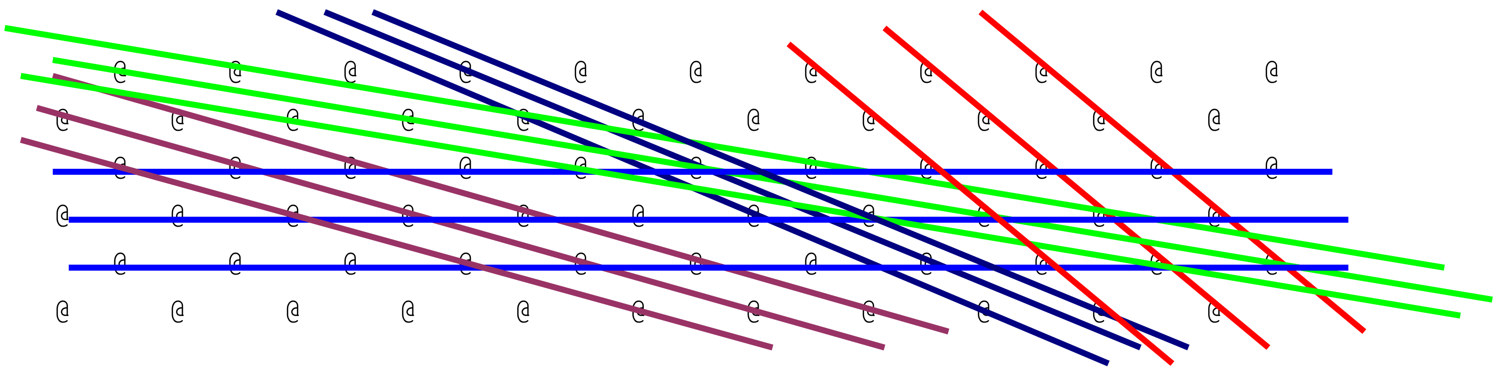
Bragg Diffraction: A rough and simple look

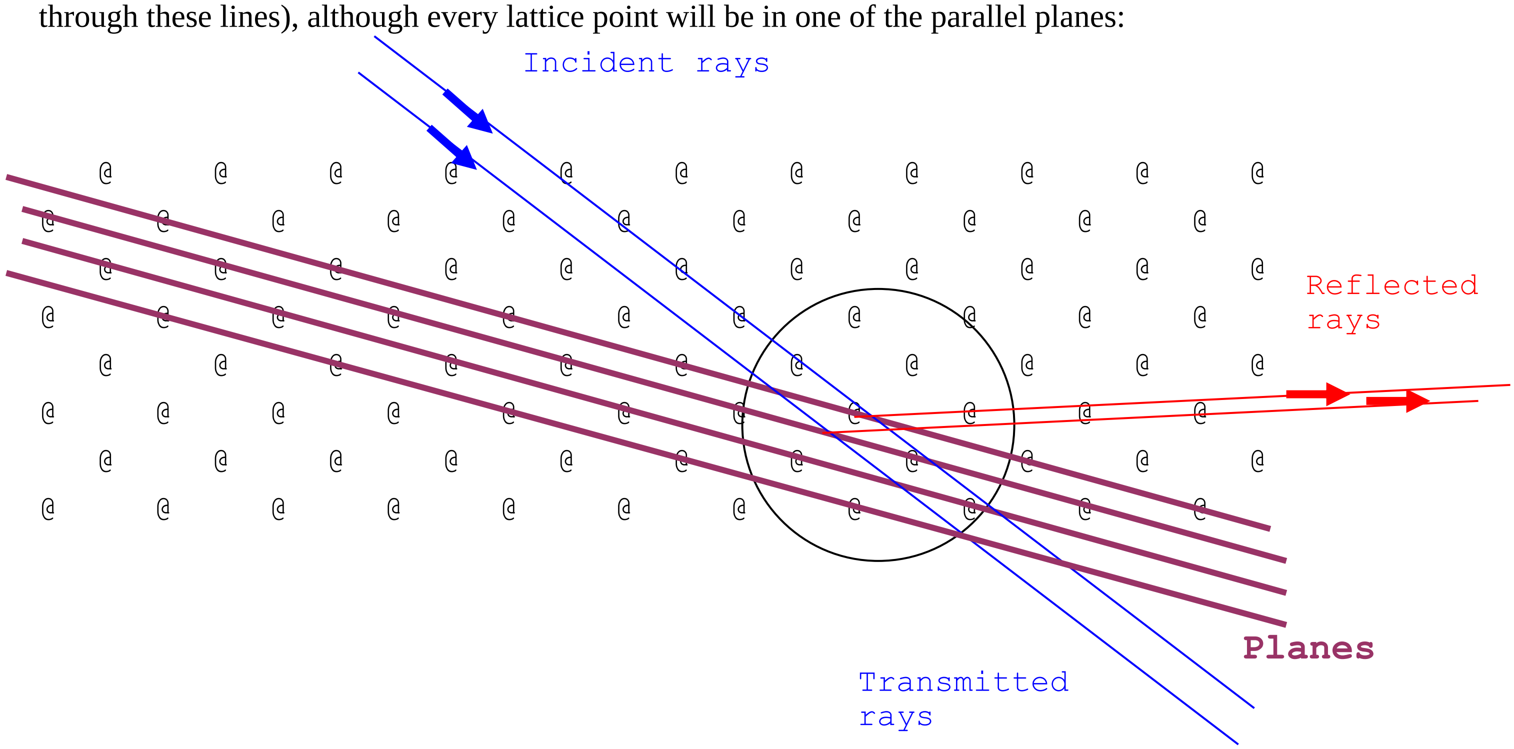
1. Assumption: Instead of discrete atoms, we will consider the lattice to be made up of **continuous planes** where each atom (more specifically, the basis) is located in the planes. Each atom (or basis) can be considered to be located in many planes, just like any point in space can be considered to be located in many planes.

2. Diagram (2-D) of lattice with @ marking positions of basis and three planes each (same color) of five of the different planes (different colors) drawn in: (3-D planes go through the lines on the 2-D diagram) To get the Miller indices of a couple of these planes, see the last page.



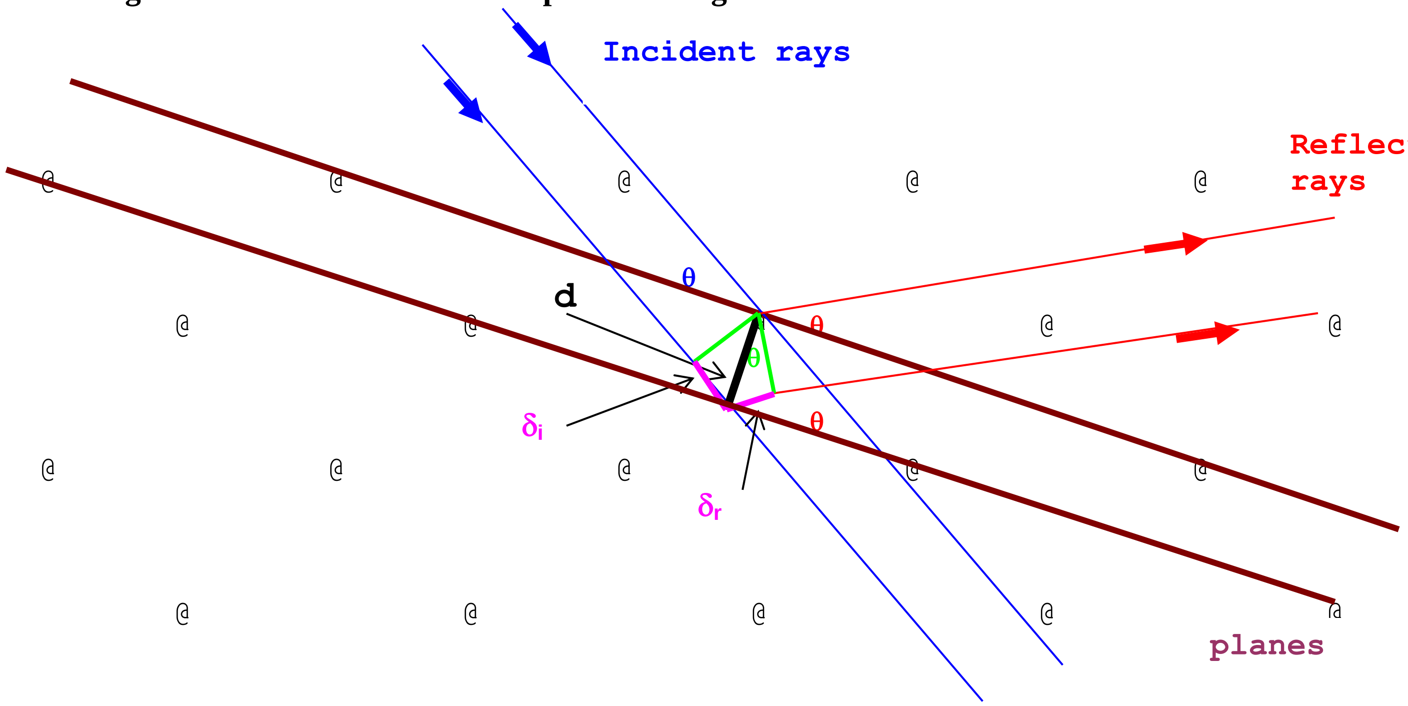
3. Basic rough and simple idea: x-rays are E&M waves that partially bounce off of each plane and partially (in fact, mainly) penetrate through each plane. The reflected parts of the waves add up and in general add up destructively. Only if the waves add up constructively will we get a reflected beam. This will happen when the path difference between any two beams hitting adjacent parallel planes is an integer of the wavelength of the incident E&M wave.

4. Diagram of diffracted beam from one set of planes (only four lines are drawn (with 3-D planes going through these lines), although every lattice point will be in one of the parallel planes:



Bragg Diffraction: a rough and simple look (cont)

5. Magnified view of circled area on previous diagram:



6. Derivation of Bragg formula from this rough and simple model:

d = distance between planes
θ = angle between the plane and the incident ray of beam; it is also the angle between the plane and the reflected ray of the beam (**θ**=**θ**)
λ = wavelength of the x-ray (E&M wave); for elastic scattering, the incoming λ should equal the outgoing λ.
n = integer
δi = extra distance incident wave travels over that in incident wave that reflects off next higher plane
δr = extra distance reflected wave travels over that in reflected wave that reflects off next higher plane

a) In order for the two reflected waves to be in phase and hence add constructively, $\delta i + \delta r = n\lambda$.

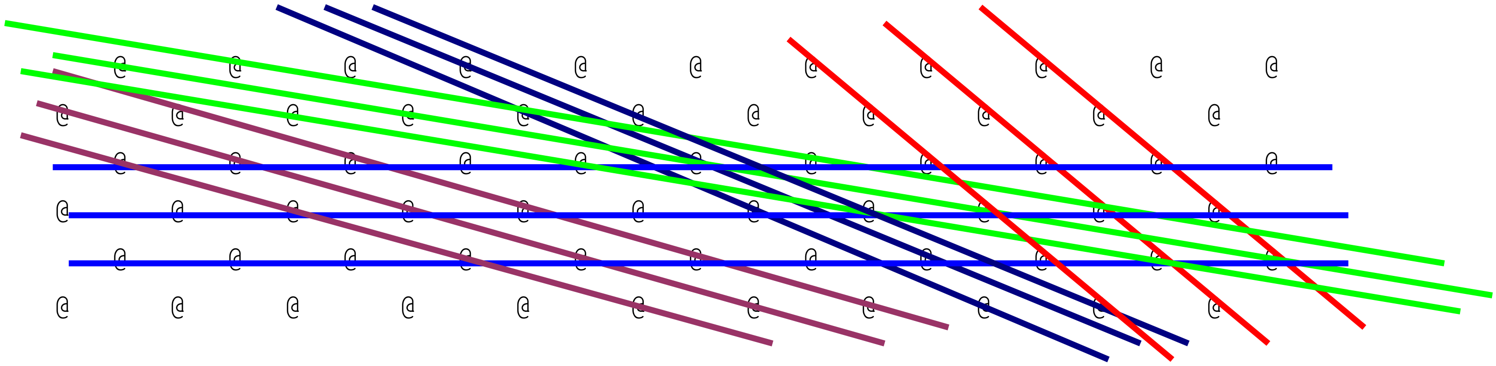
b) From the geometry, the angle **θ** = **θ**. This can be seen from the fact that the "d" line is perpendicular to the lattice plane lines and the green lines are perpendicular to the parallel x-ray lines.

c) From the definition of sine as opposite over adjacent, and using part b (**θ** = **θ**), we have $\delta i = d\sin(\theta)$ and likewise $\delta r = d\sin(\theta)$.

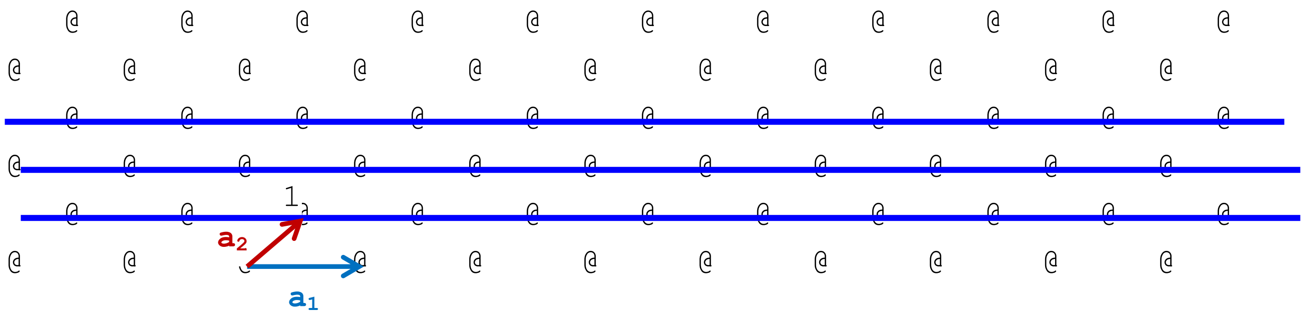
d) Therefore, using part a and part c we have our result:

$$n\lambda = 2d\sin(\theta)$$

2 - extended. Diagram (2-D) of lattice with @ marking positions of basis and three planes each (same color) of five of the different planes (different colors) drawn in: `(3-D planes go through the lines on the 2-D diagram)`

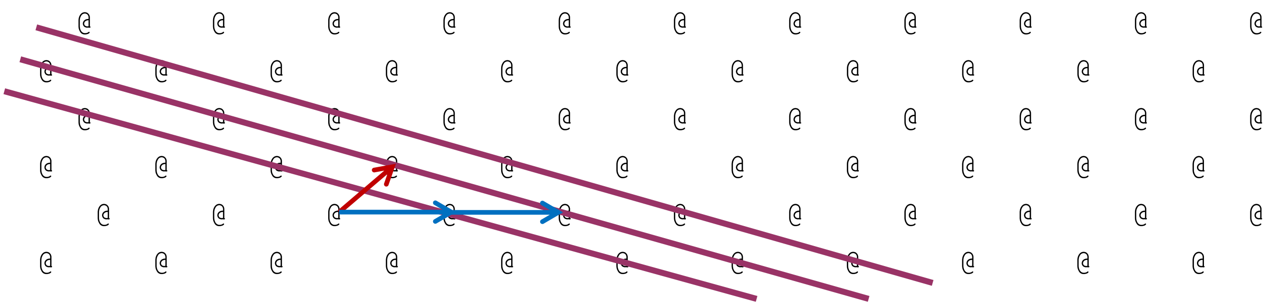


If we look at the blue planes and use the primitive lattice vectors as shown (with the third primitive lattice vector directed out of the page)



Then to get the Miller indices of the blue planes:
We can't reach the blue plane in the a_1 direction, we can the blue plane in the a_2 direction with 1**a_2**, and we'll assume we can't reach the blue plane in the a_3 direction (too hard to picture on a 2-D page). Therefore, $n = \infty$, $m=1$, and $p=\infty$, so inverting we get $1/\infty$, $1/1$, and $1/\infty$ so now we have **(010)** for the blue planes.

If we look at the brown planes and use the same primitive lattice vectors as above,



We can reach a brown plane with $2a_1$ and with $1a_2$ and we'll again assume we can't reach the brown plane in the a_3 direction. Therefore, $n=2$, $m=1$, and $p=\infty$, so inverting we get $1/2$, $1/1$, and $1/\infty$, and getting a common denominator: $1/2$, $2/2$, and $0/2$, so now we have **(120)** for the Miller indices of the brown planes.