FYS3410 - Vår 2016 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/v16/index.html

Pensum: Introduction to Solid State Physics
by Charles Kittel (Chapters 1-9 and 17, 18, 20)

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2016 FYS3410 Lectures (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17,18,20)

Module I – Periodic Structures and Defects (Chapters 1-3, 20)

M18/1: 9-12 am	**Introduction. Crystal bonding. Periodicity and lattices, Brag diffraction and Laue condition, reciprocal space**	**3h**
W20/1 cancelled		
M25/1: 9-12 am	**Ewald construction, interpretation of a diffraction experiment , Brag planes, and Brillouin zones**	**3h**
W27/1 cancelled		
M01/2: 10-12 am	**Elastic strain and structural defects in crystals**	**2h**
W03/2: 9-10 am	**Atomic diffusion in solids**	**1h**
M08/2: 10-12 am	**Summary of Module I**	**2h**

Module II – Phonons (Chapters 4 and 5)

W10/2: 9-10 am	**Vibrations in monoatomic and diatomic chains of atoms**	**1h**
M15/2: 10-12am	**Periodic boundary conditions, phonons and density of states (DOS)**	**2h**
W17/2: 9-10 am	**Planck distribution**	**1h**
M22/2 : 10-12am	**Lattice heat capacity: Dulong-Petit, Einstein, and Debye models**	**2h**
W24/2 cancelled		
M29/2: 9-12am	**Comparison of different models for lattice heat capacity, thermal conductivity with phonons**	**3h**
W02/3: 9-10 am	**Thermal expansion**	**1h**
M07/3: 10-12am	**Summary of Module II.**	**2h**

Module III – Electrons (Chapters 6, 7, 18 - pp.528-530, and Appendix D)

W09/3: 9-10 am	**Free electron gas (FEG) versus free electron Fermi gas (FEFG)**	**1h**
M14/3: 10-12am	**DOS of FEFG in 3D. Effect of temperature – Fermi-Dirac distribution**	**2h**
W16/3: 9-10 am	**Heat capacity of FEFG in 3D**	**1h**
W30/3: 9-10 am	**DOS in 2D - quantum wells**	**1h**
M04/4: 10-12am	**DOS in 1D and 0D, i.e. quantum wires and quantum dots; transport properties of electrons**	**2h**
W06/4: 9-10 am	**Origin of the energy band gap**	
M11/4: 10-12am	**Nearly free electron model. Kronig-Penney model. Empty lattice approximation.**	**2h**
W13/4: 9-10 am	**Number of orbitals in a band**	**1h**
M18/4: 10-12am	**Summary of Module III.**	**2h**

Module IV – Semiconductors and interfaces (Chapters 8, 9-pp 223-231, 17)

W20/4: 9-10 am	**Metals versus semiconductors. Surfaces and interfaces.**	**1h**
M25/4: 9-12 am	**Effective mass method.**	**3h**
W27/4: 9-10 am	**Intrinsic carrier generation – elctrons and holes.**	**1h**
M02/5: 9-12 am	**Localized levels for hydrogen-like impurities – donors and acceptors. Doping.**	**3h**
W04/5: 9-10 am	**Carrier statistics in semiconductors**	**1h**
M09/5: 9-12 am	**p-n junctions**	**3h**
W11/5: 9-10 am	**Optoelectronic semiconductor properties and devices**	**1h**
M18/5: 9-12 am	**Device demonstrations. Summary of Module IV**	**3h**

Repetition

M23/5 9-12 am	**The course in a nutshell**	**2h**
W25/5, M30/5 and W1/6 cancelled		

Exam during week 22 (tentatively 30-31/5)

Lecture 2
Ewald construction.Interpretation of a diffraction experiment.
Brag planes and Brillouin zones

- **Repetition of Brag and Laue conditions**
- **Ewald construction**
- **interpretation of diffraction experiment**
- **Brag planes and Brillouin zones**

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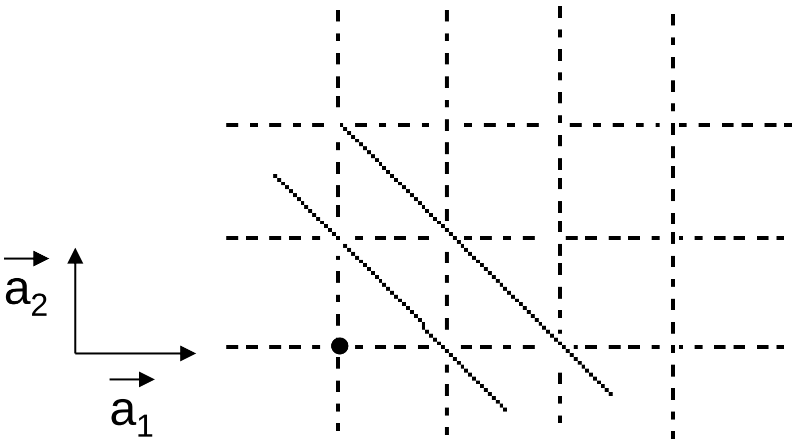
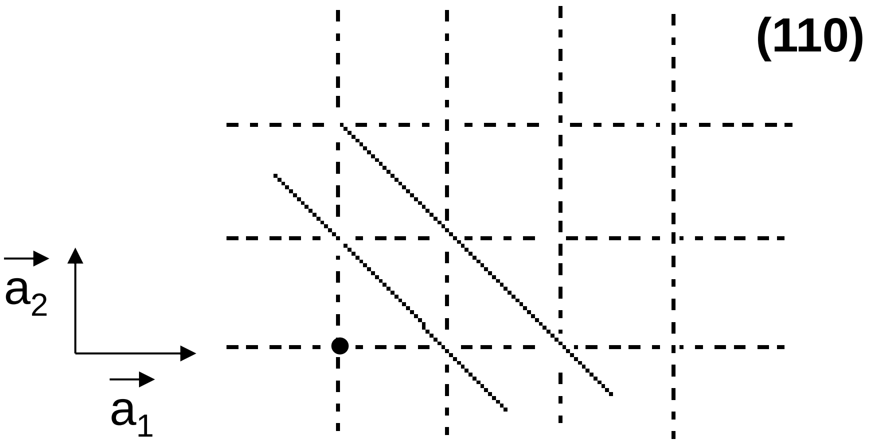
(hkl) plain indices



(hkl) plain indices



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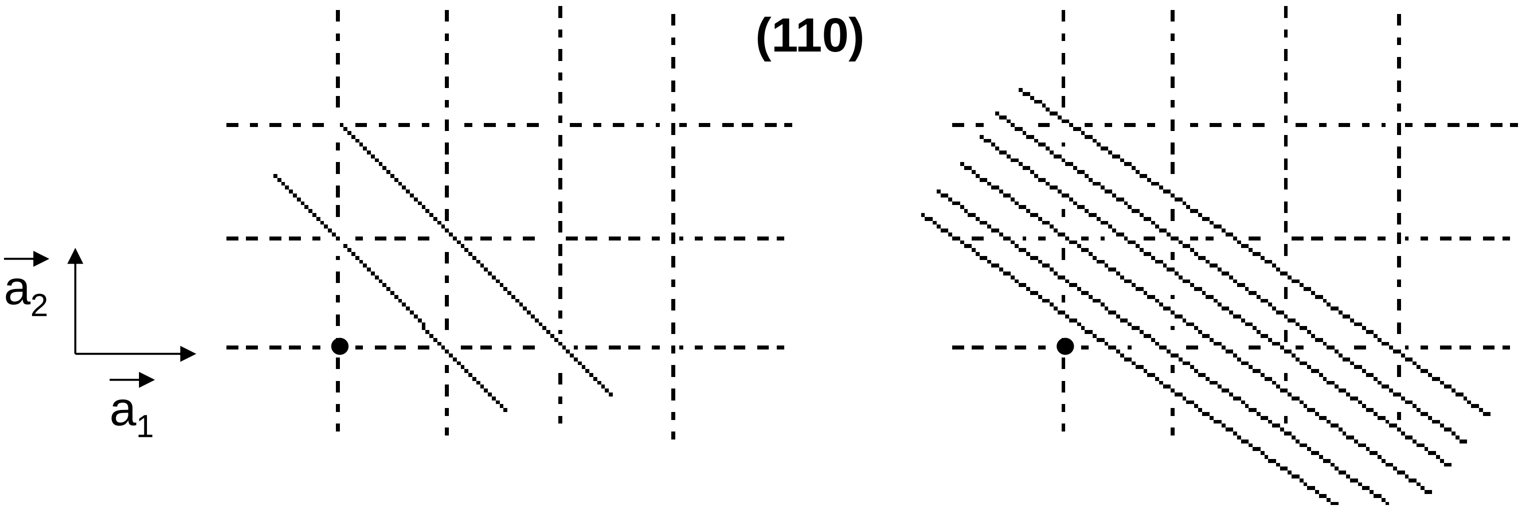
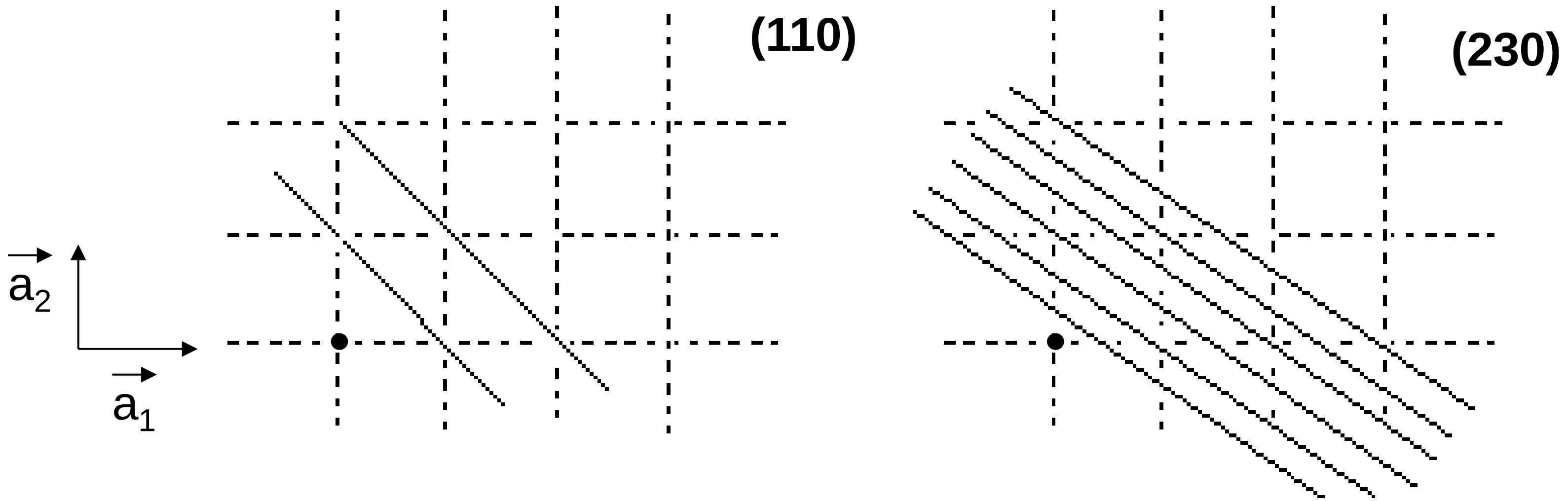


(hkl) plain indices



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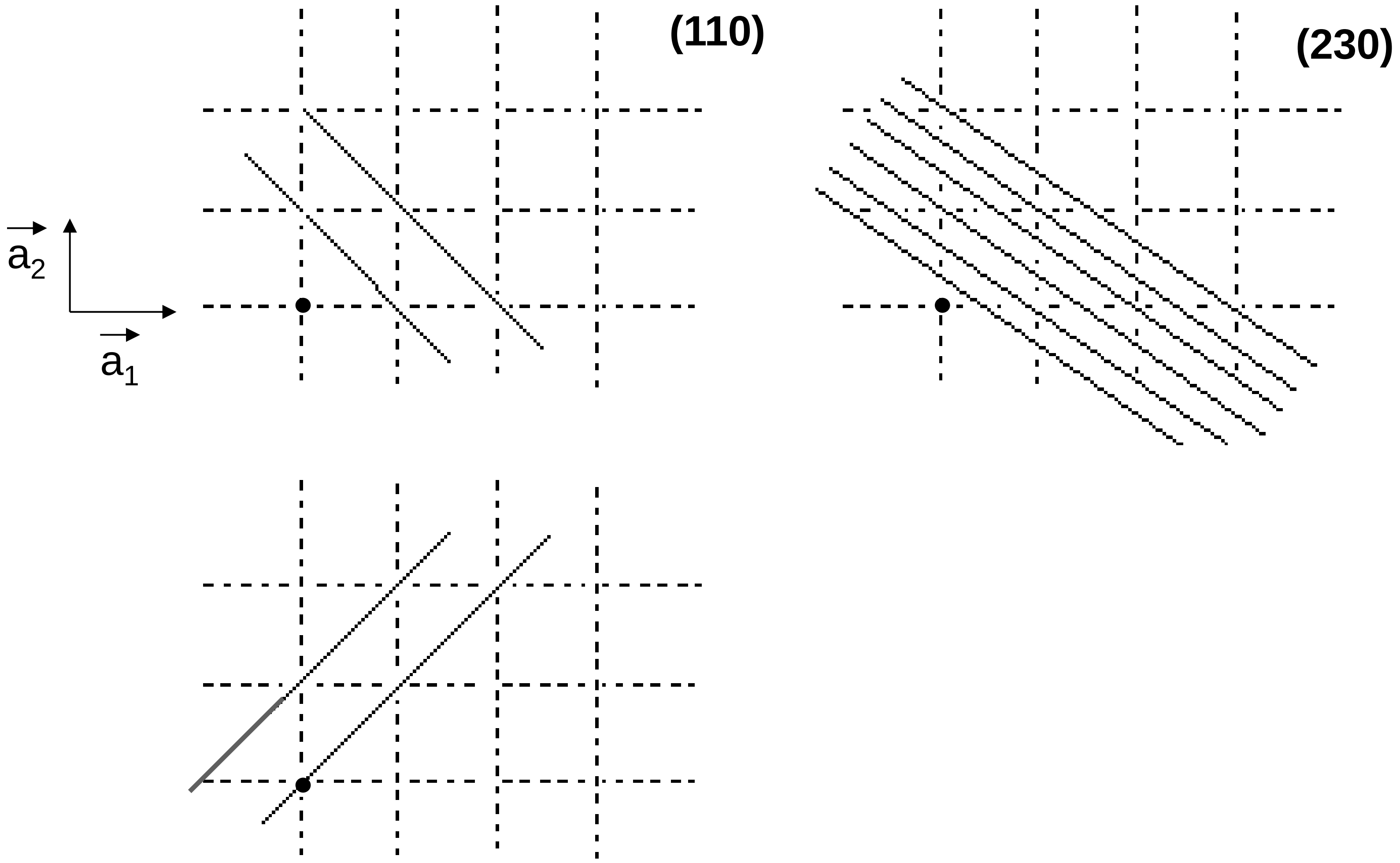

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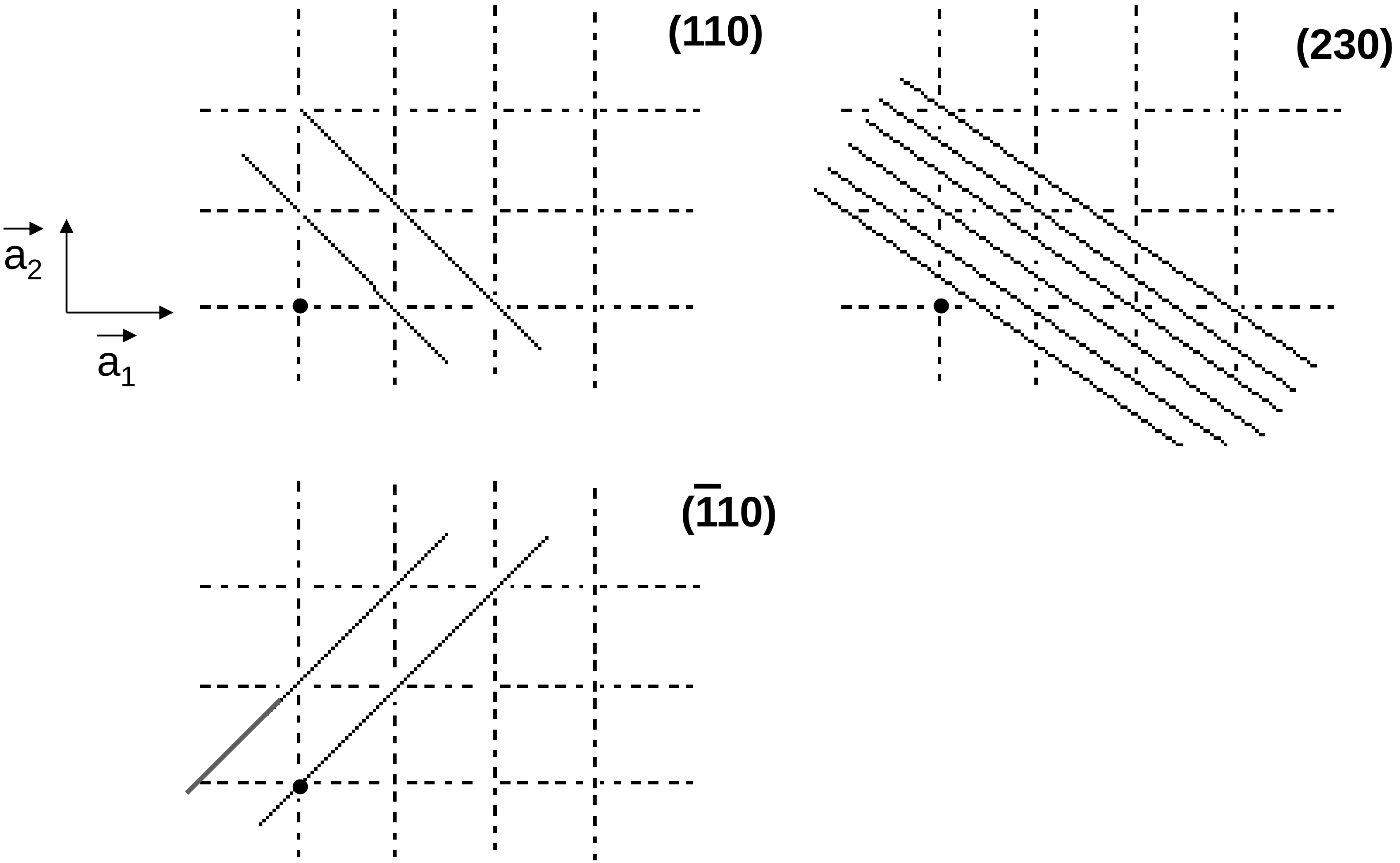
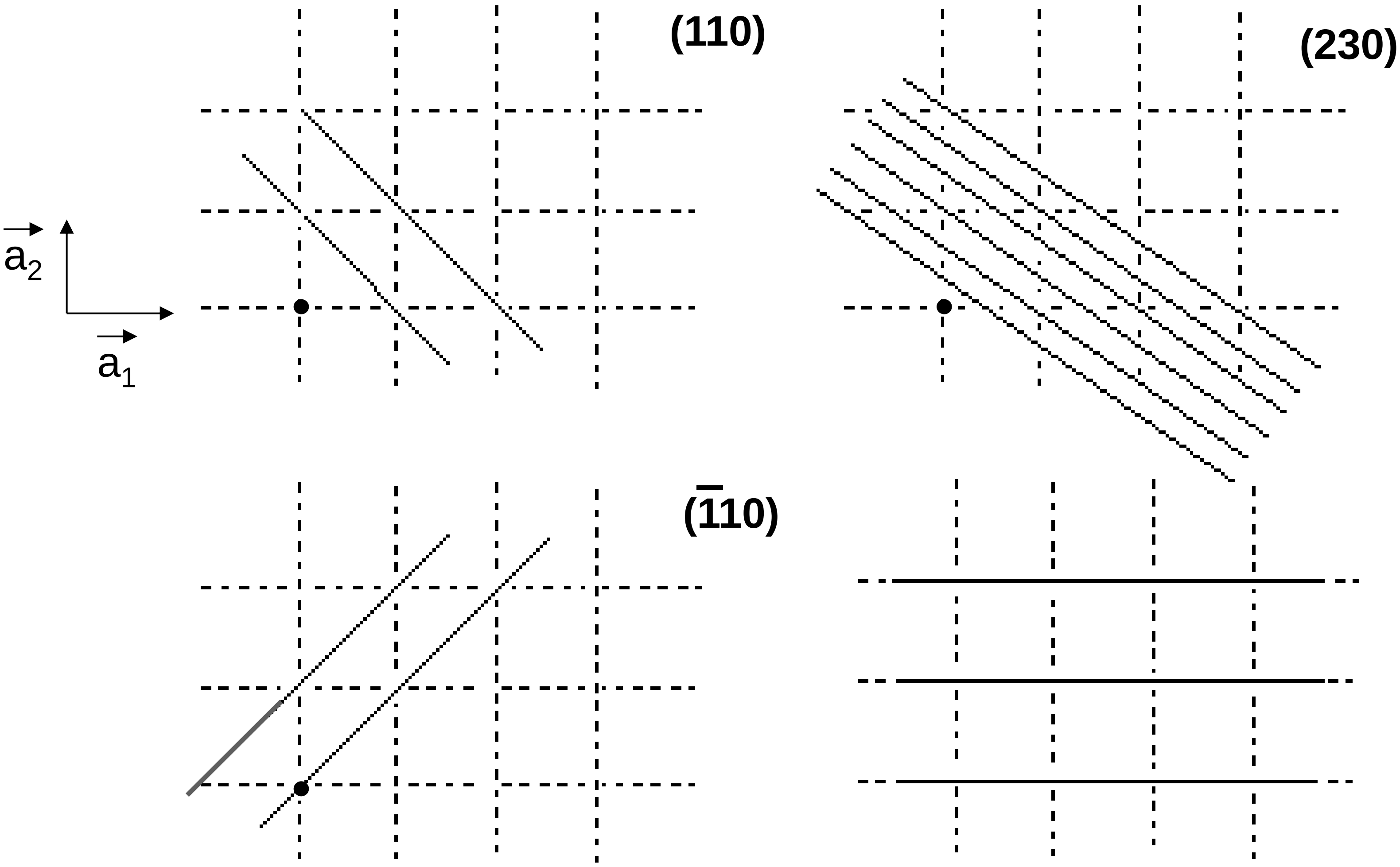


(hkl) plain indices



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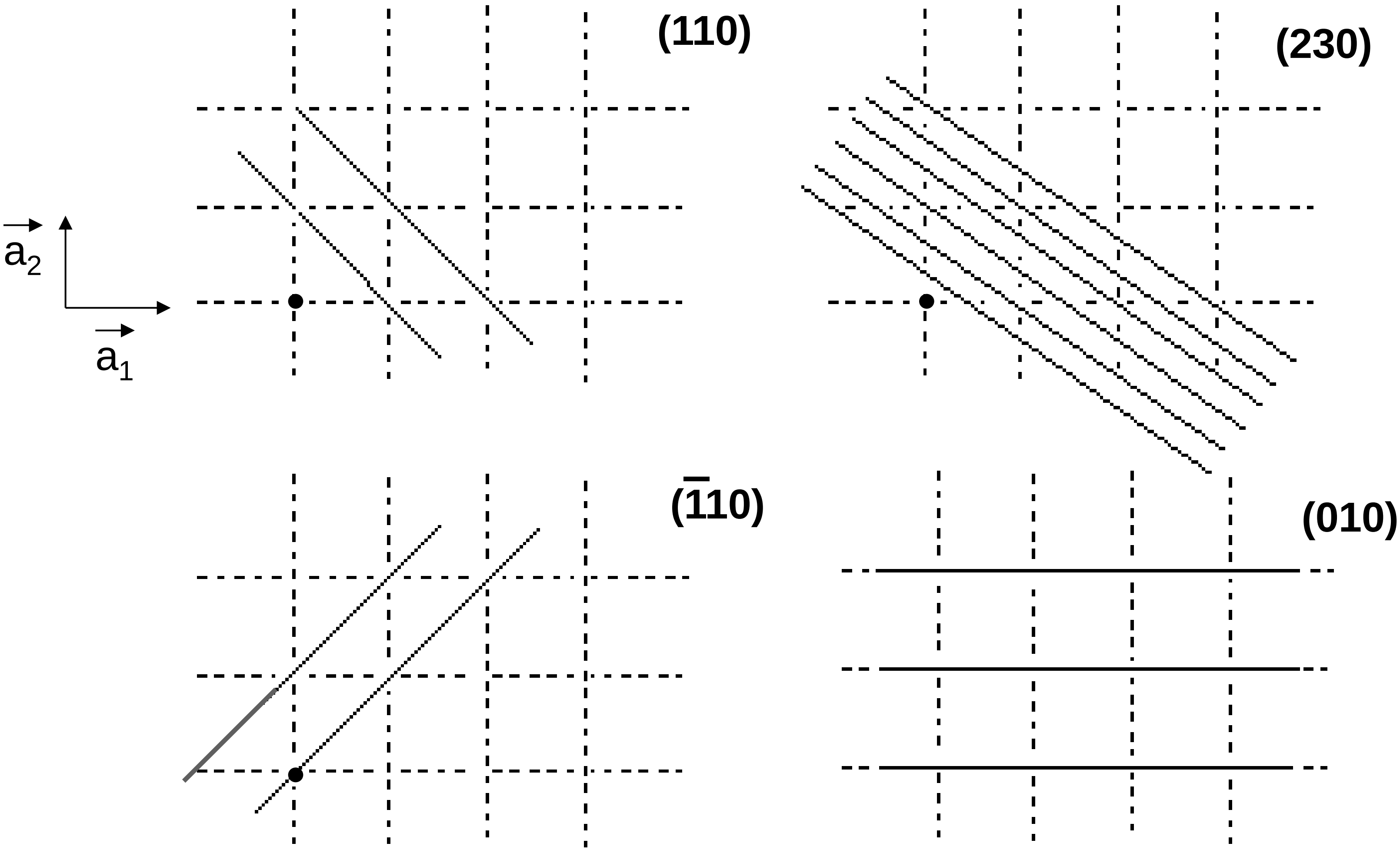
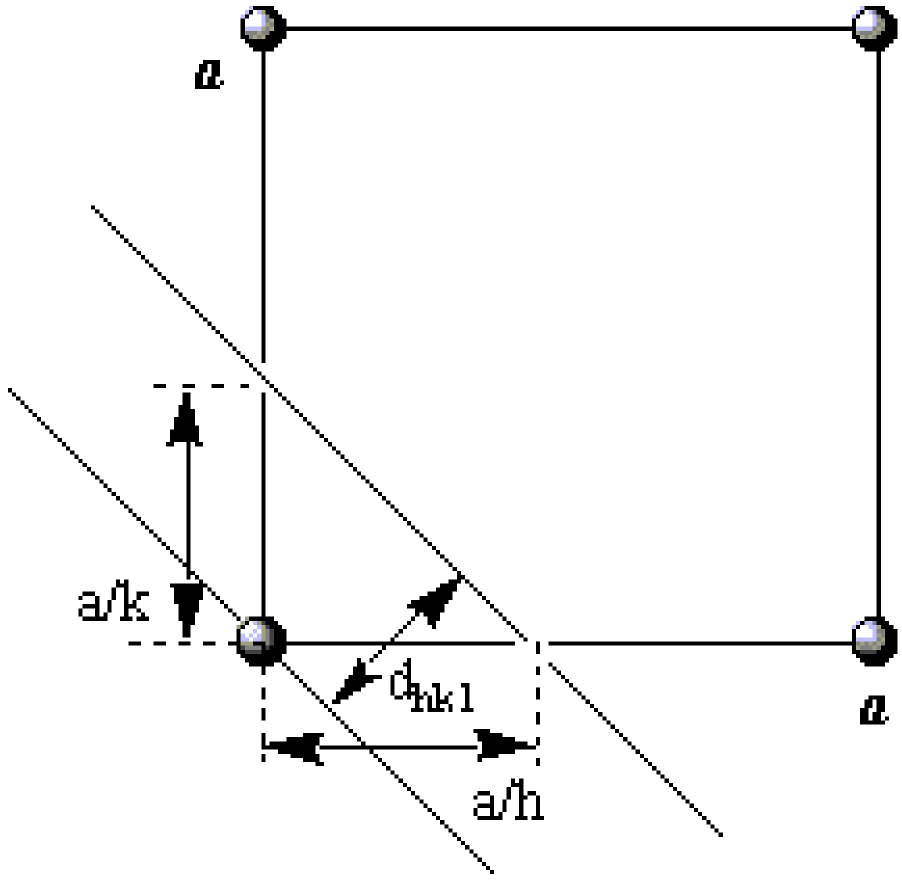
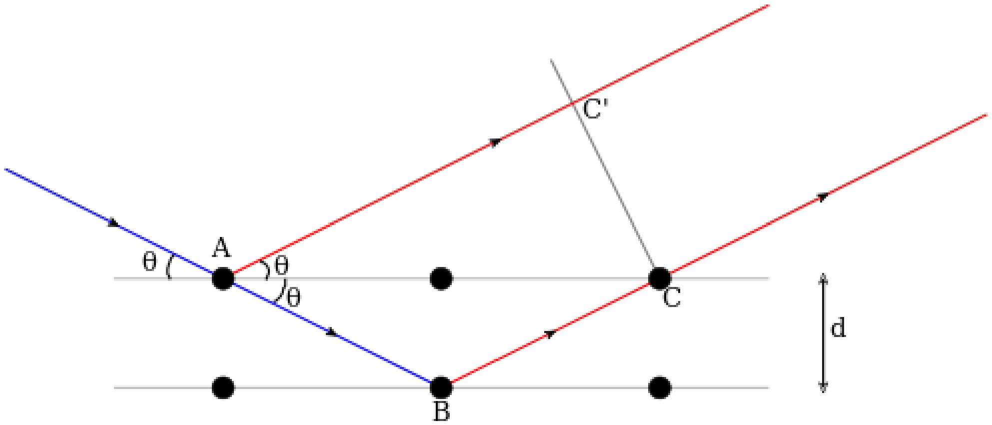


Distance between (hkl)-planes in cubic lattices



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



The two separate waves will arrive at a point with the same phase, and hence undergo constructive interference, if and only if this path difference is equal to any integer value of the wavelength, i.e.

$$(AB+BC)-(AC')=n\lambda, \qquad AB=BC=\frac{d}{\sin\theta} \qquad AC=\frac{2d}{\tan\theta},$$

.

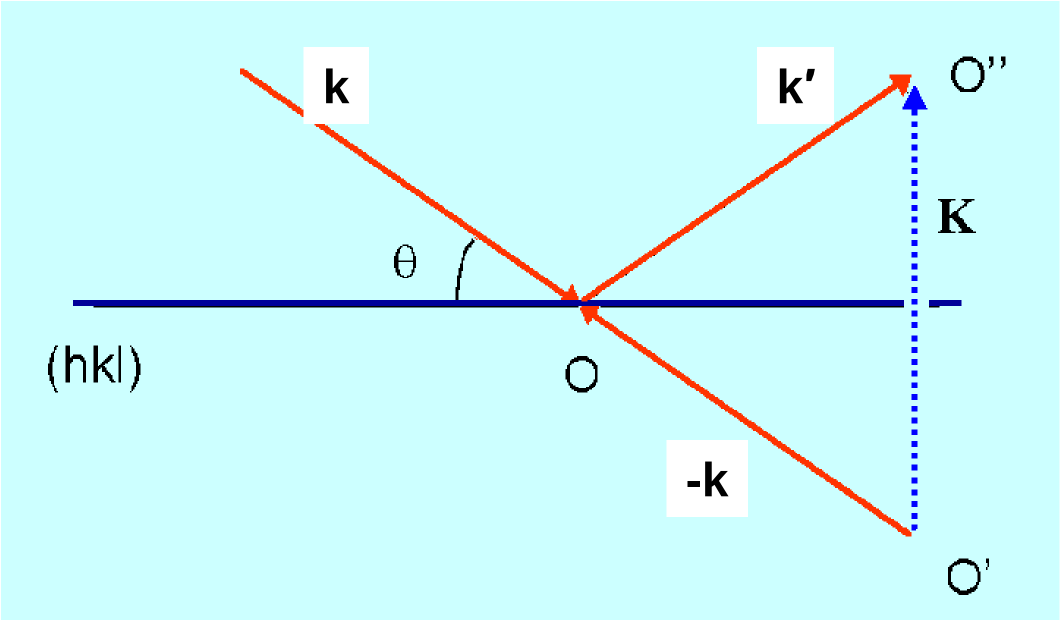
Therefore, $AC'=AC\cdot\cos\theta=\frac{2d}{\tan\theta}\cos\theta=\left(\frac{2d}{\sin\theta}\cos\theta\right)\cos\theta=\frac{2d}{\sin\theta}\cos^2\theta.$

Putting everything together,

$$n\lambda=\frac{2d}{\sin\theta}(1-\cos^2\theta)=\frac{2d}{\sin\theta}\sin^2\theta,$$

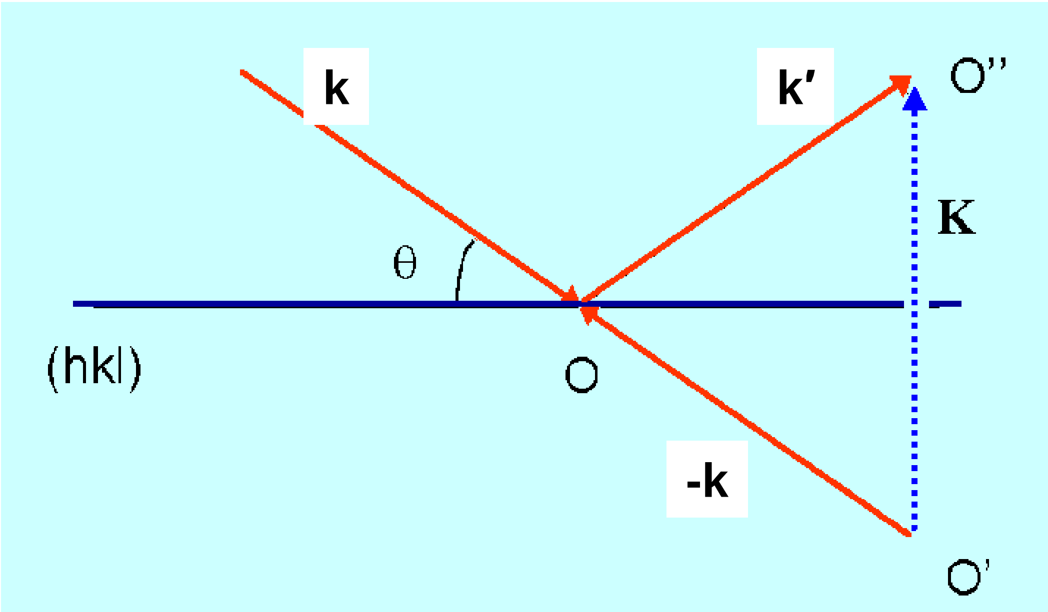
$$n\lambda=2d\sin\theta,$$

Laue condition



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

Laue condition



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

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

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

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

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

and $|G_{hkl}| = \frac{1}{d_{hkl}}$ from previous

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

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

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

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Ewald construction.Interpretation of a diffraction experiment.
Brag planes and Brillouin zones

- **Repetition of Brag and Laue conditions**

- **Ewald construction**

- **interpretation of diffraction experiment**

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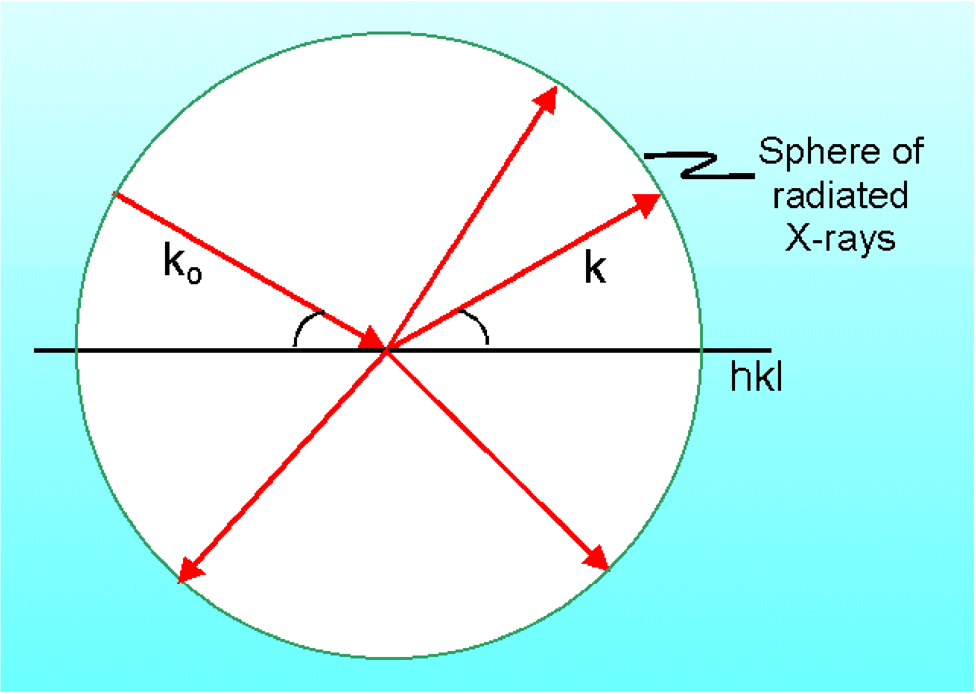
Diffraction pattern as representation of the reciprocal lattice

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

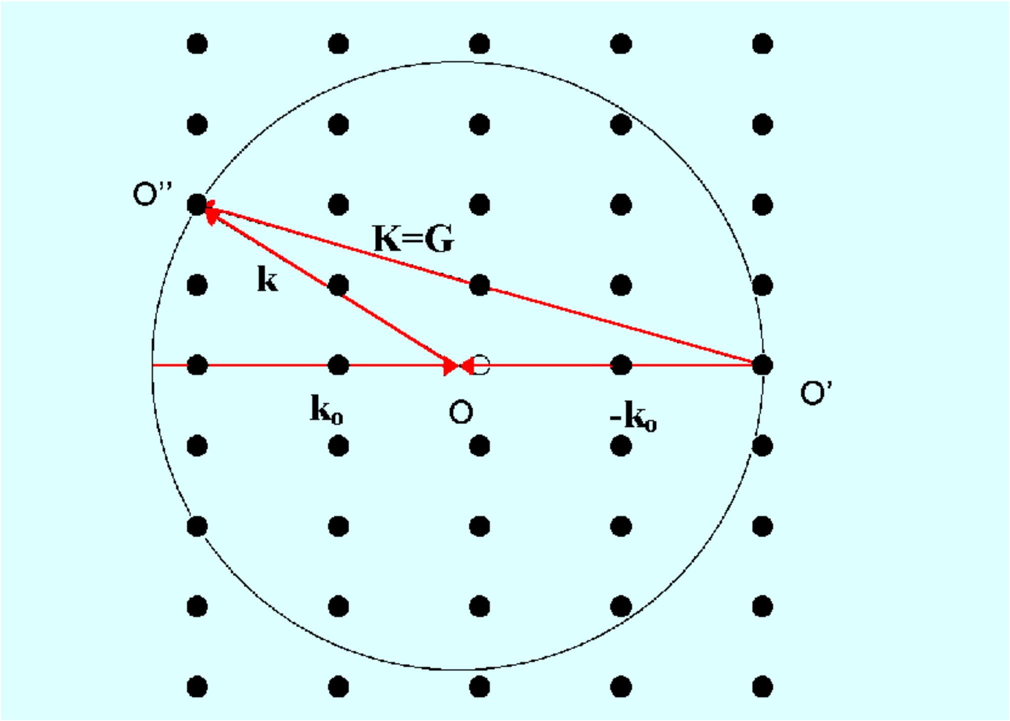


Constructive interference only occurs when the scattering vector, **K (*Δk*** *in the Kittel's notations*), coincides with a reciprocal lattice vector, **G**

This naturally leads to the Ewald Sphere construction

Ewald construction

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



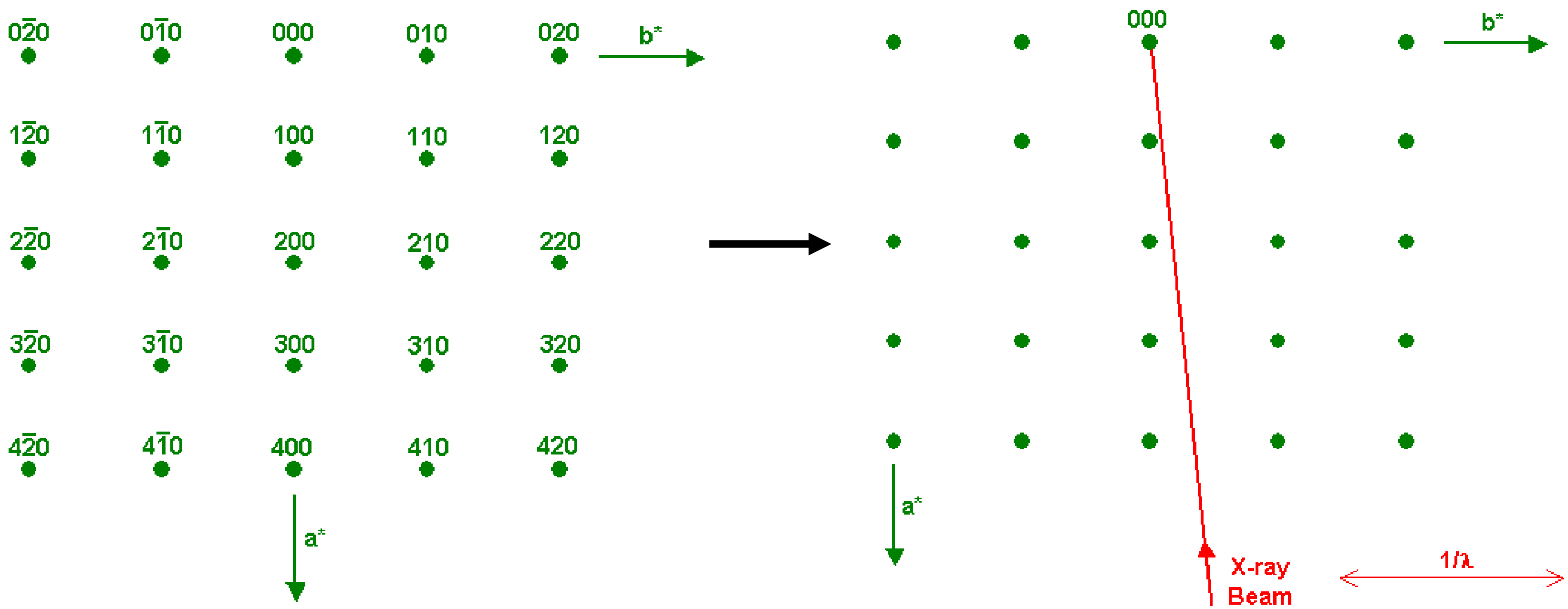
Draw sphere of radius $1/\lambda$ centred on end of $\mathbf{k_o}$

Reflection is only observed if sphere intersects a point

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

Ewald construction

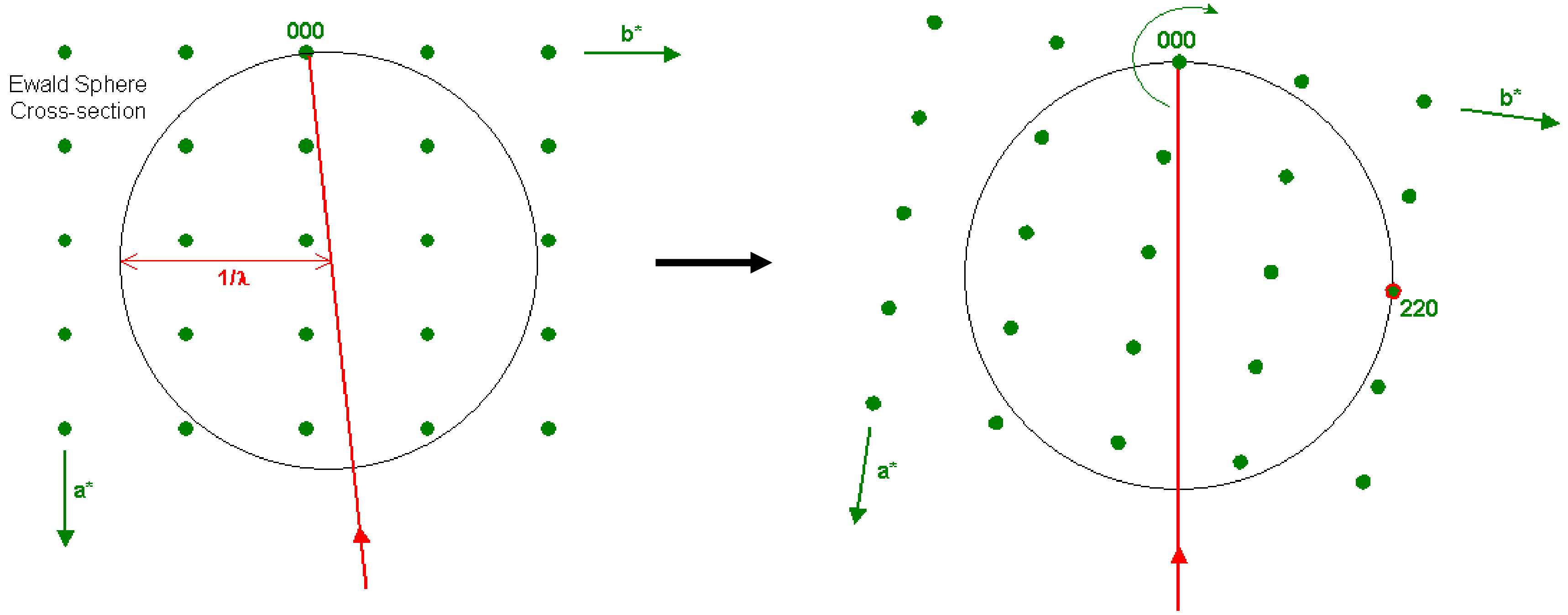
This means that when a lattice point intersects the Ewald sphere, the reflection corresponding to that family of planes will be observed and the diffraction angle will be apparent.



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.

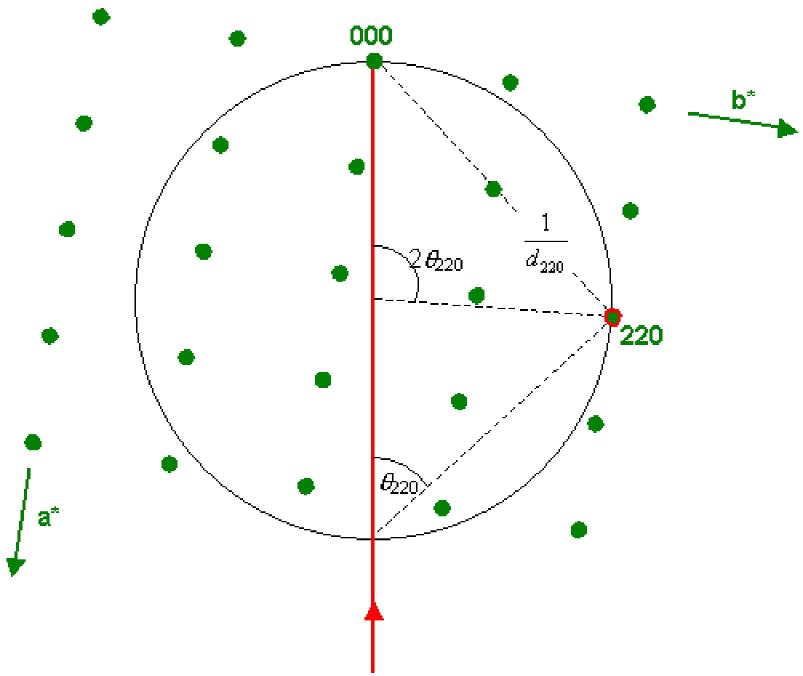
Ewald construction

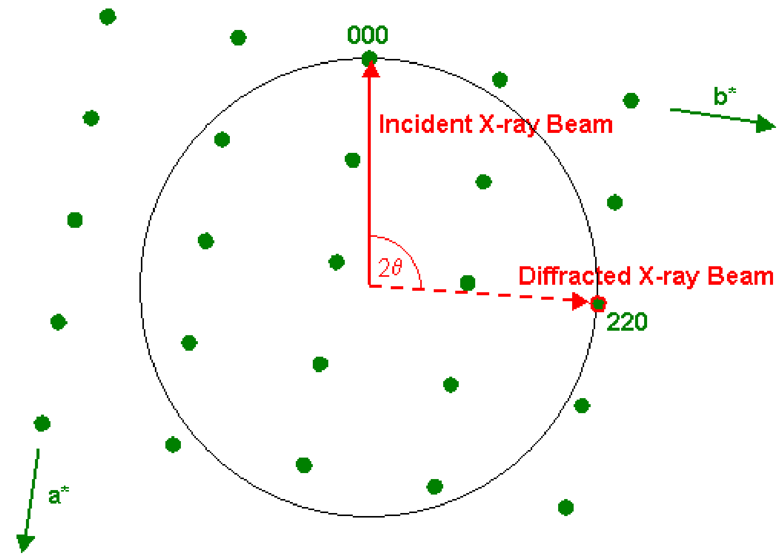
The Ewald sphere for this case is defined by making a sphere of radius 1/λ having its diameter on the X-ray beam that intersects the origin point. In the diagram on the left, no other reciprocal lattice points are on the surface of the sphere so the Bragg condition is not satisfied for any of the families 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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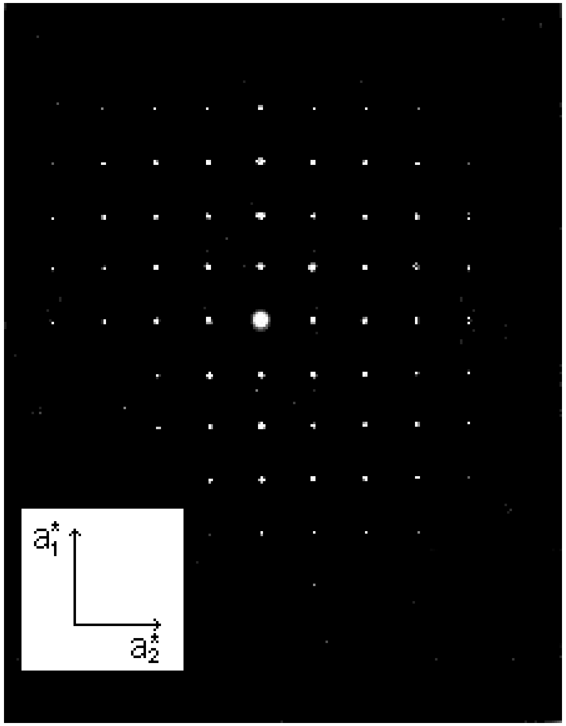
The reciprocal lattice is composed of all points lying at positions $\vec{G}_{hkl}$ from the origin, so that there is one point in the reciprocal lattice for each set of planes (hkl) in the real-space lattice.

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



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:

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

Now put it together with Bragg:

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

Finally

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

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

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

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:

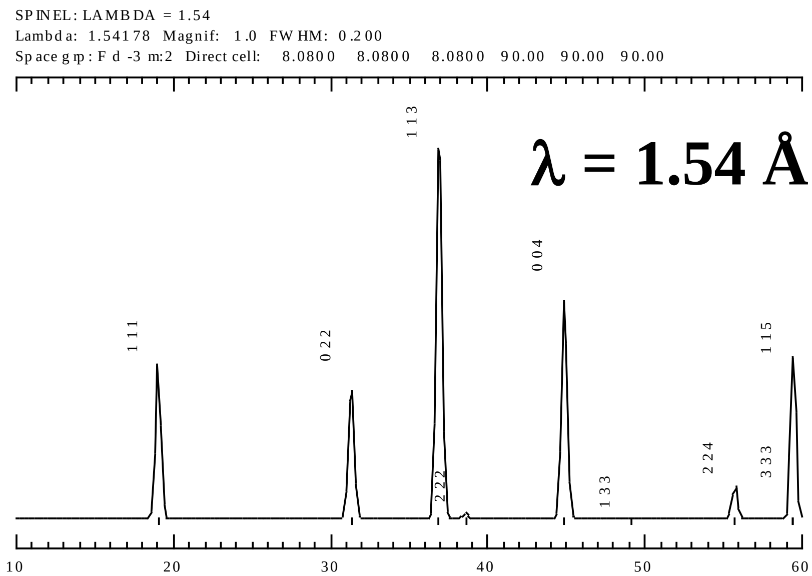
$$\left(h^2+k^2+l^2\right)\leq\frac{4a^2}{\lambda^2}$$

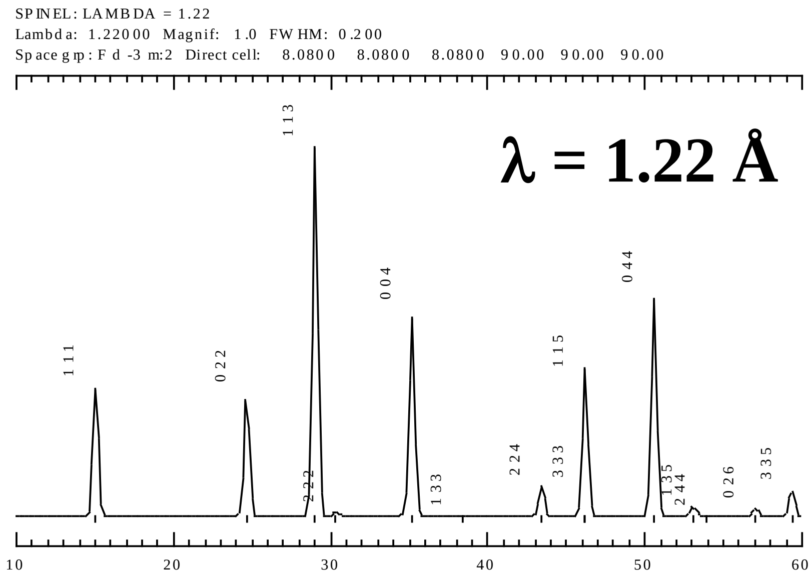
Some consequences:
how many lines = reciprocal lattice point will we see

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

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



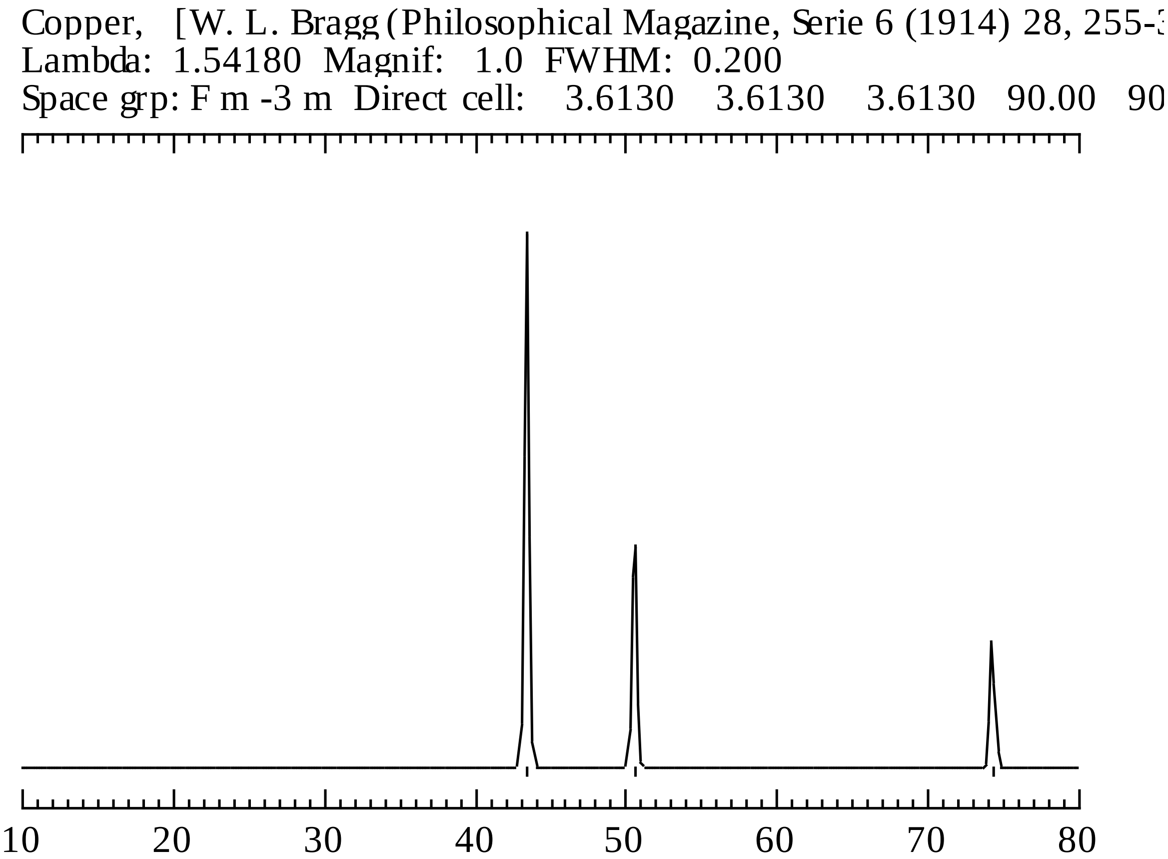


Some consequences:
how many lines = reciprocal lattice point will we see

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)?

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

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



θ= 12.32º, so 2θ = 24.64º

BUT….

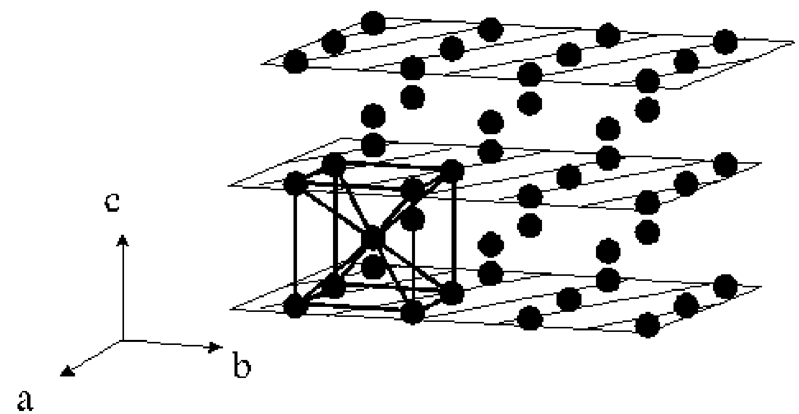
Some consequences:
how many lines = reciprocal lattice point will we see

- 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.

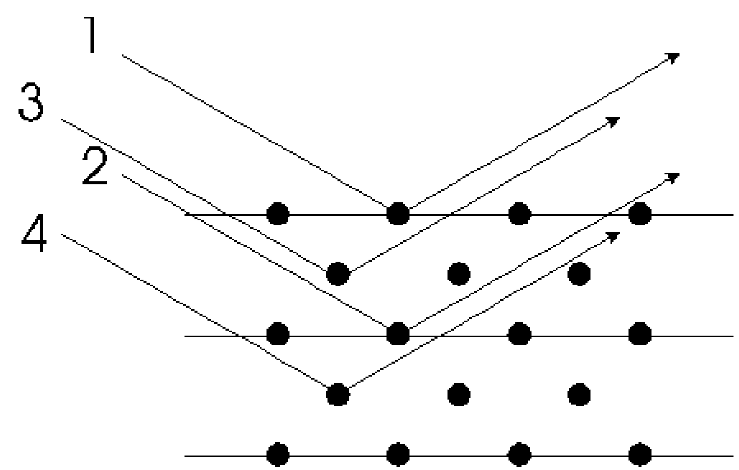
e.g. the (001) reflection in a BCC lattice is absent.



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.



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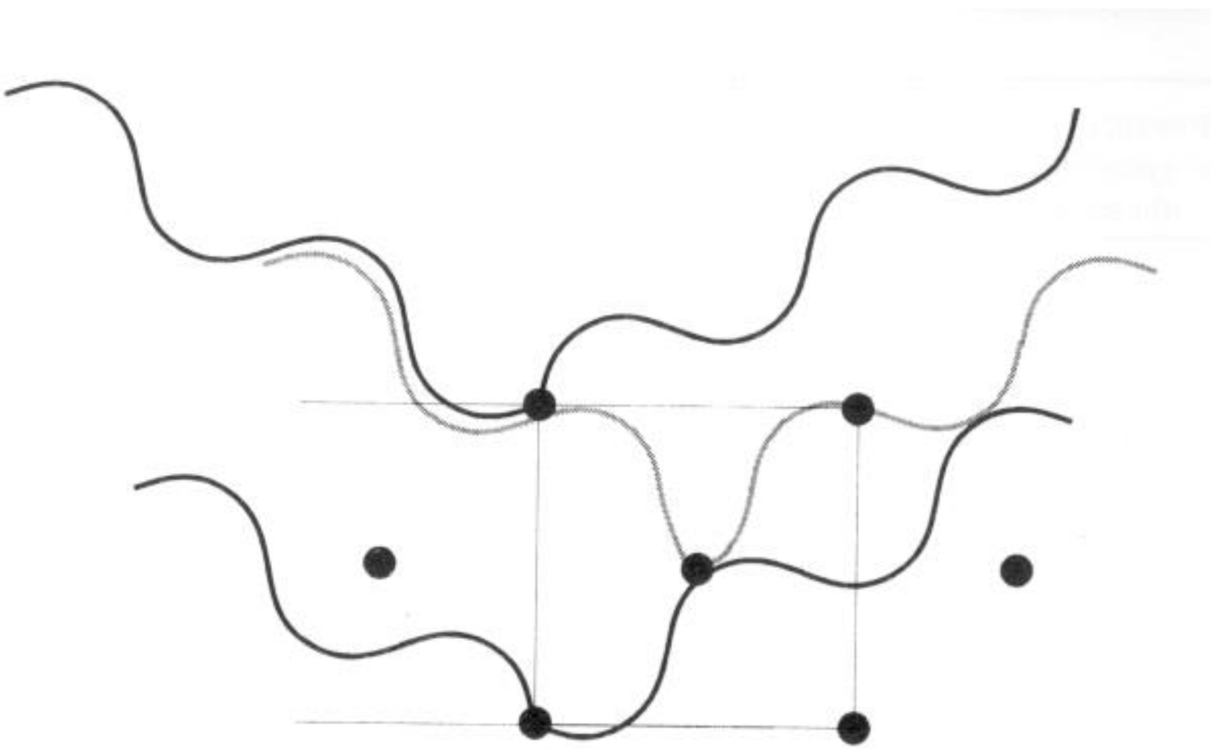

Some consequences:
how many lines = reciprocal lattice point will we see

So for each Bravais lattice:

$h^2 + k^2 + l^2$	PRIMITIVE All possible	BODY h+k+l=2n	FACE 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

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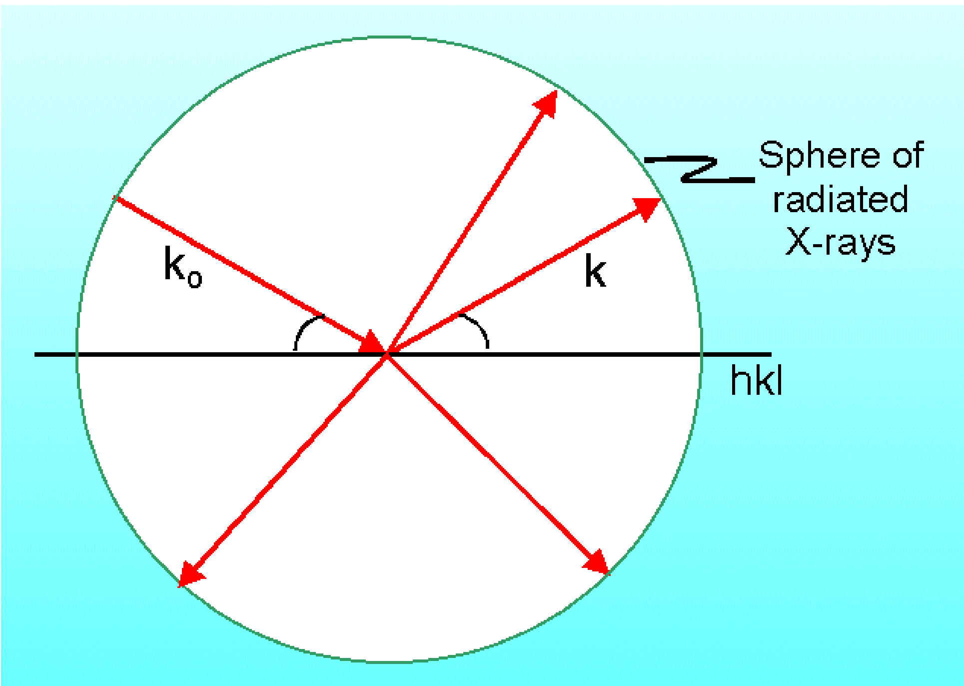
Ewald construction

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



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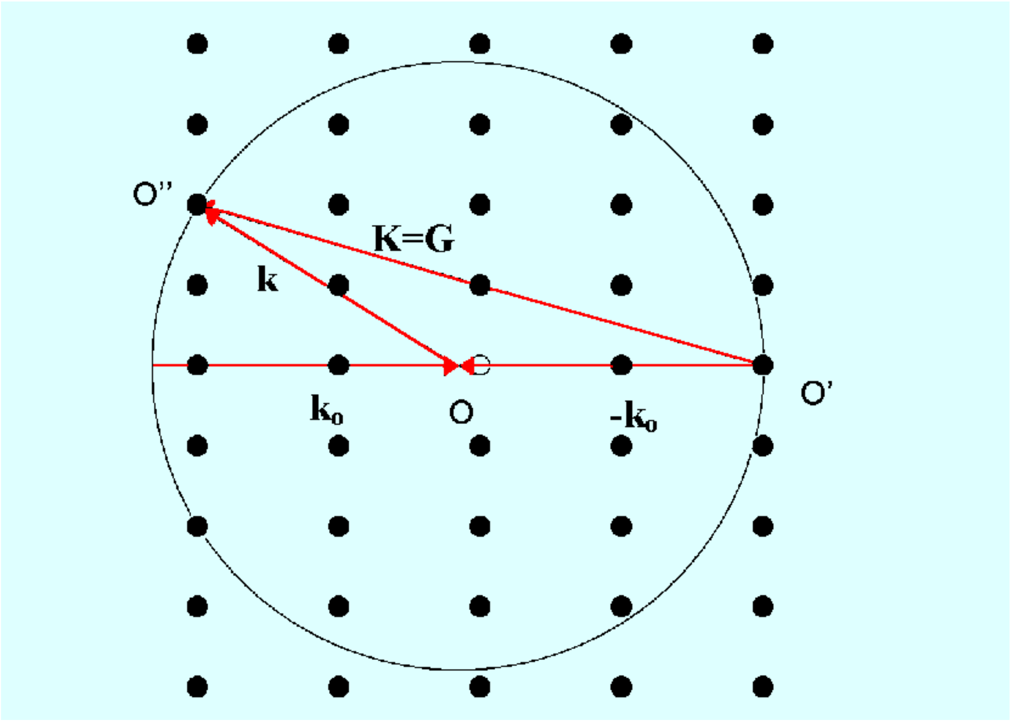
We superimpose the imaginary "sphere" of radiated radiation upon the reciprocal lattice



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**

Bragg planes and Brillouin zone construction

The construction of Bragg Planes in the context of Brillouin zones can be understood by considering Bragg's Law $\boldsymbol{\lambda = 2d\sin\theta}$. As we now know, in reciprocal space this can be expressed in the form

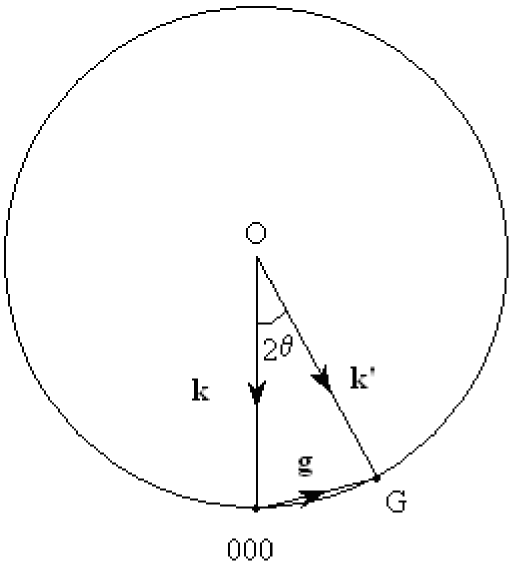
$$\mathbf{k'} - \mathbf{k} = \mathbf{g}$$

where **k** is the wave vector of the incident wave of magnitude $2\pi/\lambda$,

k' is the wave vector of the diffracted wave, also of magnitude $2\pi/\lambda$, and

g is a reciprocal lattice vector of magnitude $2\pi/d$:

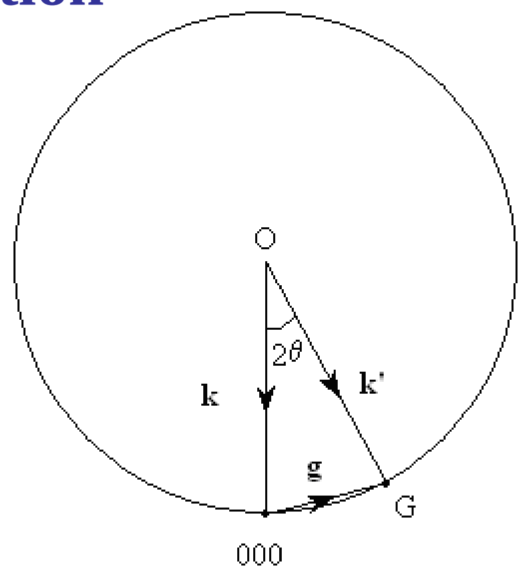
As we also know, this can be illustrated graphically using the Ewald sphere construction –
with 000 to be the origin of the reciprocal lattice and O is the centre of the sphere of radius $|\mathbf{k}|$.



Bragg planes and Brillouin zone construction

If the angle subtended at O between 000 and **G** on the diagram is 2θ, simple geometry shows that

$$\sin\theta = \frac{|\mathbf{g}|}{2|\mathbf{k}|} = \frac{\frac{2\pi}{d_{hkl}}}{2.\frac{2\pi}{\lambda}} = \frac{\lambda}{2d_{hkl}} \qquad \lambda = 2d_{hkl}\sin\theta$$



The equation

k' – k = g

can be rearranged in the form

k' = **k** + **g** so that

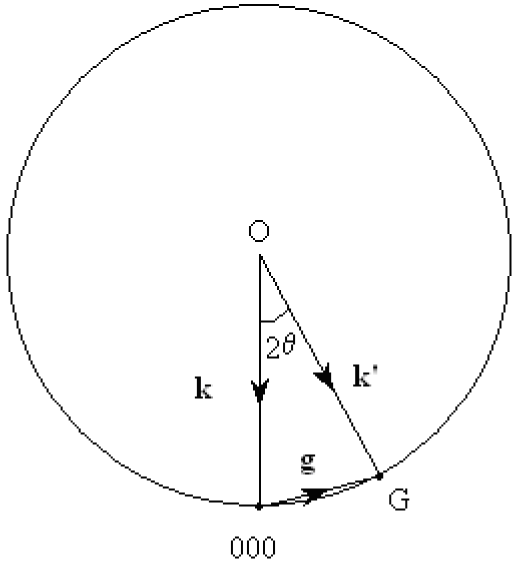
k'.k' = **(k** + **g).(k** + **g)** = **k.k** + **g.g** + **2k.g**

But **k'.k'** = **k.k** because diffraction is an elastic scattering event,

g.g + **2k.g** = 0

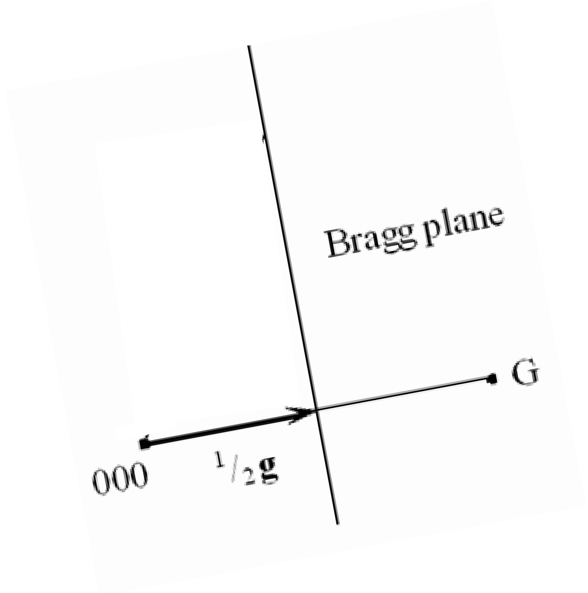
Bragg planes and Brillouin zone construction

g.g + 2k.g = 0



To construct the Bragg Plane, it is convenient to replace **k** by **-k** in this equation so that both **k** and **g** begin at the origin, 000, of the reciprocal lattice. Hence, the equation can be written in the form

k.(½g) = (½g). (½g)



Constructing the plane normal to **g** at the midpoint, **(½g)**,

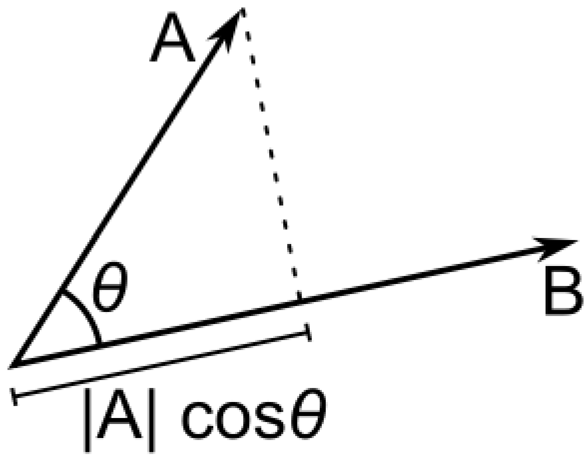
then means that **any** vector **k** drawn from the origin, 000, to a position on this plane satisfies the Bragg diffraction condition.

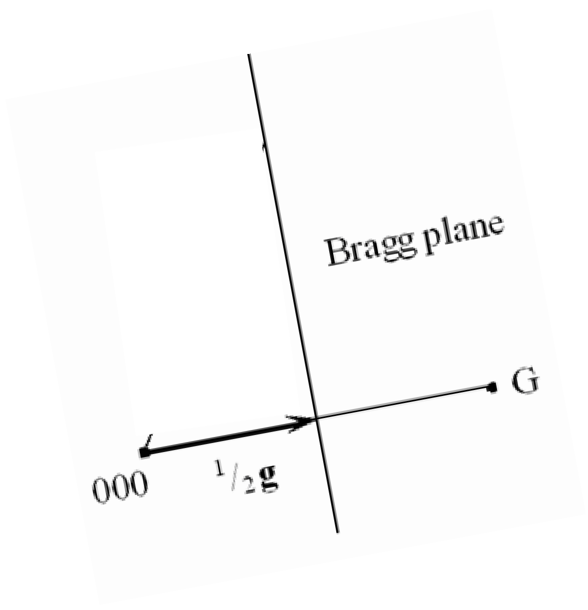
Do we undrestand this? Let's repeat

Bragg planes and Brillouin zone construction

$k.(\frac{1}{2}g) = (\frac{1}{2}g).(\frac{1}{2}g)$ **When this holds – diffraction occurs – that's the law**

Let's considering when this "dot" products will do coincide?
What the dot product by the way?

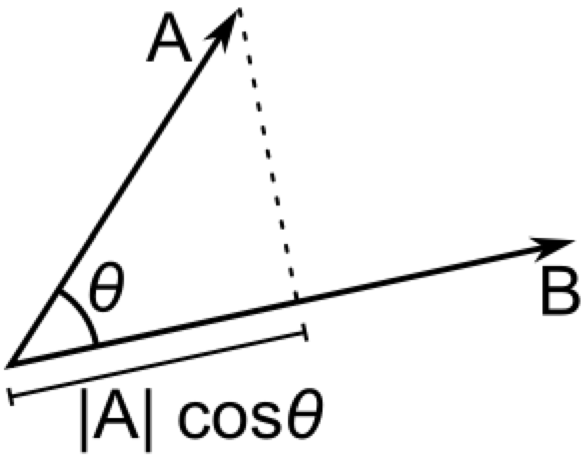


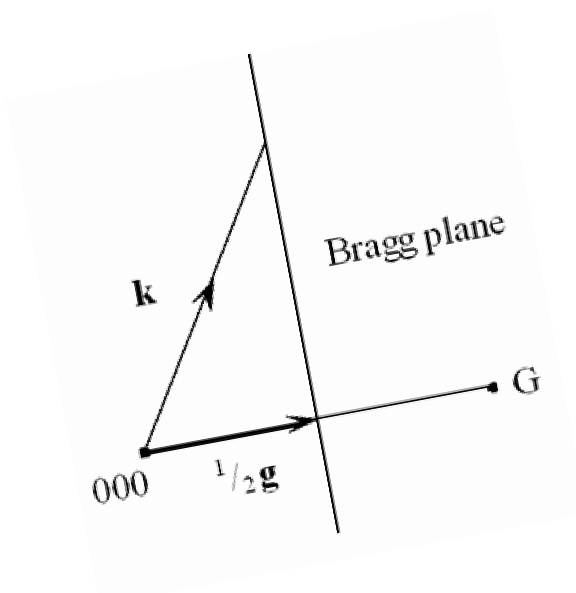


Bragg planes and Brillouin zone construction

k.(½g) = (½g). (½g) **When this holds – diffraction occurs – that's the law**

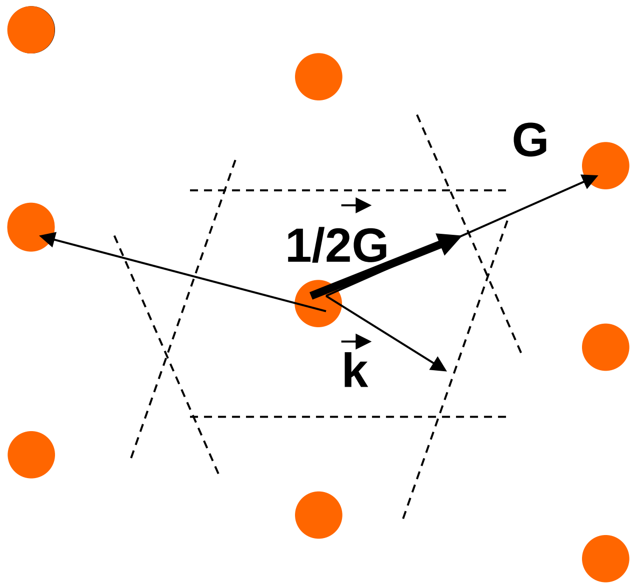
Let's considering when this "dot" products will do coincide?
What the dot product by the way?





Fundamental conslusion is:
A wave with a wafe vector < k has no chance to get diffracted

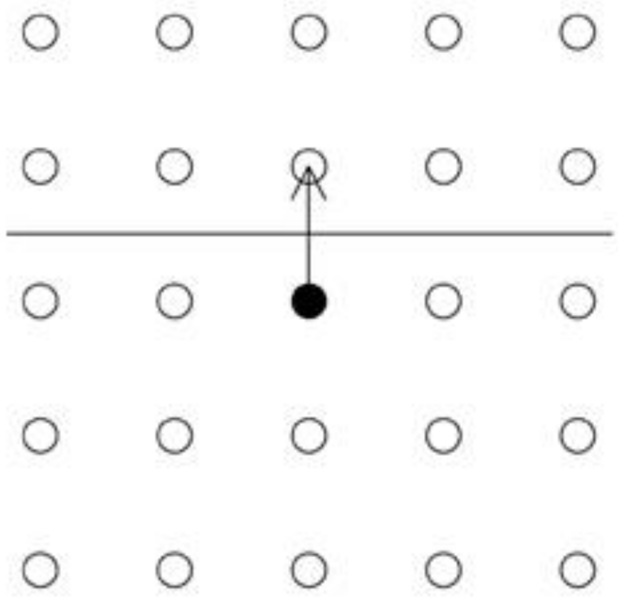
Bragg planes and Brillouin zone construction



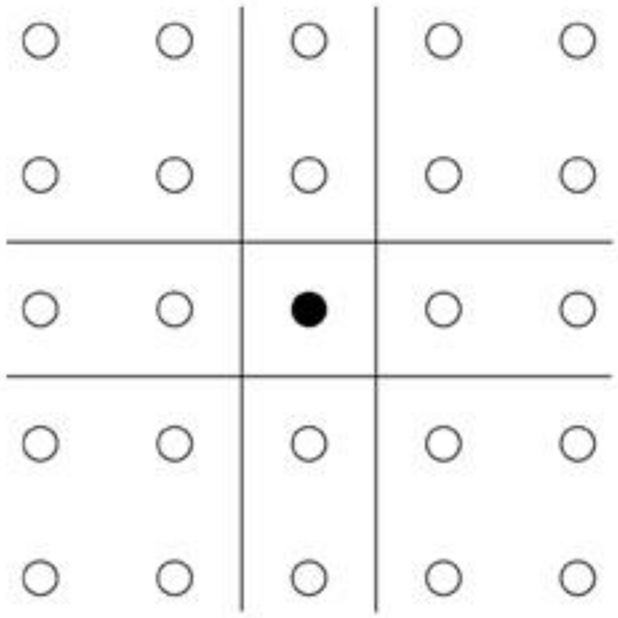
The vector k_{in} (also k_{out}) lies along the perpendicular bisecting plane of a G vector

- **Brillouin Zone formed by perpendicular bisectors of G vectors**
- **Consequence: No diffraction for any k inside the first Brillouin Zone**
- **Special role of Brillouin Zone (Wigner-Seitz cell of reciprocal lattice) as opposed to any other primitive cell**

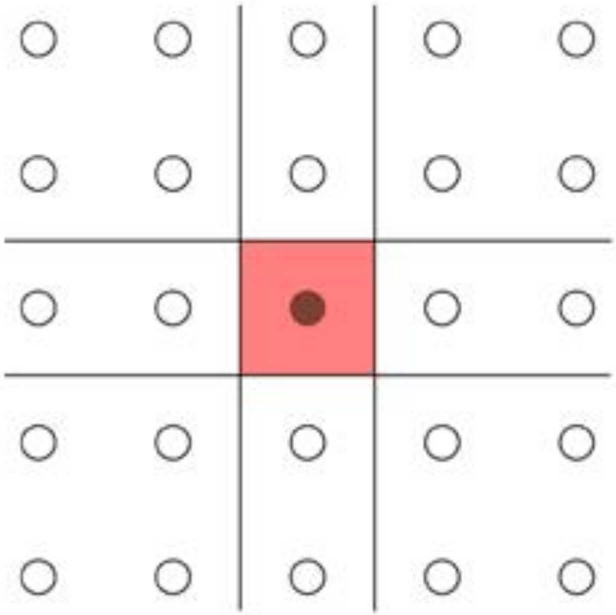
Bragg planes and Brillouin zone construction



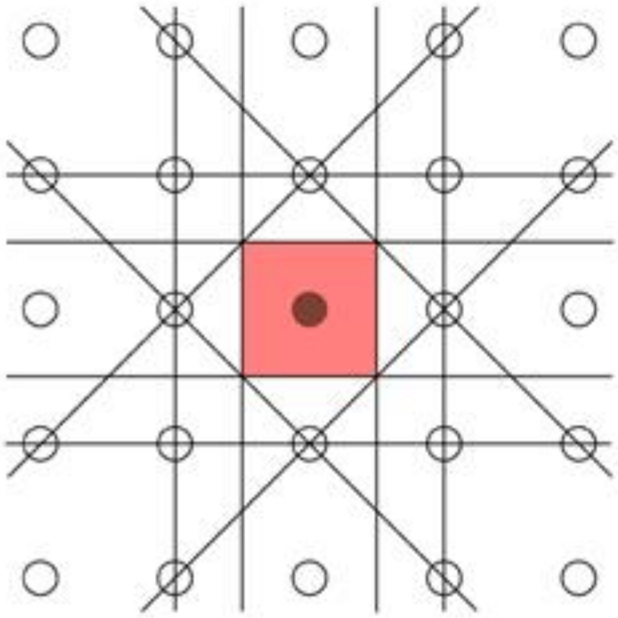
Bragg planes and Brillouin zone construction



Bragg planes and Brillouin zone construction



Bragg planes and Brillouin zone construction



Bragg planes and Brillouin zone construction