text{more specifically:} \quad n\lambda = 2d_{\text{unit cell}} \sin(\theta)$$

where  $\lambda$  is the wavelength of the x-rays,  $d$  is a dimension of the unit cell of the crystal, and  $\theta$  is the angle of the scattered ray from “Bragg Planes”, and the integer  $n$  is the number of wavelengths of path difference between a ray scattered from one side of the unit cell and a ray scattered from the opposite side of the unit cell.

The “ $n$ ” formula brings to mind vibrating string harmonics. Indeed, we will see how the electron density can be thought of as a sum of standing waves in the box of the unit cell.

This  $n$ , the order of the diffraction, is useful for fiber diffraction and is reasonably convenient for small molecule crystals with very small unit cells, BUT can be very confusing when thinking about diffraction from macromolecular crystals. (For convenience, the examples drawn in text books and lecture notes show small unit cells, so drawings with the “ $n$ ” form seem to make sense. However, in real life, or with general equations, dealing with large unit cells, everything is done in terms of uniquely indexed Bragg planes, i.e. uniquely indexed diffraction events.).