# FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml

Based on Introduction to Solid State Physics by Kittel

## Course content

- **Periodic structures, understanding of diffraction experiment and reciprocal lattice**
- **Imperfections in crystals: diffusion, point defects, dislocations**
- **Crystal vibrations: phonon heat capacity and thermal conductivity**
- **Free electron Fermi gas: density of states, Fermi level, and electrical conductivity**
- **Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators**
- **Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions**
- **Metals: Fermi surfaces, temperature dependence of electrical conductivity**

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**FYS3410 lecture schedule and exams: Spring 2010**

| | | |
|---|---|---|
| M/18/1/2010: | Introduction and motivation. Periodicity and lattices | 2h |
| W/20/1/2010: | Index system for crystal planes. Crystal structures | 1h |
| M/25/1/2010: | Reciprocal space, Laue condition and Ewald construction | 2h |
| W/27/1/2010: | Interpretation of a diffraction experiment | 1h |
| M/01/2/2010: | Crystal binding and introduction to elastic strain | 2h |
| W/03/2/2010: | Point defects, case study – vacancies | 1h |
| M/08/2/2010: | Point defects and atomic diffusion | 2h |
| W/10/2/2010: | Diffusion (continuation); dislocations | 1h |
| M/15/2/2010: | Crystal vibrations and phonons | 2h |
| W/17/2/2010: | Crystal vibrations and phonons | 1h |
| M/22/2/2010: | Planck distribution and density of states | 2h |
| W/24/2/2010: | Debye model | 1h |
| M/01/3/2010: | Einstein model and general result for density of states | 2h |
| W/03/3/2010: | Thermal conductivity | 1h |
| M/08/3/2010: | Free electron Fermi gas in 1D and 3D – ground state | 2h |
| W/10/3/2010: | Density of states, effect of temperature – FD distribution | 1h |
| M/15/3/2010: | Heat capacity of FEFG | 2h |
| W/17/3/2010: | Repetition | 1h |
| 22/3/2010: | Mid-term exam | |

| | | |
|---|---|---|
| **M/14/4/2010:** | **Electrical and thermal conductivity in metals** | **2h** |
| **W/12/4/2010:** | **Bragg reflection of electron waves at the boundary of BZ** | **1h** |
| **M/19/4/2010:** | **Energy bands, Kronig - Penny model** | **2h** |
| **W/21/4/2010:** | **Empty lattice approximation; number of orbitals in a band** | **1h** |
| **M/26/4/2010:** | **Semiconductors, effective mass method, intrinsic carriers** | **2h** |
| **W/28/4/2010:** | **Impurity states in semiconductors and carrier statistics** | **1h** |
| **M/03/5/2010:** | **p-n junctions and heterojunctions** | **2h** |
| **W/05/5/2010:** | **surface structure, surface states, Schottky contacts** | **2h** |
| **M/10/5/2010:** | **no lectures** | |
| **W/12/5/2010:** | **no lectures** | |
| **W/19/5/2010:** | **Repetition** | **2h** |
| **W26/5/2010:** | **Repetition** | **2h** |

**28/5/2010: Final Exam** **(sensor: Prof. Arne Nylandsted Larsen at the Århus University, Denmark,** http://person.au.dk/en/anl@phys.au.dk**)**

**Lecture 3: Reciprocal space, Laue condition and Ewald construction**

- **(hkl) plain indices and distance between plains in cubic, tetragonal and orthorombic lattices;**
- **introduction of the reciprocal lattice;**
- **Bragg diffraction, Laue condition and Ewald construction;**
- **Some consequences: how many lines = reciprocal lattice point will we see**

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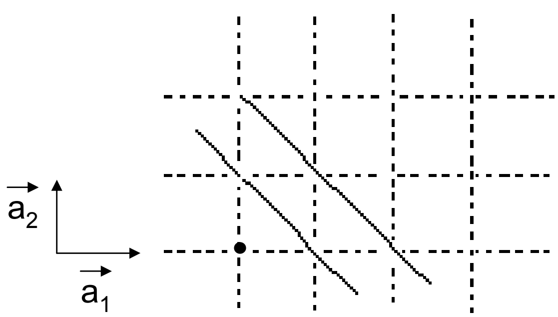
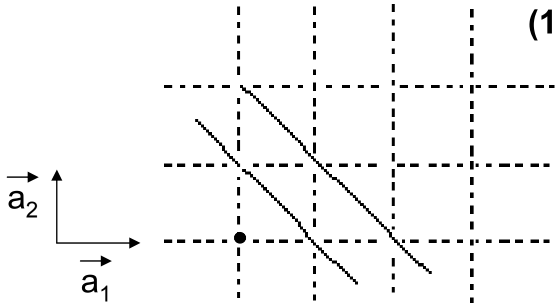
## (hkl) plain indices



## (hkl) plain indices

(110)

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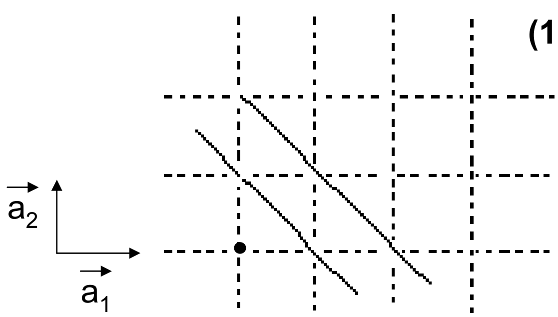
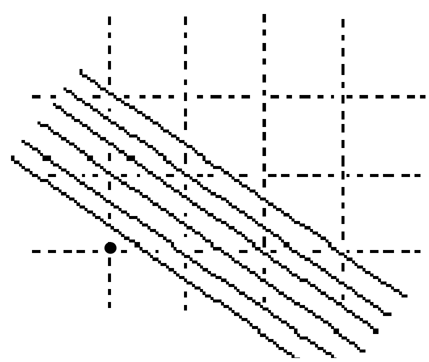
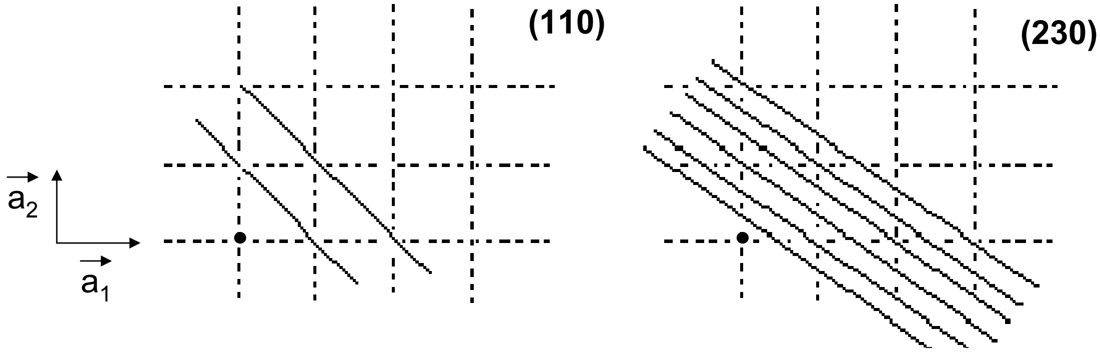
(110)



# (hkl) plain indices

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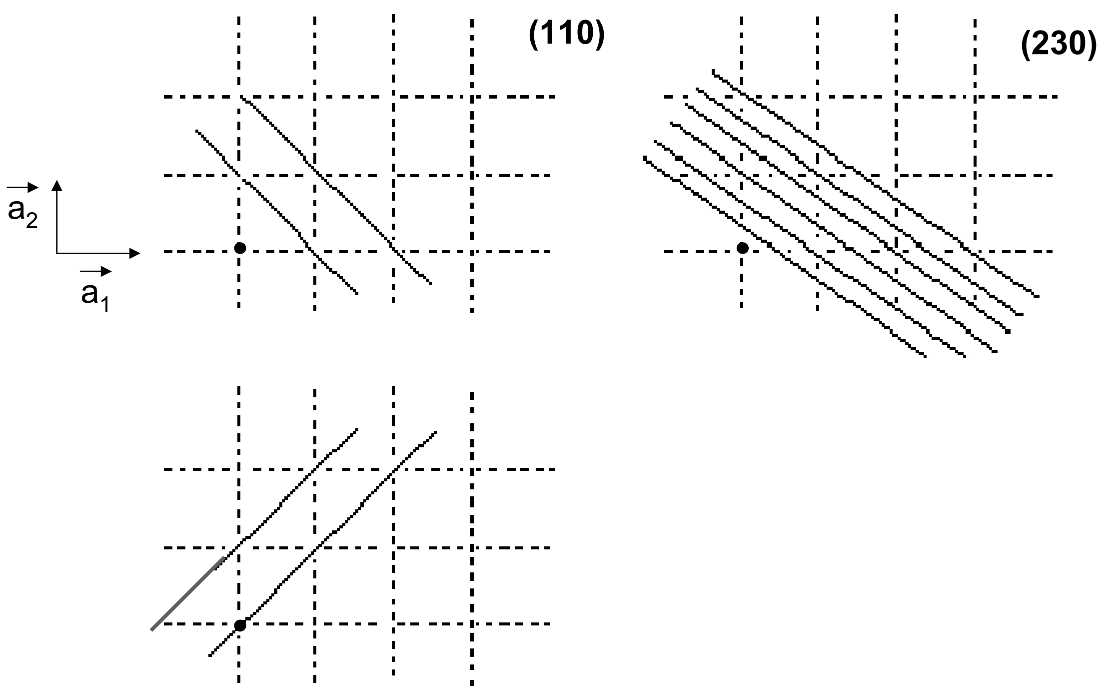

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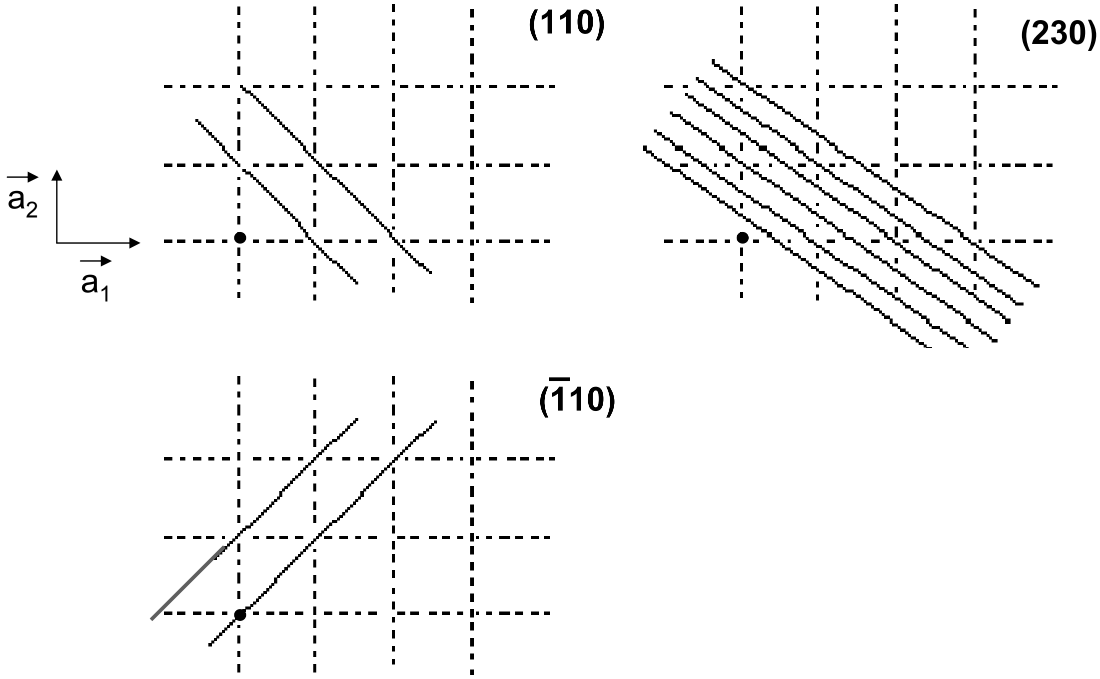
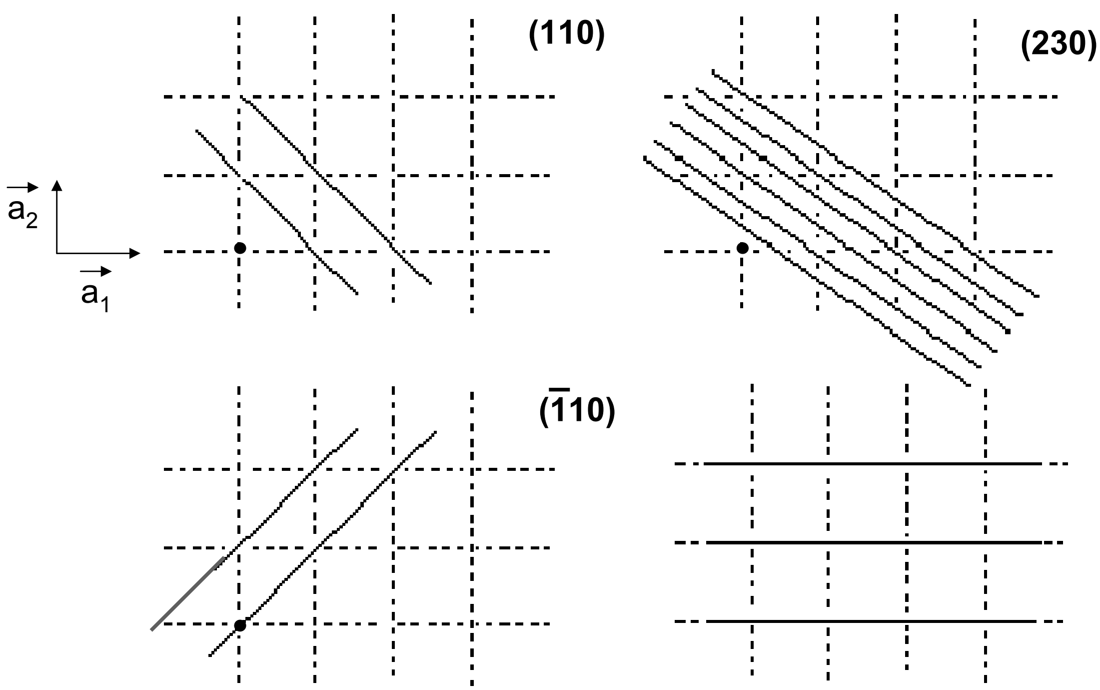
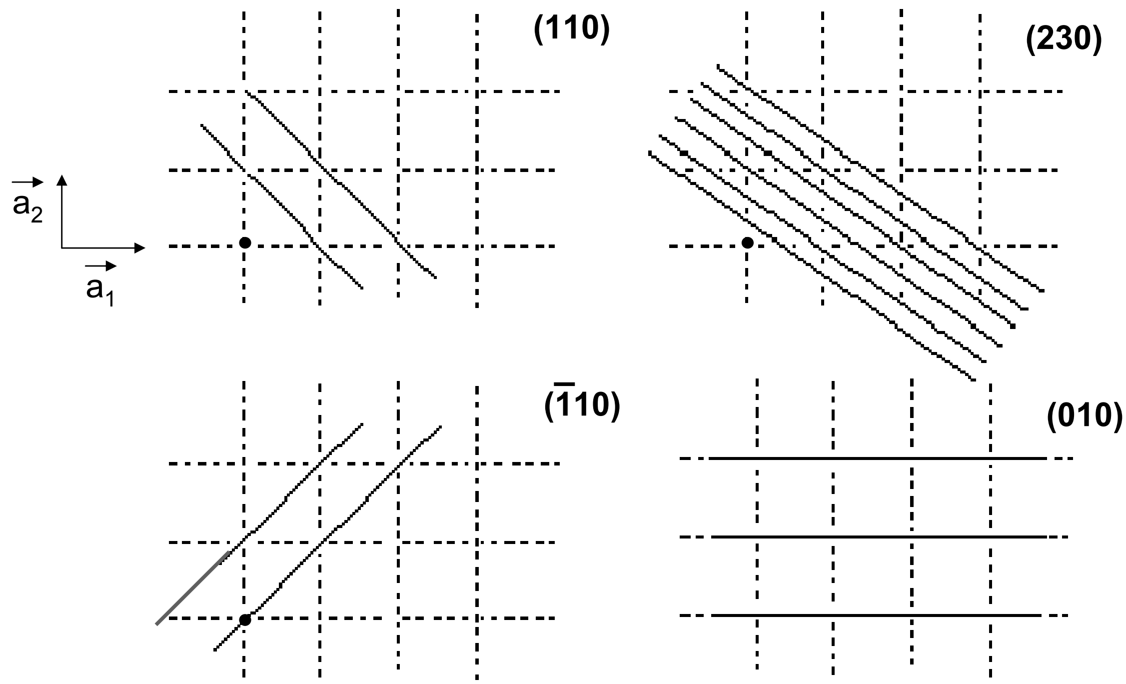


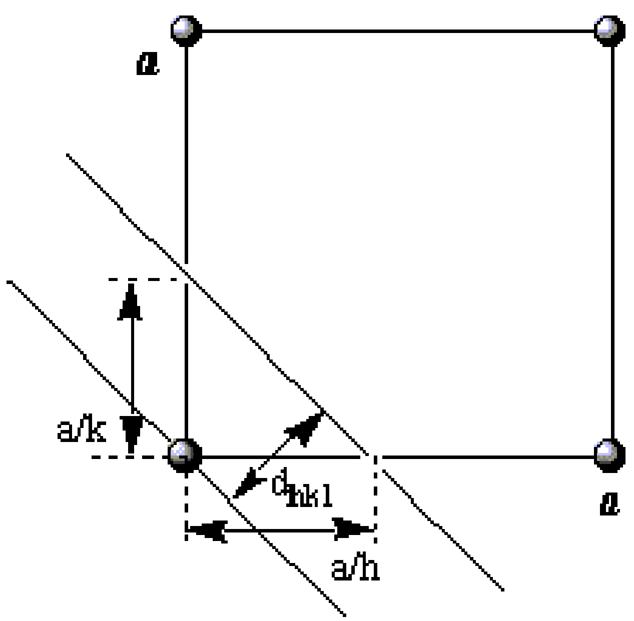

# (hkl) plain indices



## (hkl) plain indices




## Distance between (hkl)-plains in cubic lattices




$$d_{hkl} = \frac{a}{\sqrt{\left(h^2 + k^2 + l^2\right)}}$$

**Lecture 3: Reciprocal space, Laue condition and Ewald construction**

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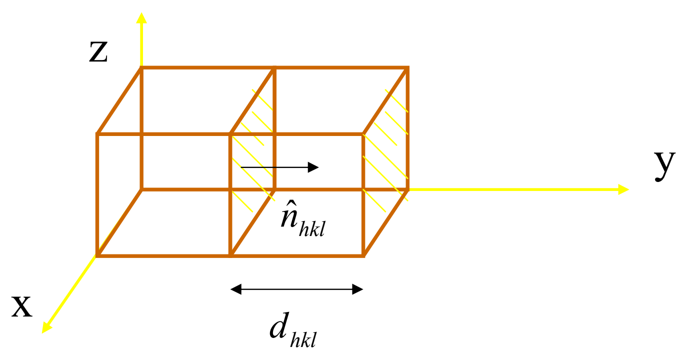
## Reciprocal lattice

Crystal planes (hkl) in the real-space or direct lattice are characterized by the normal vector $\hat{n}_{hkl}$ and the interplanar spacing $d_{hkl}$ :




Defining a different lattice in reciprocal space whose points lie at positions given by the vectors

$$\vec{G}_{hkl} \equiv \frac{2\pi\hat{n}_{hkl}}{d_{hkl}}$$

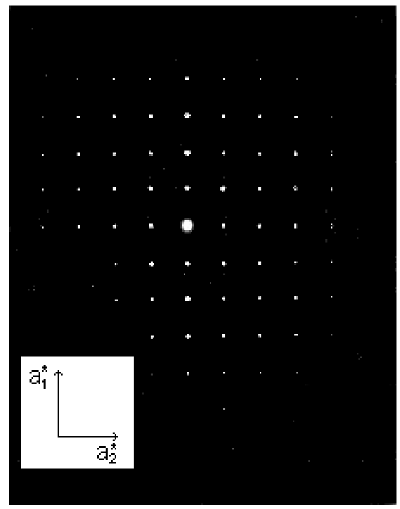
These vectors are parallel to the [hkl] direction but has magnitude $2\pi/d_{hkl}$, which is a reciprocal distance

## Reciprocal lattice

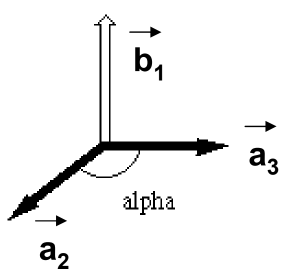
The <u>reciprocal lattice</u> is composed of all points lying at positions $\vec{G}_{hkl}$ from the origin, so that there is one point in the reciprocal lattice for each set of planes (hkl) in the real-space lattice.

This seems like an unnecessary abstraction. What is the payoff for defining such a reciprocal lattice? No, the reciprocal lattice simplifies the interpretation of x-ray diffraction from crystals because:

- **Diffraction pattern is not a direct representation of the crystal lattice**
- **Diffraction pattern is a representation of the *reciprocal lattice***




## Reciprocal lattice




**Generallizing,we introduce a set of new unit vectors so that they are normal to the plains determined by the previously introduced translation vectors**

### Definition of reciprocal translation vectors

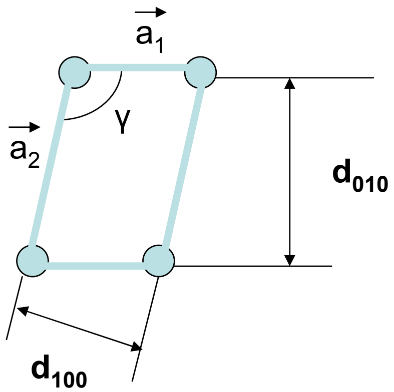
$\vec{b}_1 = (\vec{a}_2 \times \vec{a}_3)\, 2\pi/V_c$ $\quad$ $\vec{b}_2 = (\vec{a}_3 \times \vec{a}_1)\, 2\pi/V_c$ $\quad$ $\vec{b}_3 = (\vec{a}_1 \times \vec{a}_2)\, 2\pi/V_c$

$V_c = \vec{a}_1 \bullet (\vec{a}_2 \times \vec{a}_3)$ – **volume of a unit cell**

$$\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$$

# Reciprocal lattice

**Reciprocal lattice is nothing with ”anti-matter” or ”black holes” to do – it is determined by a set of vectors with specific magnitudes just having a bit unusual dimentions – 1/length. It is actually relatively straightforward – as long as we understood the definitions – to schetch the reciprocal lattice.**

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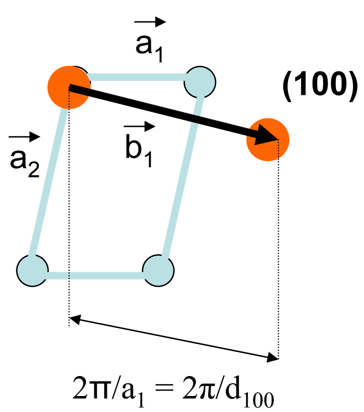


**The important part is that $b_1$ should be normal to a plain determined by $[a_2 \times a_3]$ and having a magnitude of $1/a_1$ – just by definition - or $1/d_{100}$, where $d_{100}$ is the interplain distance between (100) family of plains. NB, for any plain from (100) familly the point in the reciprocal space is exactly the same meaning that any reciprocal lattice point represents its own family of plains in the real space.**

$$\vec{b}_1 = (\vec{a}_2 \times \vec{a}_3)\, 2\pi/V_c$$

$$V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

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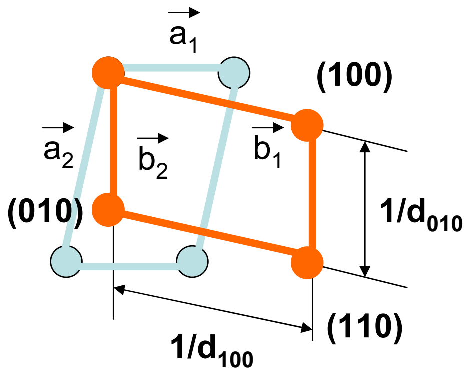


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**Similar excercise can be done with vector $b_2$ which points out to a reciprocal lattice point representing (010) family of plains.**

**In adition (110) family of plaines in the real space would naturally result in to (110)-points in the reciprocal space.**

**The procedure can be repeated any type of plain cuts in the real space**

# Reciprocal lattice

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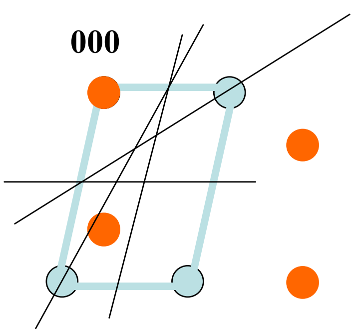


$$d_{hkl} = \frac{a}{\sqrt{\left(h^2 + k^2 + l^2\right)}}$$

## Reciprocal lattice

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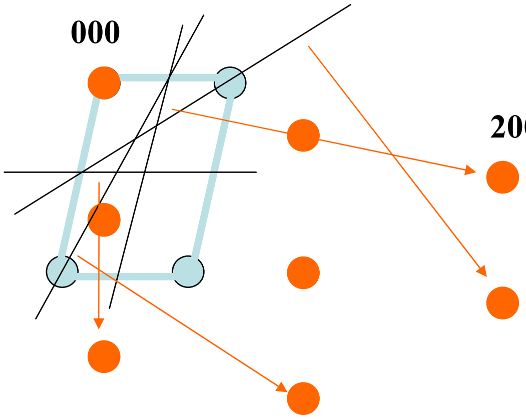


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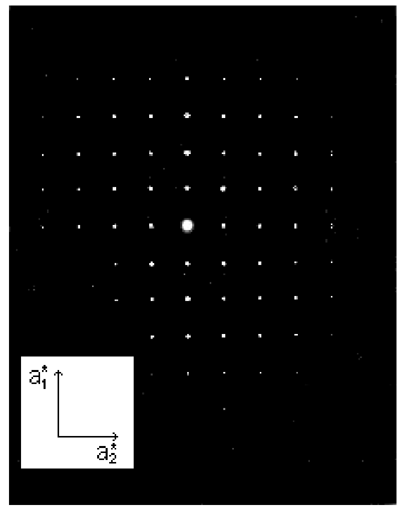

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- (hkl) plain indices and distance between plains in cubic, tetragonal and orthorombic lattices;
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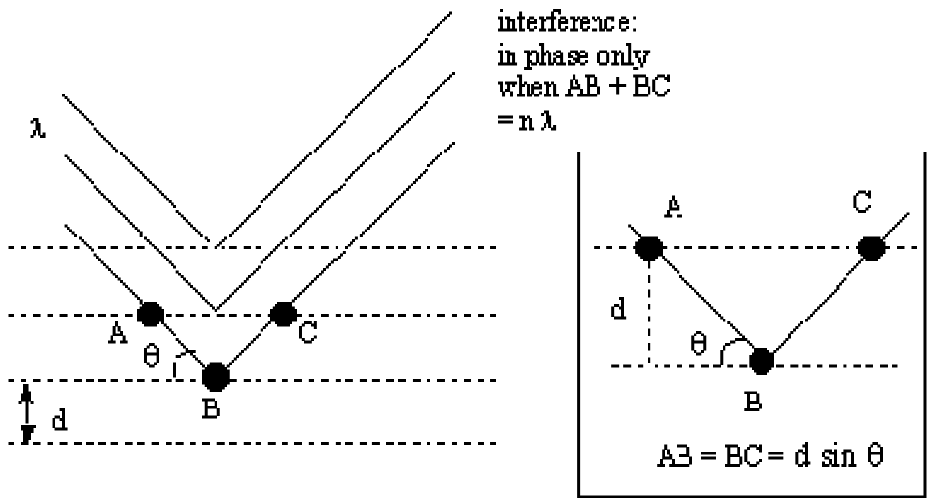
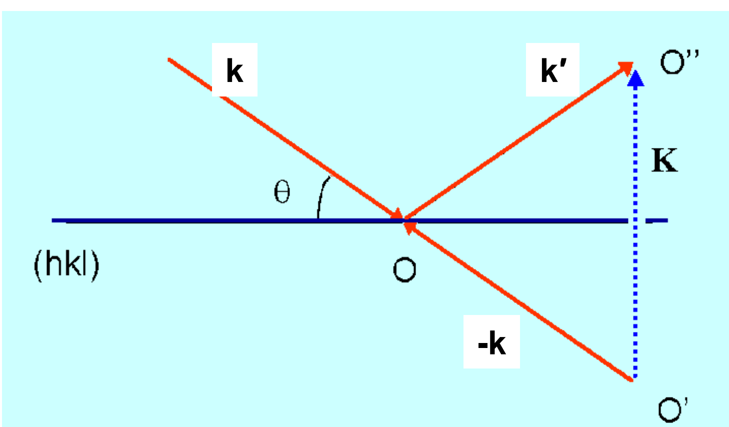
## Bragg diffraction




**The conditions leading to diffraction are given by the Bragg's law, relating the angle of incidence of the radiation (theta) to the wavelength (lambda) of the incident radiation and the spacing between the crystal lattice planes (d):**

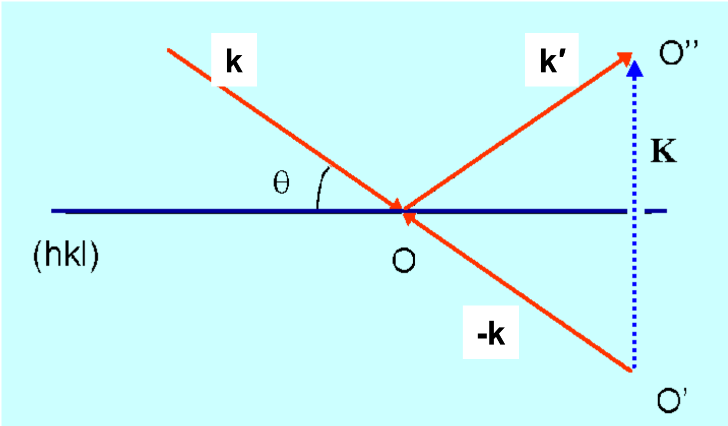
**2 d sin (theta) = n lambda**

## Laue condition




$$|K| = 2|k|\sin\theta_{hkl} = \frac{2\sin\theta_{hkl}}{\lambda}$$

# Laue condition

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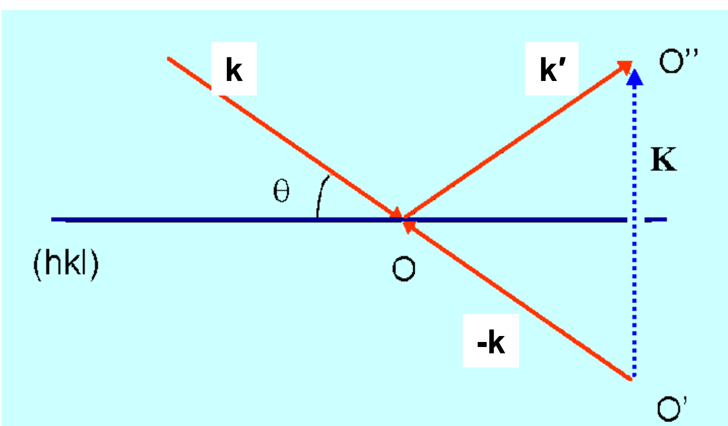
$\vec{\mathbf{K}}$ is perpendicular to the (hkl) plane, so can be defined as:

$$\vec{K} = \left[\frac{2\sin\theta_{hkl}}{\lambda}\right]\hat{\mathbf{n}}$$

# Laue condition

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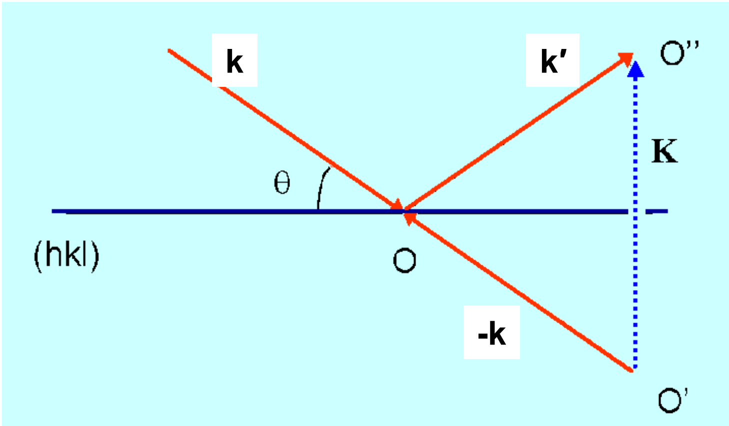
**G** is also perpendicular to (hkl) so $\hat{\mathbf{n}} = \frac{G_{hkl}}{|G_{hkl}|}$

## Laue condition

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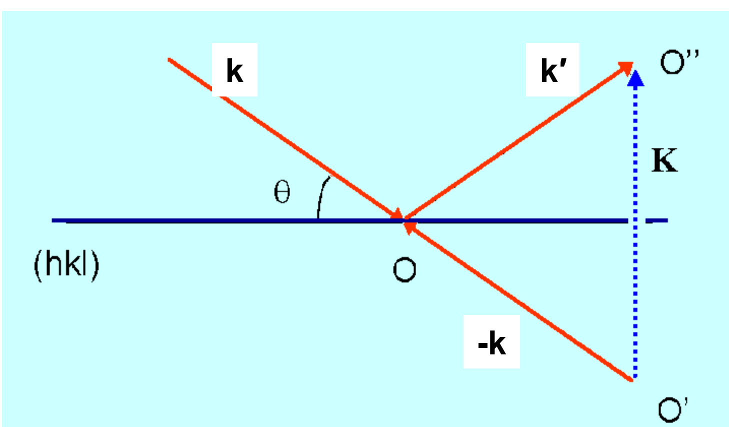
$$\Rightarrow \quad K = \frac{2}{\lambda|G_{hkl}|}\sin\theta_{hkl} G_{hkl}$$ and $|G_{hkl}| = \frac{1}{d_{hkl}}$ from previous

## Laue condition

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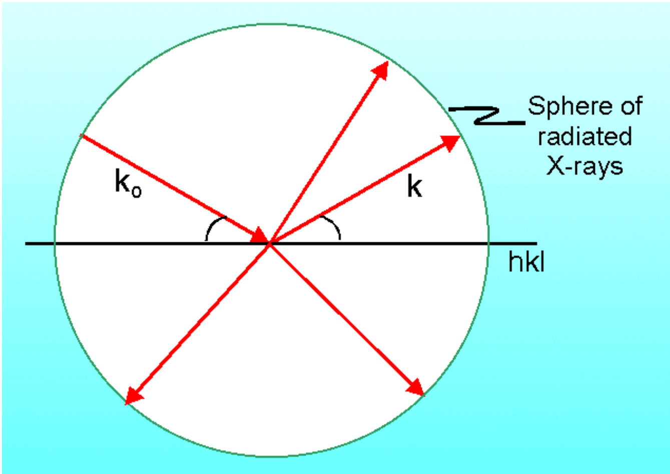
$$\Rightarrow K = \frac{2d_{hkl}\sin\theta_{hkl}}{\lambda} G_{hkl}$$

But Bragg: $2d\sin\theta = \lambda$

**$K = G_{hkl}$ the Laue condition**

## Diffraction pattern as representation of the reciprocal lattice

**Laue assumed that each set of atoms could radiate the incident radiation in all directions**

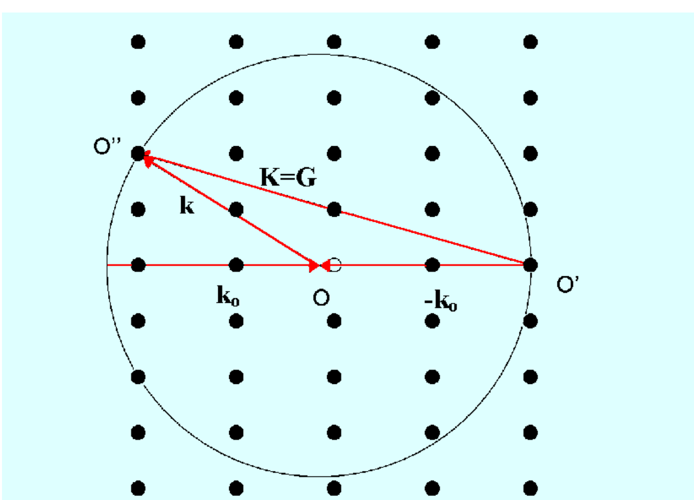



Constructive interference only occurs when the scattering vector, **K** (***Δk*** *in the Kittel's notations*), coincides with a reciprocal lattice vector, **G**

This naturally leads to the Ewald Sphere construction

## Ewald construction

We superimpose the imaginary "sphere" of radiated radiation upon the reciprocal lattice



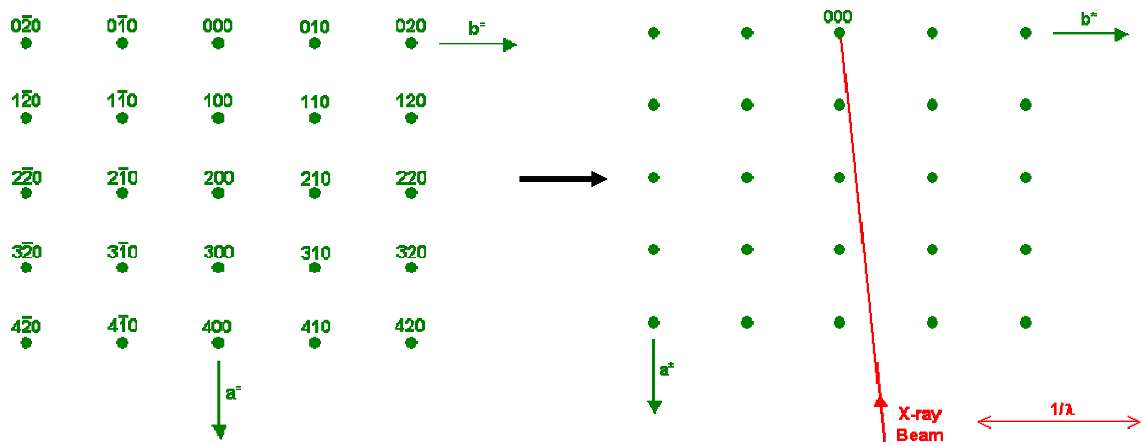

Draw sphere of radius $1/\lambda$ centred on end of $\mathbf{k_o}$

Reflection is only observed if sphere intersects a point

i.e. where **K=G**

# Ewald construction

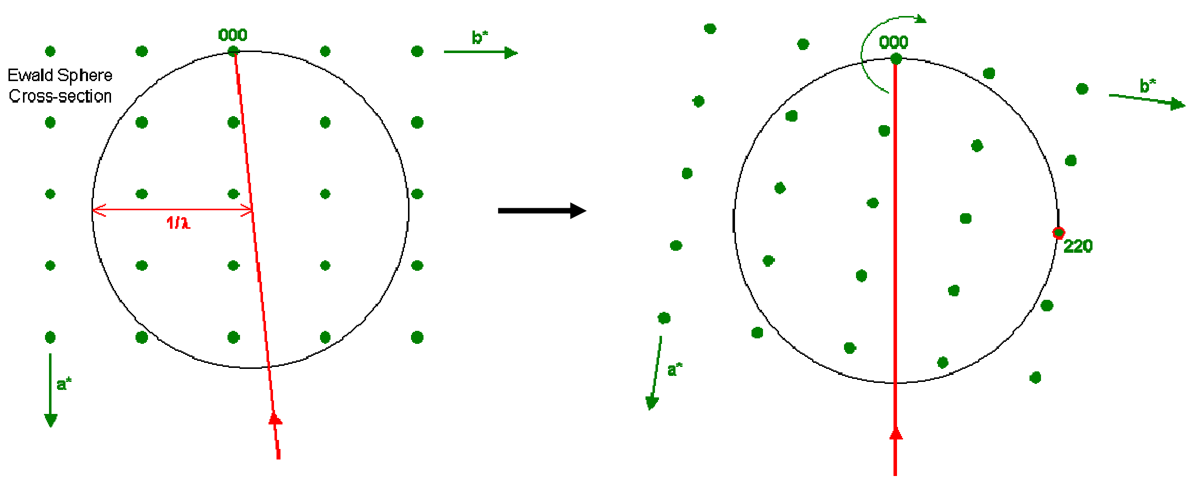
This means that when a lattice point intersects the Ewald sphere, the reflection corresponding to that family of planes will be observed and the diffraction angle will be apparent.




Starting with an indexed reciprocal lattice, an incident x-ray beam must pass through the origin (000) point, corresponding to the incident beam of x-rays.

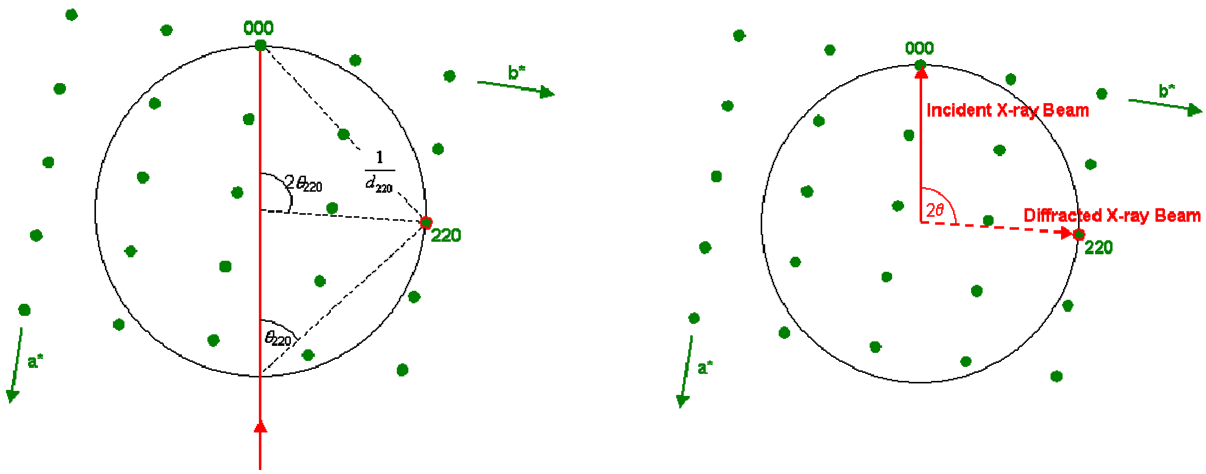
# Ewald construction

The Ewald sphere for this case is defined by making a sphere of radius 1/λ having its diameter on the X-ray beam that intersects the origin point. In the diagram on the left, no other reciprocal lattice points are on the surface of the sphere so the Bragg condition is not satisfied for any of the families of planes.




To observe reflections, the reciprocal lattice must be rotated until an reciprocal lattice point contacts the surface of the sphere. Note: it would be easier to rotate the sphere on paper, but in practice, we rotate the crystal lattice and the RL.

## Ewald construction




When a reciprocal lattice point intersects the Ewald sphere, a reflection will occur and can be observed at the 2θ angle of the inscribed triangle. To be able to collect as many different reflections as possible, it is thus necessary to be able to rotate the reciprocal lattice to a great extent…

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- **Some consequences: how many lines = reciprocal lattice point will we see**

## Some consequences:
## how many lines = reciprocal lattice point will we see

In the experiment we just correlate the increased intencity with the angle

In cubic crystal: $$d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}}$$

Now put it together with Bragg: $$2\frac{a}{\sqrt{(h^2 + k^2 + l^2)}}\sin\theta = \lambda$$

Finally $$\sqrt{(h^2 + k^2 + l^2)} = \frac{2a}{\lambda}\sin\theta$$

## Some consequences:
## how many lines = reciprocal lattice point will we see

$$\sqrt{(h^2 + k^2 + l^2)} = \frac{2a}{\lambda}\sin\theta$$

| h k l | $h^2 + k^2 + l^2$ | h k l | $h^2 + k^2 + l^2$ |
|---|---|---|---|
| 1 0 0 | 1 | 2 2 1, 3 0 0 | 9 |
| 1 1 0 | 2 | 3 1 0 | 10 |
| 1 1 1 | 3 | 3 1 1 | 11 |
| 2 0 0 | 4 | 2 2 2 | 12 |
| 2 1 0 | 5 | 3 2 0 | 13 |
| 2 1 1 | 6 | 3 2 1 | 14 |
| 2 2 0 | 8 | 4 0 0 | 16 |

**Is there anything limiting ($h^2 + k^2 + l^2$) values of the "last" reflection?**

**Yes it it's the wavelength. Why?**

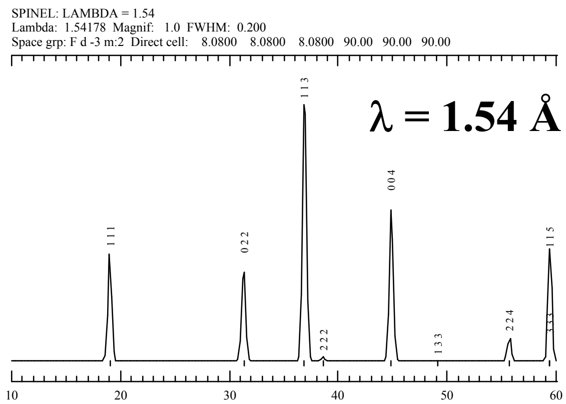
$$\left(h^2 + k^2 + l^2\right) = \frac{4a^2}{\lambda^2}\sin^2\theta$$

**$\sin^2\theta$ has a limiting value of 1, so for this limit:**

$$\left(h^2 + k^2 + l^2\right) \leq \frac{4a^2}{\lambda^2}$$

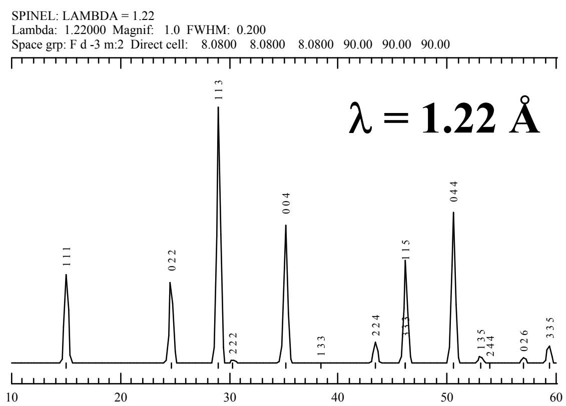
## Some consequences:
## how many lines = reciprocal lattice point will we see

$$\left(h^2 + k^2 + l^2\right) \leq \frac{4a^2}{\lambda^2}$$




Still if one knows the lattice it should quite stright to index the peaks, but…

| h k l | $h^2 + k^2 + l^2$ | h k l | $h^2 + k^2 + l^2$ |
|---|---|---|---|
| 1 0 0 | 1 | 2 2 1, 3 0 0 | 9 |
| 1 1 0 | 2 | 3 1 0 | 10 |
| 1 1 1 | 3 | 3 1 1 | 11 |
| 2 0 0 | 4 | 2 2 2 | 12 |
| 2 1 0 | 5 | 3 2 0 | 13 |
| 2 1 1 | 6 | 3 2 1 | 14 |
| 2 2 0 | 8 | 4 0 0 | 16 |




## Some consequences:
## how many lines = reciprocal lattice point will we see

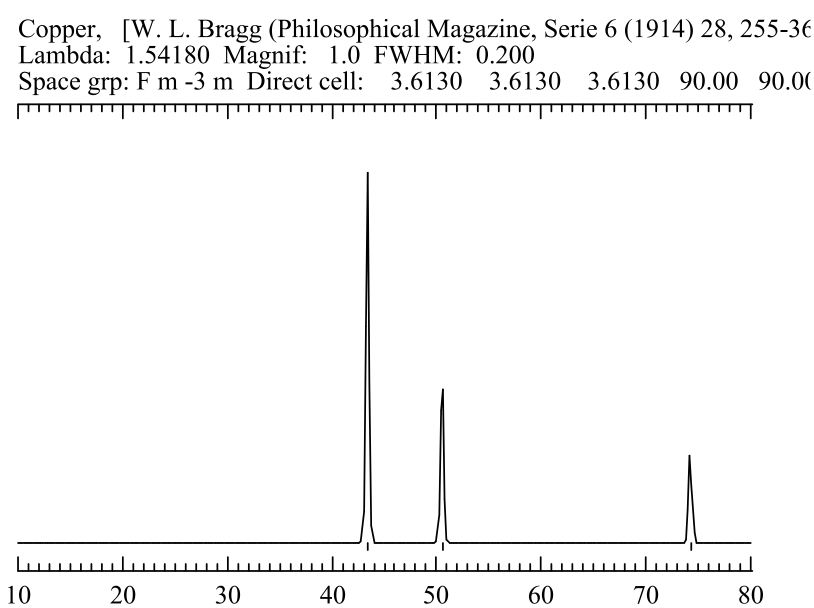
Let's take an example: The unit cell of copper is 3.613 Å. What is the Bragg angle for the (100) reflection with Cu Kα radiation (λ = 1.5418 Å)?

$$\theta = \sin^{-1}\left(\frac{\lambda}{2d_{hkl}}\right)$$

$$d_{hkl} = \frac{a}{\sqrt{\left(h^2 + k^2 + l^2\right)}}$$

$\theta$= 12.32°, so 2$\theta$ = 24.64°

**BUT….**



## Some consequences:
## how many lines = reciprocal lattice point will we see

- Due to symmetry, certain reflections cancel each other out.
- These are non-random – hence "**systematic absences**"
- For each Bravais lattice, there are thus rules for allowed reflections:

## Relation to real diffraction experiment

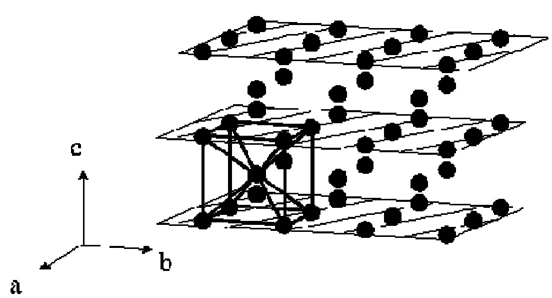
**The presence of translational symmetry elements and centering in the real lattice causes some series of reflections to be absent – can be accurately derived from the expressions of the structure factors.**

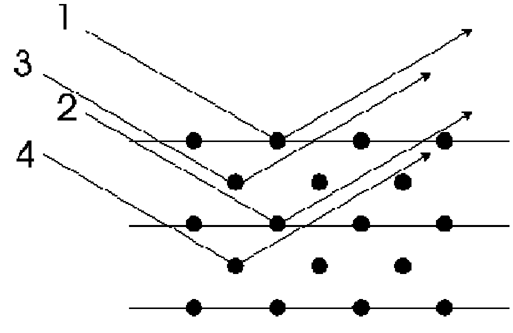
**e.g. the (001) reflection in a BCC lattice is absent.**

**Consider the additional path lengths vs. beam "1":**

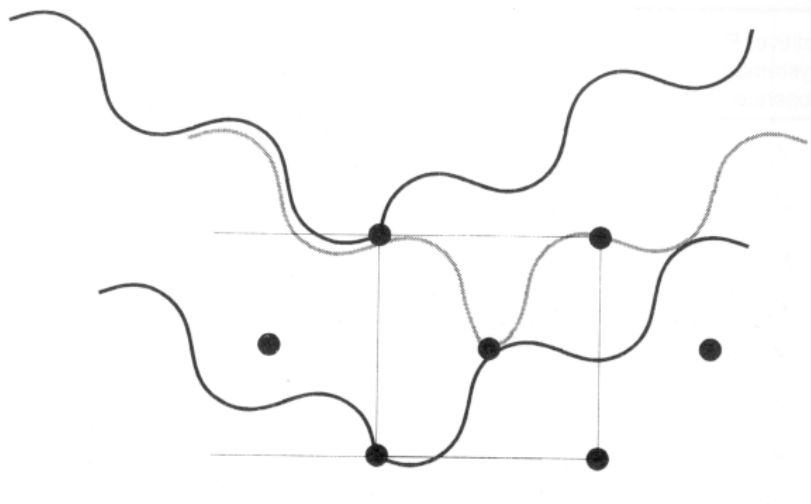
**For "2" it is 2d sin(q);**

**For "3" it is 2(d/2) sin(q), thus the rays from "3" will be exactly out-of-phase with those of "2" and no reflection will be observed.**



# Relation to real diffraction experiment



# Some consequences: how many lines = reciprocal lattice point will we see

So for each Bravais lattice:

| | PRIMITIVE | BODY | FACE |
|---|---|---|---|
| $h^2 + k^2 + l^2$ | All possible | h+k+l=2n | h,k,l all odd/even |
| 1 | 1 0 0 | | |
| 2 | 1 1 0 | 1 1 0 | |
| 3 | 1 1 1 | | 1 1 1 |
| 4 | 2 0 0 | 2 0 0 | 2 0 0 |
| 5 | 2 1 0 | | |
| 6 | 2 1 1 | 2 1 1 | |
| 8 | 2 2 0 | 2 2 0 | 2 2 0 |
| 9 | 2 2 1, 3 0 0 | | |
| 10 | 3 1 0 | 3 1 0 | |
| 11 | 3 1 1 | | 3 1 1 |
| 12 | 2 2 2 | 2 2 2 | 2 2 2 |
| 13 | 3 2 0 | | |
| 14 | 3 2 1 | 3 2 1 | |
| 16 | 4 0 0 | 4 0 0 | 4 0 0 |