Lecture 4- Reciprocal lattice and diffraction

- **Review reciprocal lattice and properties of reciprocal lattice vectors**
- **Bragg condition**
- **Laue condition**

Review of reciprocal lattice:

Definition

Consider direct lattice defined by vectors $\boldsymbol{R} = u_1\boldsymbol{a_1} + u_2\boldsymbol{a_2} + u_3\boldsymbol{a_3}$ where u_1, u_2, u_3 are integers and $\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3}$ are primitive translation vectors

The reciprocal lattice is defined by (primitive) vectors $\boldsymbol{b_1}, \boldsymbol{b_2}, \boldsymbol{b_3}$ defined in the following way:

$$\boldsymbol{b_1} = 2\pi \frac{\boldsymbol{a_2} \times \boldsymbol{a_3}}{\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}}$$

$$\boldsymbol{b_2} = 2\pi \frac{\boldsymbol{a_3} \times \boldsymbol{a_1}}{\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}}$$

$$\boldsymbol{b_3} = 2\pi \frac{\boldsymbol{a_1} \times \boldsymbol{a_2}}{\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}}$$

The reciprocal lattice is also a lattice, with all points accessed by reciprocal lattice vector

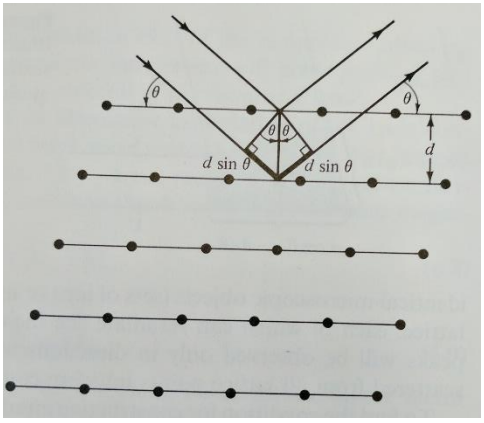
$$\boldsymbol{G} = \nu_1\boldsymbol{b_1} + \nu_2\boldsymbol{b_2} + \nu_3\boldsymbol{b_3}$$

Where ν_1, ν_2, ν_3 are integers

Another important property of the reciprocal lattice is that $\boldsymbol{R} \cdot \boldsymbol{G} = 2\pi n$ where n is an integer. This statement can be derived from the property that $\boldsymbol{b_i} \cdot \boldsymbol{a_j} = 2\pi\delta_{ij}$ where $\delta_{ij} = 0$ if $i \neq j$ and $\delta_{ij} = 1$ if $i = j$ (and you can use this property to double check that you have really found the reciprocal lattice)

Scattering: application of reciprocal lattice

Old way:



Ray 1 travels a distance $2dsin\theta$ longer than ray 2

For them to **constructively interfere,** this path length difference, must be an integer multiple of the wavelength of light, $n\lambda$

This gives the usual formulation of Bragg's law, $2dsin\theta = n\lambda$

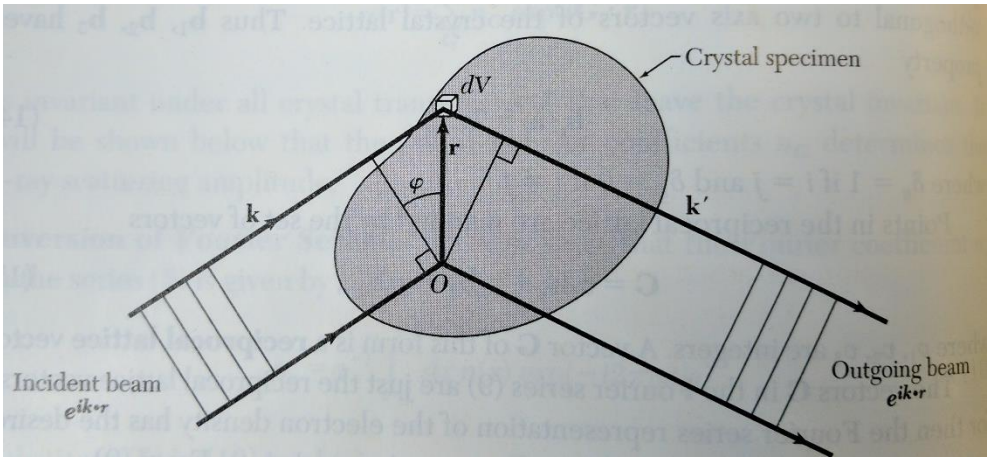
Detour: actual numbers

Bragg's law will work if d is of similar magnitude to λ

Object	**Source of diffracted wave**
Diffraction grating in class ($d \sim 1\mu m$)	Laser pointer, $\lambda = 532\ nm$
Planes of crystal ($d \sim 1 - 10\text{Å}$)	x-rays, $\lambda \sim 0.1 - 10\text{Å}$
Planes of crystal ($d \sim 1 - 10\text{Å}$)	Neutrons, $\lambda = \frac{h}{p} \sim 0.3 - 2\text{Å}$
Planes of crystal ($d \sim 1 - 10\text{Å}$)	Electrons, $\lambda = \frac{h}{p} \sim 0.1 - 1\text{Å}$

Bragg's law can be reformulated using the reciprocal lattice

Theorem: the set of reciprocal lattice vectors **G** determines the possible x-ray reflections



In the figure above, the incident beam is a plane wave given by $e^{i\mathbf{k}\cdot r}$. We consider the wave scattered from two different positions in the solid: the origin (given by O) and a volume element **r** away, called dV. The wavevector **k** encodes the wavelength of the light $k = 2\pi/\lambda$ and also its propagation direction.

Step 1: find **phase** difference of the **incoming** beams as they travel to O as compared to dV (confusing point in figure: k and r have different units)

The **path length** difference is given by $rsin\phi$

Lets express that path length difference as a phase difference (what fraction of 2pi?)

In words, the phase difference is given by $\frac{\text{path length difference}}{\text{wavelength}} * 2\pi$. The first term gives the number of wavelengths which fit in the path length difference (not necessarily an integer) and the factor of 2π tells you what fraction of a full wave cycle this path length difference corresponds to. This gives a phase difference of $2\pi r\ sin\phi/\lambda$

Remember, $k = \frac{2\pi}{\lambda}$ (definition of wave number)

Thus, the **phase difference** of the incoming beam going to O vs going to dV is $\boldsymbol{k} \cdot \boldsymbol{r}$

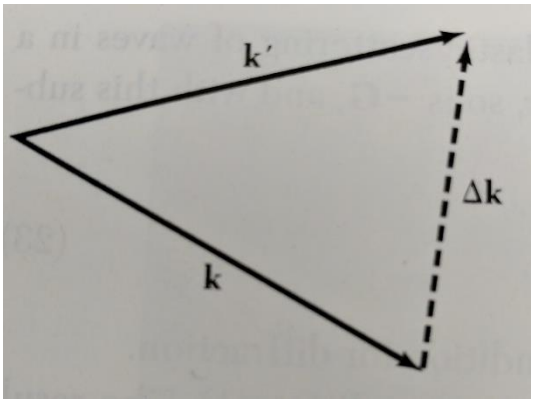
Step 2: find phase difference of diffracted beam from O vs dV

For the diffracted beam, if we go through the same exercise, we will get $-\boldsymbol{k}' \cdot \boldsymbol{r}$ (the negative factor comes because **k'** points in the opposite direction relative to **r**; also, there is a typo in your textbook in labeling the outgoing beam, it should be $e^{i\boldsymbol{k}\prime \cdot \boldsymbol{r}}$)

Thus the total phase angle difference is $(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{r}$

The wave scattered from dV has a phase factor of $e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot \boldsymbol{r}}$ relative to the wave scattered from the origin located distance **r** away.

Define $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$



Now, we have to account for the fact that we are not just considering two scatterers, but we are considering an array of scatterers. The relative positions of all of these scatters are given by the lattice vectors: $\boldsymbol{R} = u_1\boldsymbol{a_1} + u_2\boldsymbol{a_2} + u_3\boldsymbol{a_3}$

The total phase factor from this array of scatterers is given by:

$$F(\Delta\boldsymbol{k}) = \sum_j e^{i\Delta\boldsymbol{k}\cdot\boldsymbol{r_j}}$$

The **intensity** of the scattered beam:

$$|F(\Delta\boldsymbol{k})|^2 = \sum_{i,j} e^{i\Delta\boldsymbol{k}\cdot(\boldsymbol{r_i}-\boldsymbol{r_j})}$$

The separation between any two scatterers in a bravais lattice is given by a translation vector of the lattice:

$$|F(\Delta\boldsymbol{k})|^2 = \sum_{i,j} e^{i\Delta\boldsymbol{k}\cdot(u_1a_1+u_2a_2+u_3a_3)}$$

Each of the exponential terms will be equal to 1 if $\boxed{\Delta \boldsymbol{k} = \boldsymbol{G}}$ where **G** is a vector of the **reciprocal lattice**. This is called the **laue condition**.

Most scattering experiments used to determine crystal structure are **elastic** experiments, meaning the energy (and wavelength) of the incoming and outgoing beam are the same. This also means that the magnitudes of the wavevectors are equal:

$|\boldsymbol{k}| = |\boldsymbol{k}'|$ and $k^2 = k'^2$

With this, the diffraction condition can be re-written as:

$$\boldsymbol{G} = \boldsymbol{k}' - \boldsymbol{k}$$

$$(\boldsymbol{k} + \boldsymbol{G})^2 = k'^2 = k^2$$

$$(k^2 + 2\boldsymbol{k} \cdot \boldsymbol{G} + G^2) = k^2$$

$$2\boldsymbol{k} \cdot \boldsymbol{G} + G^2 = 0$$

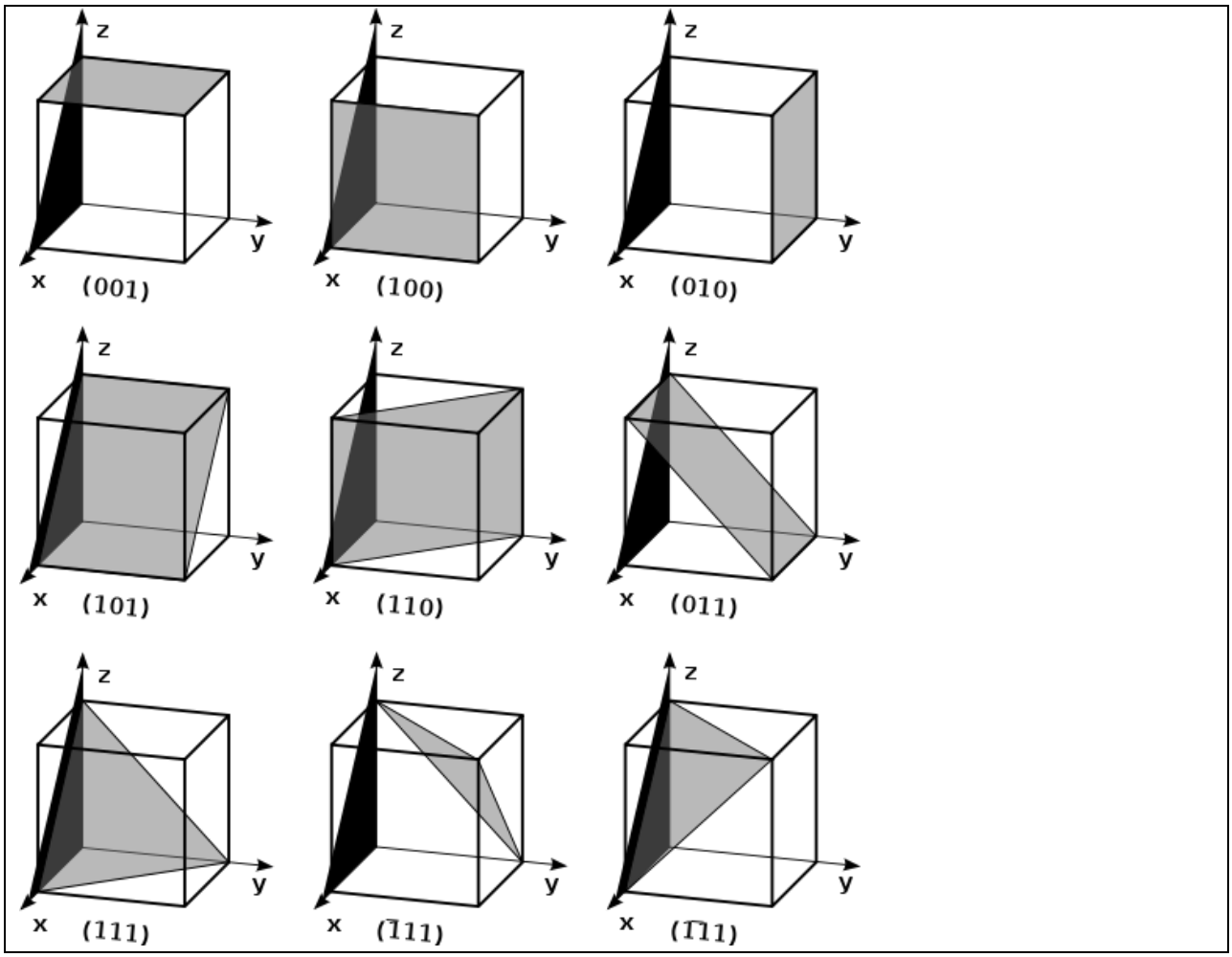
$2\boldsymbol{k} \cdot \boldsymbol{G} = G^2$ (we can do this because if **G** is a vector of the reciprocal lattice, so is **–G**)

Detour: reminder about Miller indices

The process of finding miller indices:

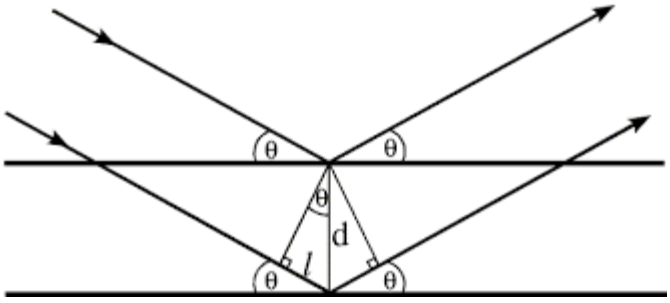
1. Find the intercepts on the axes in terms of the lattice constants a_1, a_2, a_3; Integer or fractional intercepts are fine
2. Take the reciprocals of these numbers and reduce to 3 smallest integers
3. Express result as 3 numbers in parentheses, usually no commas (hkl)

Below: examples for cubic lattice



Remember, a crystal lattice can be divided up into equivalent **planes**, a concept which is formalized via miller indices in Ch 1 of your textbook. The spacing between adjacent planes with a specific miller index is called d(hkl).

It turns out that $d(hkl) = 2\pi/|\boldsymbol{G}|$ where $\boldsymbol{G} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3}$ is **normal** to the plane of interest (we will show this for specific examples shortly).



Plugging this result back in to $2\boldsymbol{k} \cdot \boldsymbol{G} = G^2$ we get

$$2\left(\frac{2\pi}{\lambda}\right)(sin\theta)\frac{2\pi}{d(hkl)} = \left(\frac{2\pi}{d(hkl)}\right)^2$$

(θ is the angle of the incident beam relative to the planes. The sine comes in because **G** is normal to the plane of interest, and the dot product takes the component of one vector along the direction of the other)

Simplifying the expression above:

$$\frac{4\pi sin\theta}{\lambda} = \frac{2\pi}{d(hkl)}$$

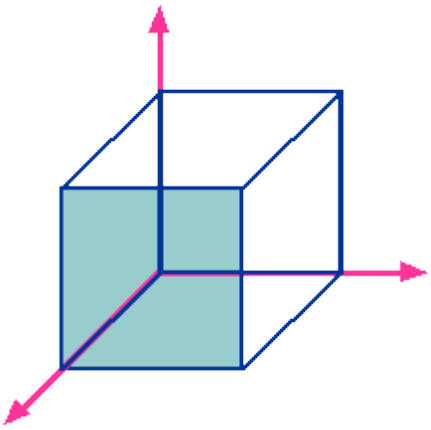
$$2d(hkl)sin\theta = \lambda$$

This is basically the Bragg condition, sans a factor of integer n in front of λ . This is missing because the definition of miller indices we use explicitly removes common integer divisors. E.g. (h/n,k/n,l/n) would be reduced to just the (hkl) plane by the definition.

Thus, we have shown the equivalency of Bragg's law and a scattering formalism using the reciprocal lattice.

Example problem: show equivalence of Bragg's law and Laue condition for simple cubic lattice with lattice spacing a

a) 100 planes



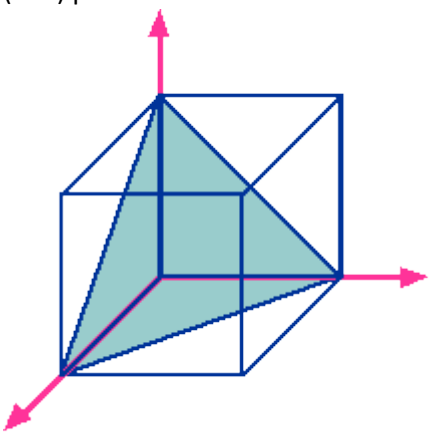
the spacing between (100) planes in adjacent unit cell is just the lattice spacing a
We want to show that $d(hkl) = 2\pi/|\boldsymbol{G}|$ and $\boldsymbol{G} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3}$ is normal to the plane of interest
Step 1: extract reciprocal lattice vectors (for simple cubic and other primitive orthogonal crystal systems, we can just do this by inspection; reminder $\boldsymbol{R} = u_1 a\hat{\boldsymbol{x}} + u_2 a\hat{\boldsymbol{y}} + u_3 a\hat{\boldsymbol{z}}$).

$$\boldsymbol{b_1} = \frac{2\pi}{a}\hat{\boldsymbol{x}}, \boldsymbol{b_2} = \frac{2\pi}{a}\hat{\boldsymbol{y}}, \boldsymbol{b_3} = \frac{2\pi}{a}\hat{\boldsymbol{z}}$$

For the given values of hkl, we get $\boldsymbol{G} = \boldsymbol{b_1} = \frac{2\pi}{a}\hat{\boldsymbol{x}}$

a. $d(100) = \frac{2\pi}{\frac{2\pi}{a}} = a$
b. **G** points in the x direction which is indeed orthogonal to the plane drawn above (by inspection)

b) (111) planes



First, let's calculate the minimum spacing between 111 planes in cubic crystal system using geometry. There is an equivalent plane connecting three other vertices of the cube above, and each plane is 1/3 of the way along the orthogonal cube diagonal (not so easy to visualize, huh). The length of the diagonal of a cube is given by $a\sqrt{3}$ and the spacing between adjacent 111 planes is $\frac{a\sqrt{3}}{3} = \frac{a}{\sqrt{3}}$

a. $\boldsymbol{G} = \frac{2\pi}{a}\hat{\boldsymbol{x}} + \frac{2\pi}{a}\hat{\boldsymbol{y}} + \frac{2\pi}{a}\hat{\boldsymbol{z}}$
$\frac{2\pi}{|\boldsymbol{G}|} = \frac{2\pi}{\frac{2\pi}{a}\sqrt{3}} = \frac{a}{\sqrt{3}}$ (much easier to calculate than figuring out the spacing between planes not oriented along crystal axes)

b. Is $\boldsymbol{G} = \frac{2\pi}{a}\hat{\boldsymbol{x}} + \frac{2\pi}{a}\hat{\boldsymbol{y}} + \frac{2\pi}{a}\hat{\boldsymbol{z}}$ normal to the (111) plane? By inspection, it looks like it is, since it points along the cube diagonal. Lets double check by choosing any vector in the plane and making sure that it is orthogonal to **G**
Choose the vector $-\hat{\boldsymbol{z}} + \hat{\boldsymbol{x}}$. This yields zero when it is dotted with **G**