FYS3410 - Vår 2011 (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**

Andrej Kuznetsov, Dept of Physics and Centre for Material Science and Nanothechnology
Postboks 1048 Blindern, 0316 OSLO
Tel: +47-22852870, e-post: andrej.kuznetsov@fys.uio.no
visiting address: MiNaLab, Gaustadaleen 23b

FYS3410 lecture schedule and exams: Spring 2011

W/19/1/2011:	Introduction and motivation. Periodicity and lattices	1h
M/24/1/2011:	Index system for crystal planes. Crystal structures	2h
W/26/1/2011:	Reciprocal space, Laue condition and Ewald construction	1h
M/31/1/2011:	Brillouin Zones. Interpretation of a diffraction experiment	2h
W/02/2/2011:	Crystal binding, elastic strain and waves	1h
M/07/2/2011:	Elastic waves in cubic crystals; defects in crystals	2h
W/09/2/2011:	Defects in crystals; case study – vacancies; diffusion	2h
M/14/2/2011:	Crystal vibrations and phonons	2h
W/16/2/2011:	Lattice heat capacity: Dulong-Petit and Einstein models	2h
M/21/2/2011:	Phonon density of states (DOS) and Debye model	2h
W/23/2/2011:	General result for DOS; role of anharmonic interactions	2h
M/28/2/2011:	Thermal conductivity and repetition of crystal vibrations	2h
W/02/3/2011:	no lectures	
M/07/3/2011:	no lectures	
W/09/3/2011:	no lectures	
M/14/3/2011:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/17/3/2011:	Density of states, effect of temperature – FD distribution	1h
M/21/3/2011:	Heat capacity of FEFG	2h
W/23/3/2011:	Repetition	1h
M/28/3/2011:	Mid-term exam	

M/04/4/2011:	**Electrical and thermal conductivity in metals**	**2h**
W/06/4/2011:	**Bragg reflection of electron waves at the boundary of BZ**	**2h**
M/11/4/2011:	**Energy bands, Kronig - Penny model**	**2h**
W/13/4/2011:	**Empty lattice approximation; number of orbitals in a band**	**2h**
Påsk uppehåll		
W/27/4/2011	**no lectures**	
M/02/5/2011:	**no lectures**	
W/04/5/2011:	**no lectures**	
M/09/5/2010:	**Semiconductors, effective mass method, intrinsic carriers**	**2h**
W/11/4/2010:	**Impurity states in semiconductors and carrier statistics**	**2h**
M/16/5/2010:	**p-n junctions, Schottky contacts and heterojunctions**	**2h**
W/18/5/2010:	**Metals and Fermi surfaces**	**1h**
M/23/5/2010:	**Repetition**	**2h**
26-27/5/2010:	**Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Aarhus University, Denmark, http://person.au.dk/en/anl@phys.au.dk)**	

Lecture 3: Bragg plains and Brillouin zones.
Use of diffraction experiment in research

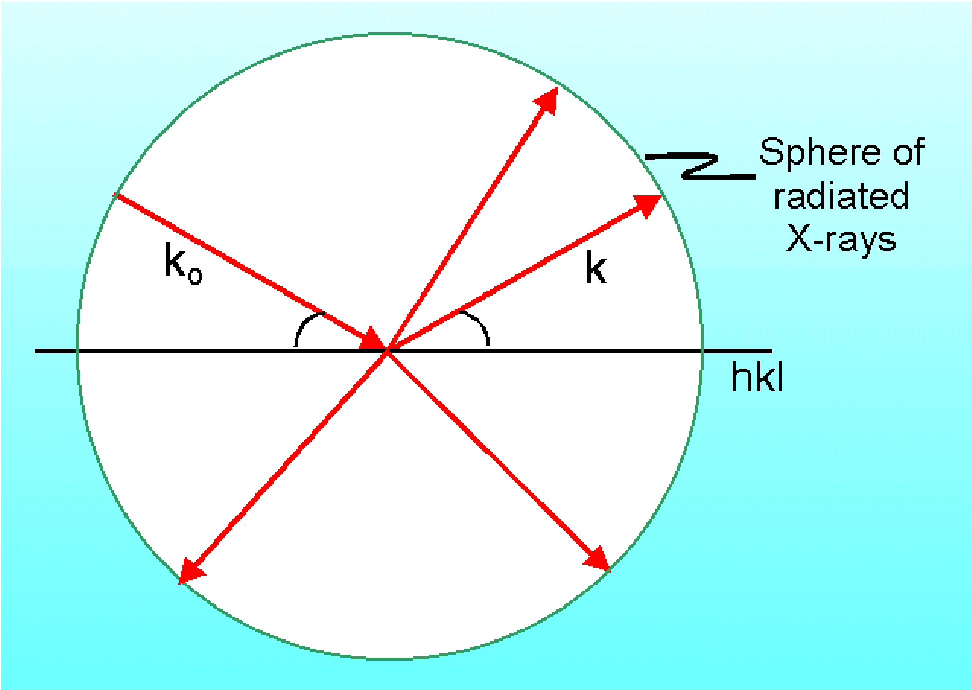
- repetition of Laue condition and Ewald construction;
- Introduction and interpretation of Brillouin zones;
- Use of diffraction experiment in research

Lecture 3: Bragg plains and Brillouin zones.
Use of diffraction experiment in research

- **repetition of Laue condition and Ewald construction;**
- **Introduction and interpretation of Brillouin zones;**
- **Interpretation of x-ray diffraction measurements**

Ewald construction

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

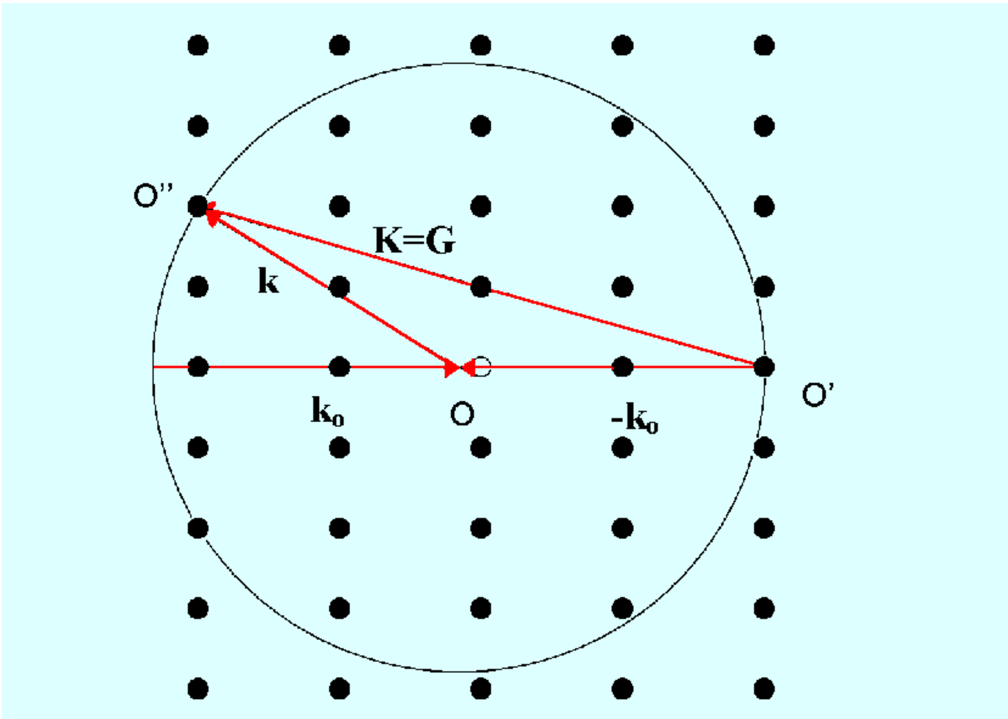


Constructive interference only occurs when the scattering vector, **K (*Δk*** *in the Kittel's notations*), coincides with a reciprocal lattice vector, **G**

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**

Lecture 3: Brillouin zones. Interpretation of a diffraction experiment

- repetition of Laue condition and Ewald construction;
- **Introduction and interpretation of Brillouin zones;**
- Interpretation of x-ray diffraction measurements

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 **$\lambda = 2d\sin\theta$**. As we now know, in reciprocal space this can be expressed in the form

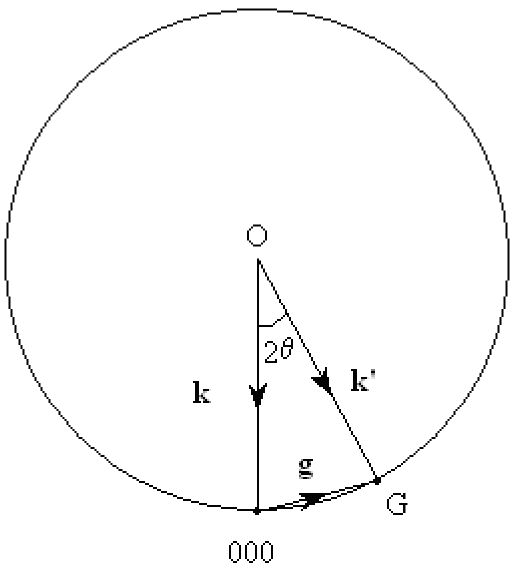
$\mathbf{k'} - \mathbf{k} = \mathbf{g}$

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 $2\pi/d$:

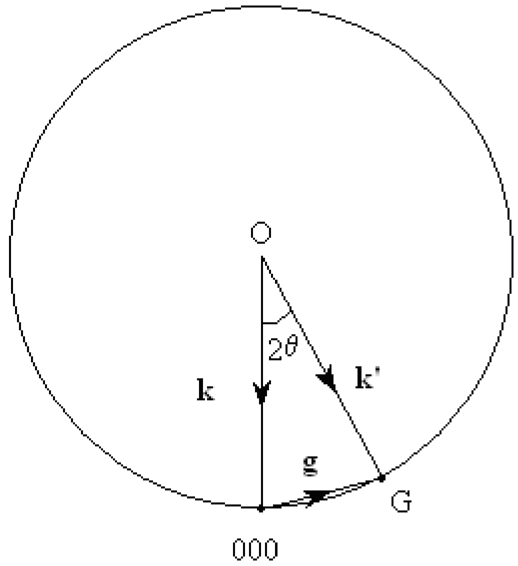
As we also know, this can be illustrated graphically using the Ewald sphere construction –
with 000 to be the origin of the reciprocal lattice and O is the centre of the sphere of radius $|\mathbf{k}|$.



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

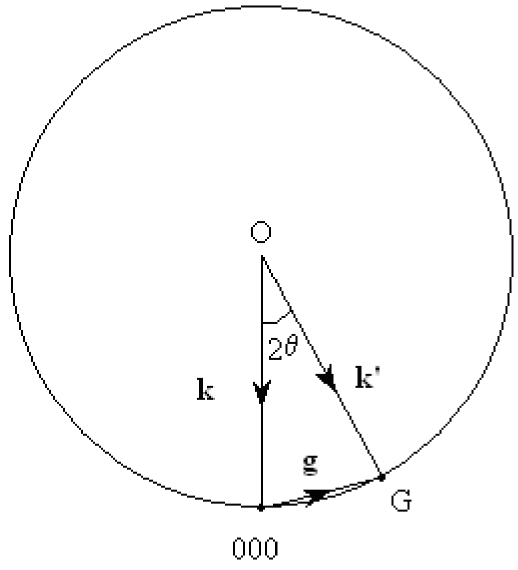
k'.k' = (k + g).(k + g) = k.k + g.g + 2k.g

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

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

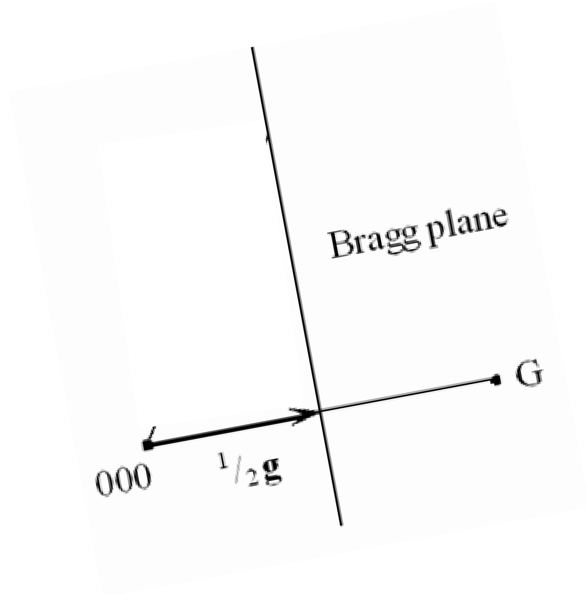
Bragg planes and Brillouin zone construction

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)**,

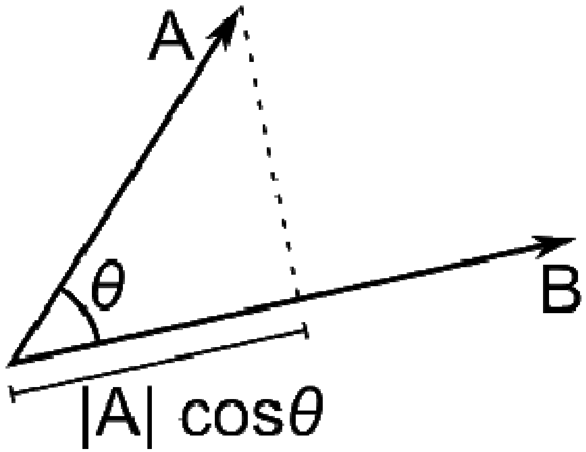
then means that **any** vector **k** drawn from the origin, 000, to a position on this plane satisfies the Bragg diffraction condition.

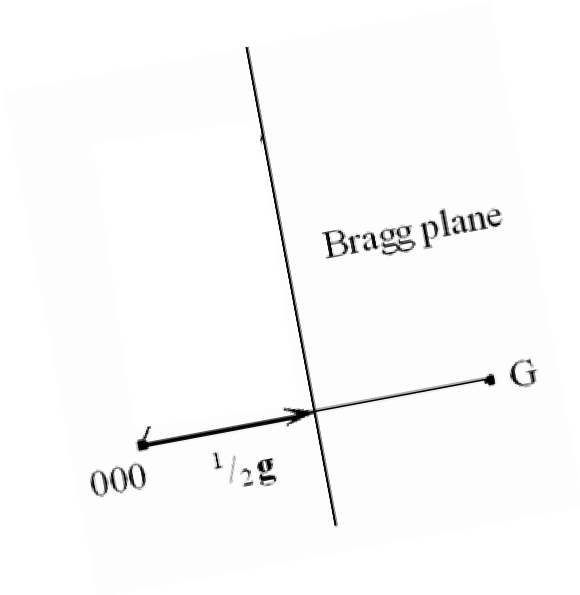
Do we undrestand this? Let's repeat

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?

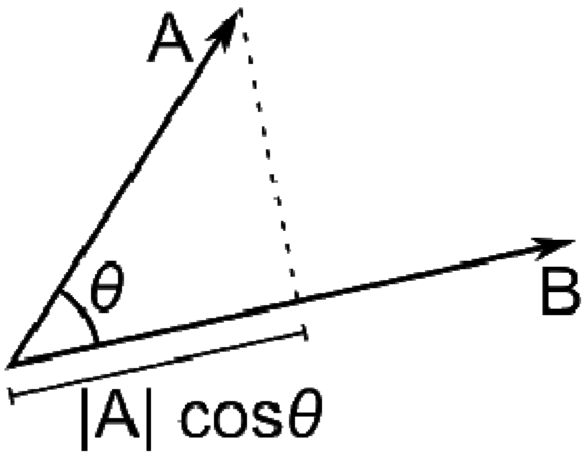


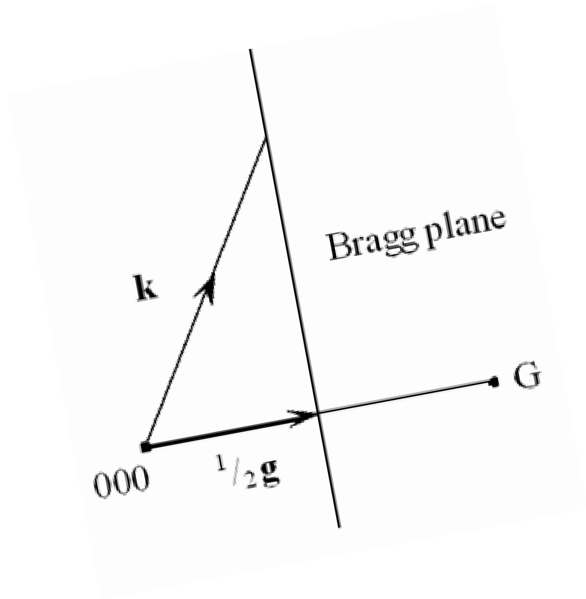


Bragg planes and Brillouin zone construction

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

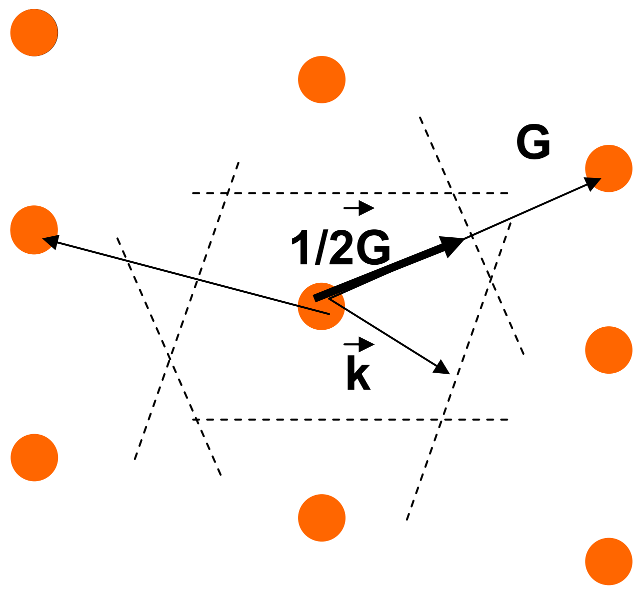
Let's considering when this "dot" products will do coincide?
What the dot product by the way?





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

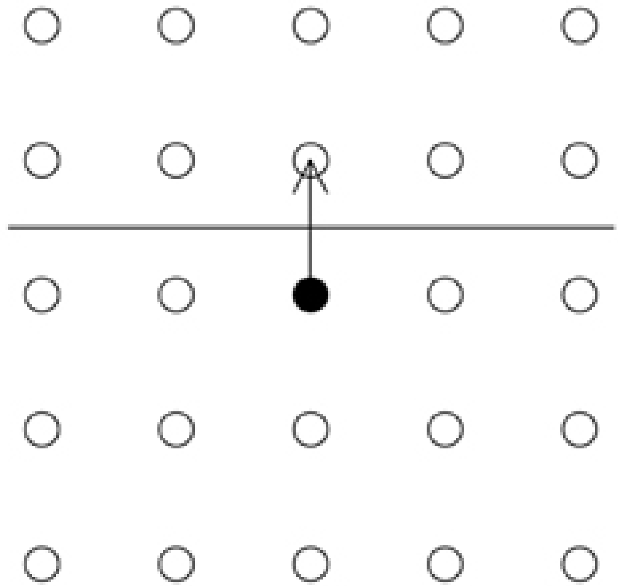
Bragg planes and Brillouin zone construction



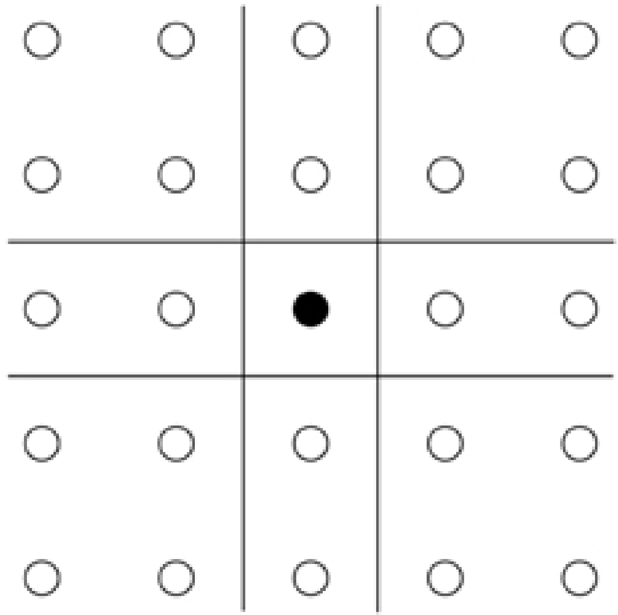
The vector k_{in} (also k_{out}) lies along the perpendicular bisecting plane of a G vector

- 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

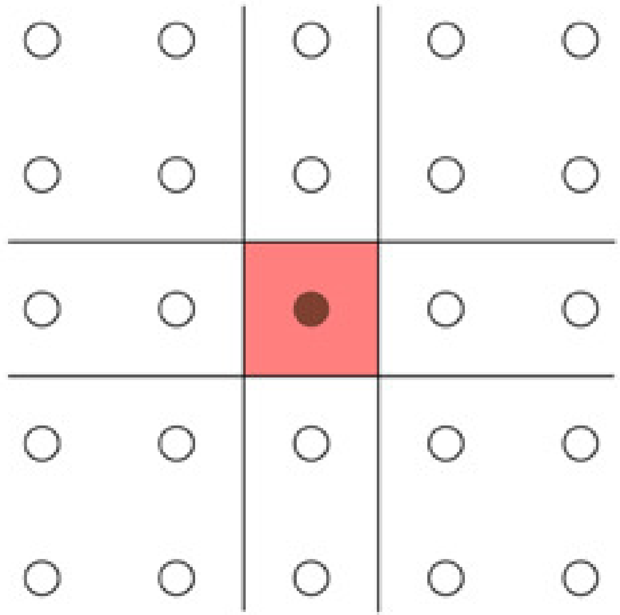
Bragg planes and Brillouin zone construction



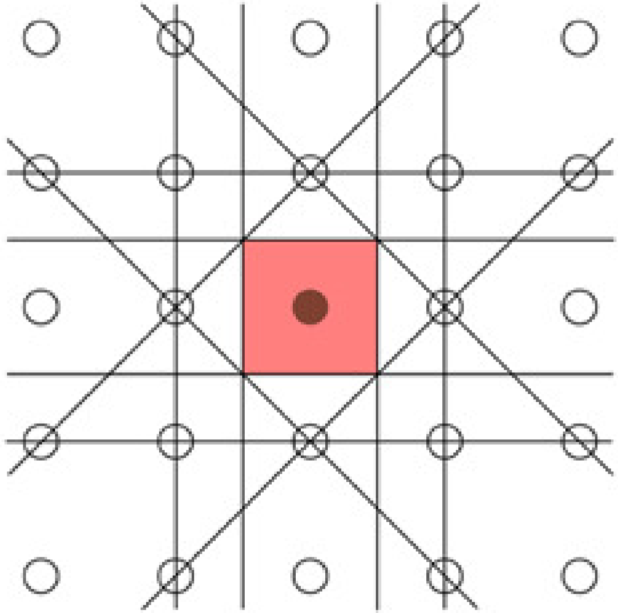
Bragg planes and Brillouin zone construction



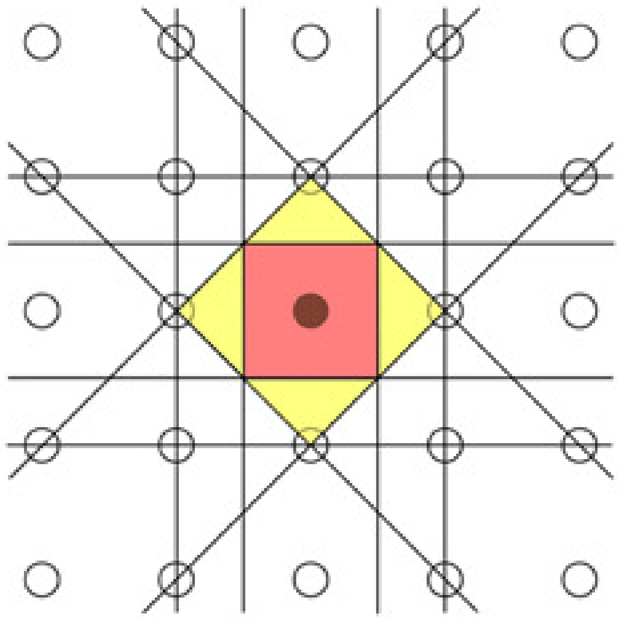
Bragg planes and Brillouin zone construction



Bragg planes and Brillouin zone construction



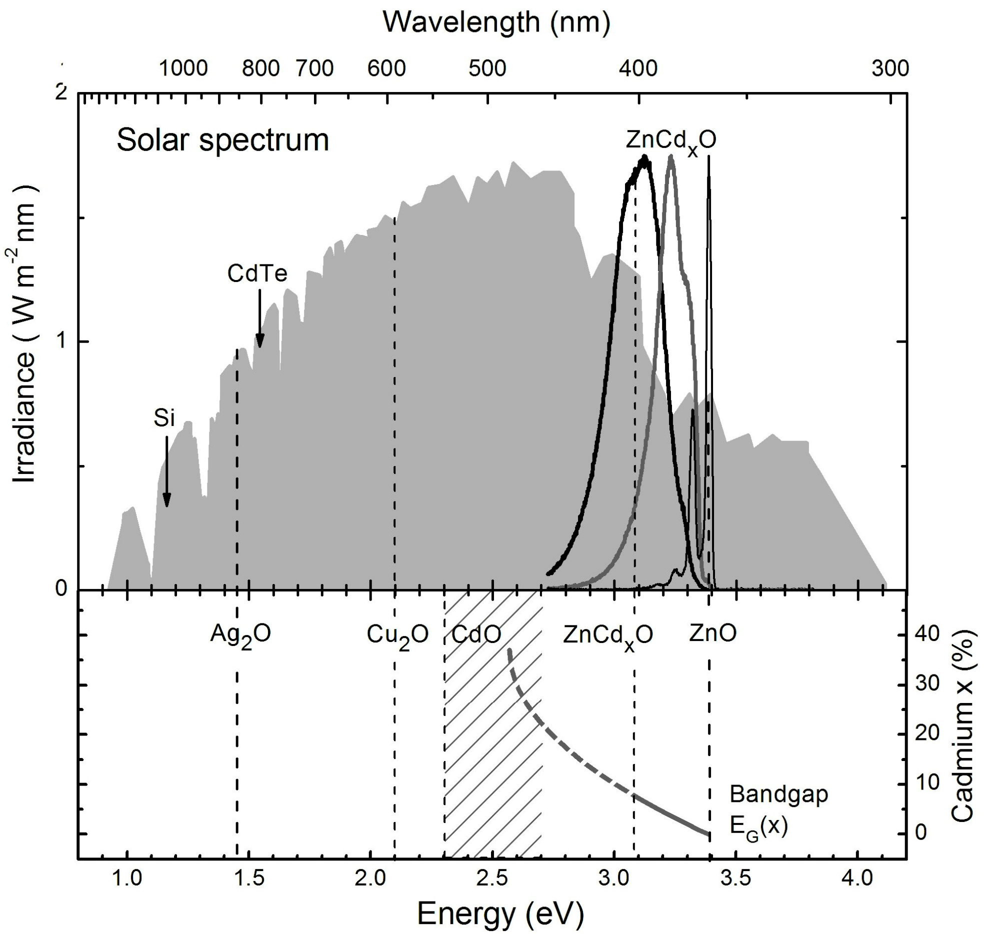
Bragg planes and Brillouin zone construction



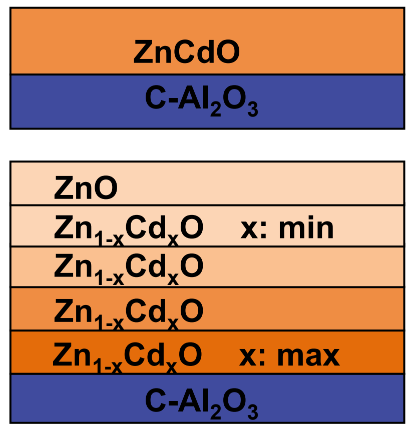
Lecture 3: Bragg plains and Brillouin zones.
Use of diffraction experiment in research

- repetition of Laue condition and Ewald construction;
- Introduction and interpretation of Brillouin zones;
- Use of diffraction experiment in research

Use of diffraction experiment in research

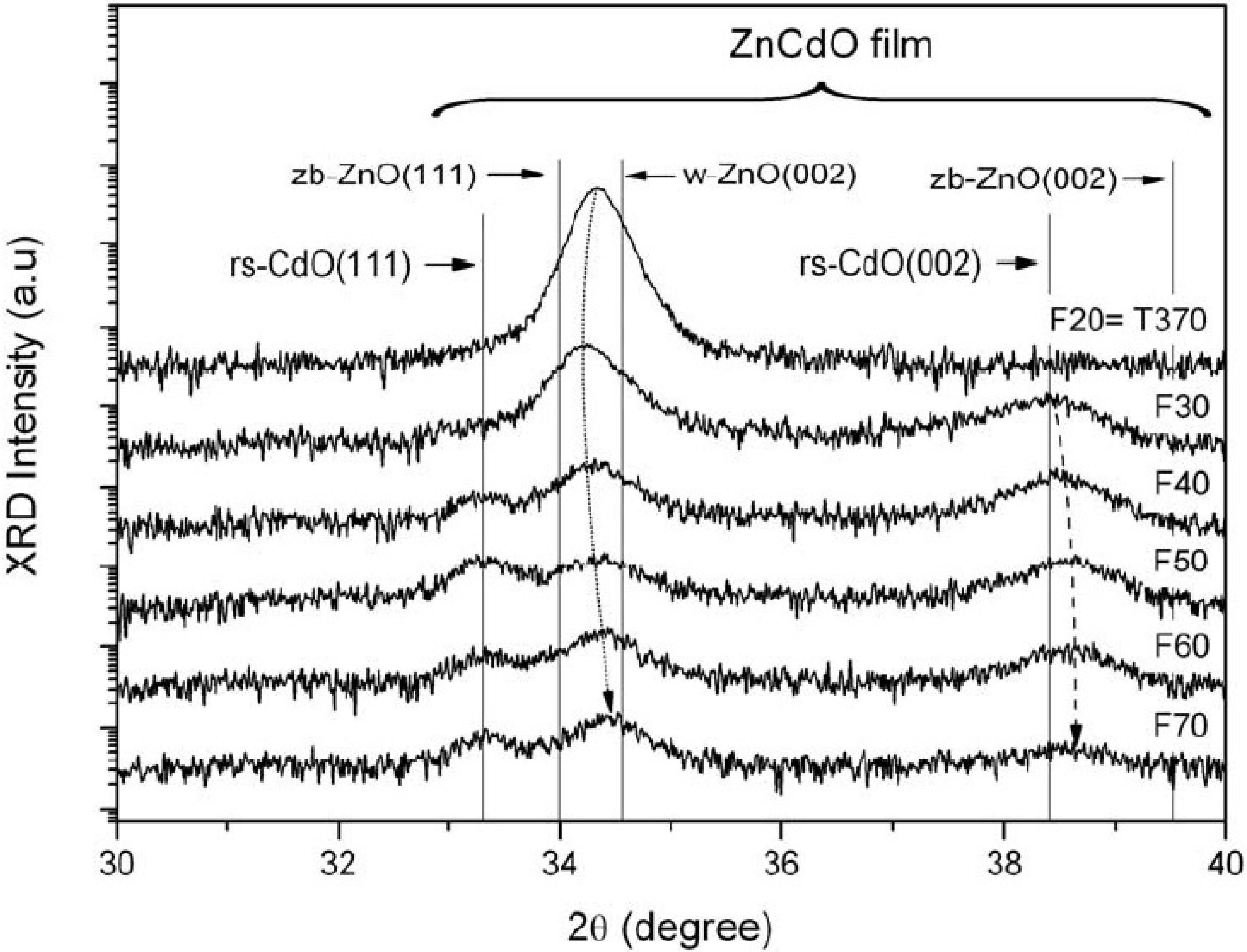


Schematic of the structures studied

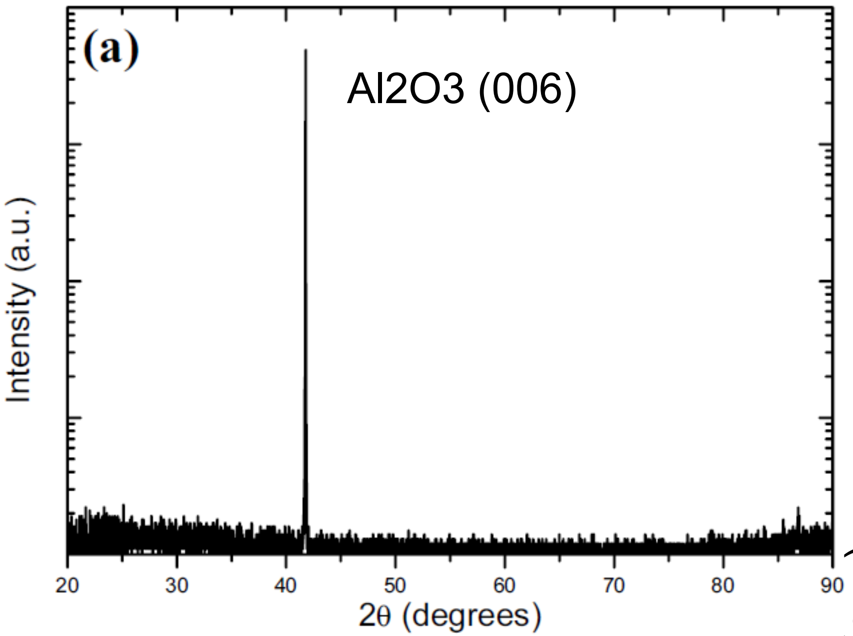


single layer

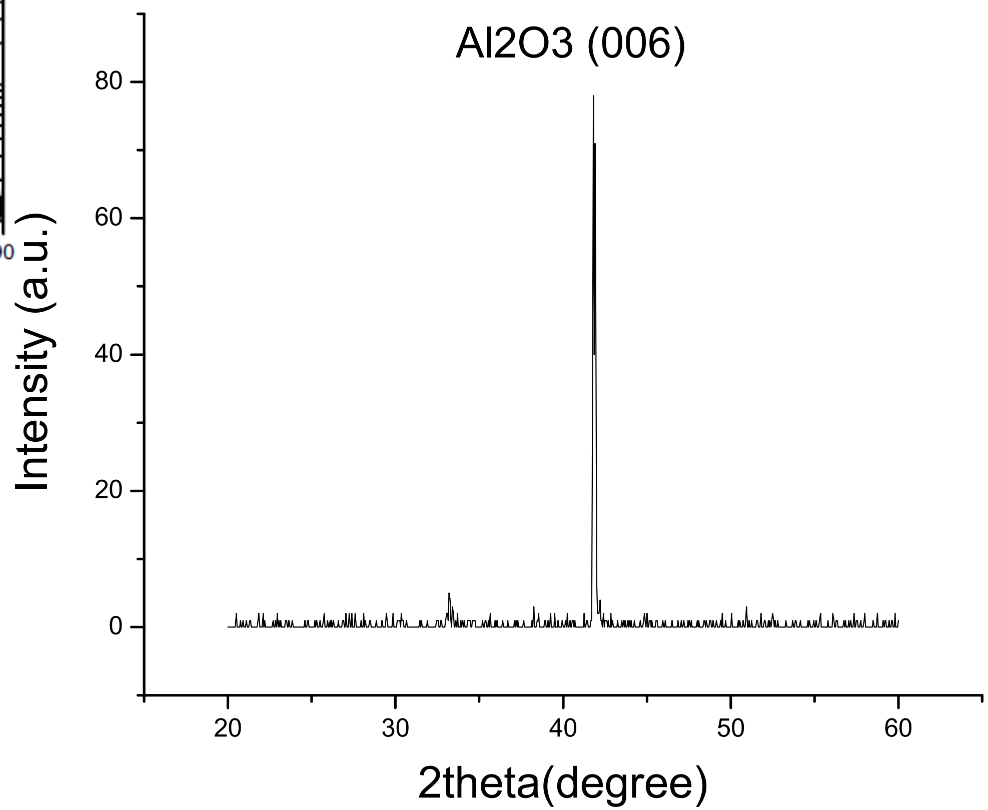
multilayer


ZnCdO film
zb-ZnO(111)
w-ZnO(002)
zb-ZnO(002)
rs-CdO(111)
rs-CdO(002)
F20= T370
F30
F40
F50
F60
F70
XRD Intensity (a.u)
30
32
34
36
38
40
2θ (degree)

Use of diffraction experiment in research



From reference
CdO [025] // Al2O3 [0001]



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:

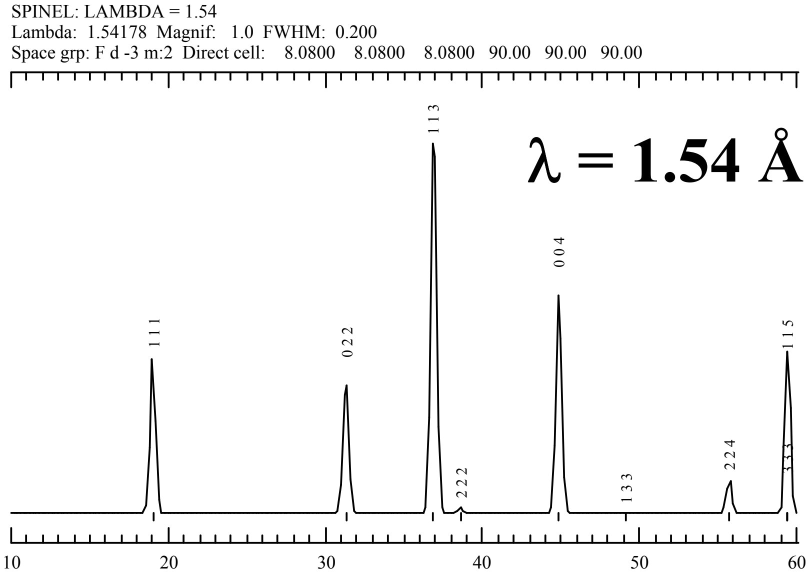
$$\left(h^2+k^2+l^2\right)\leq\frac{4a^2}{\lambda^2}$$

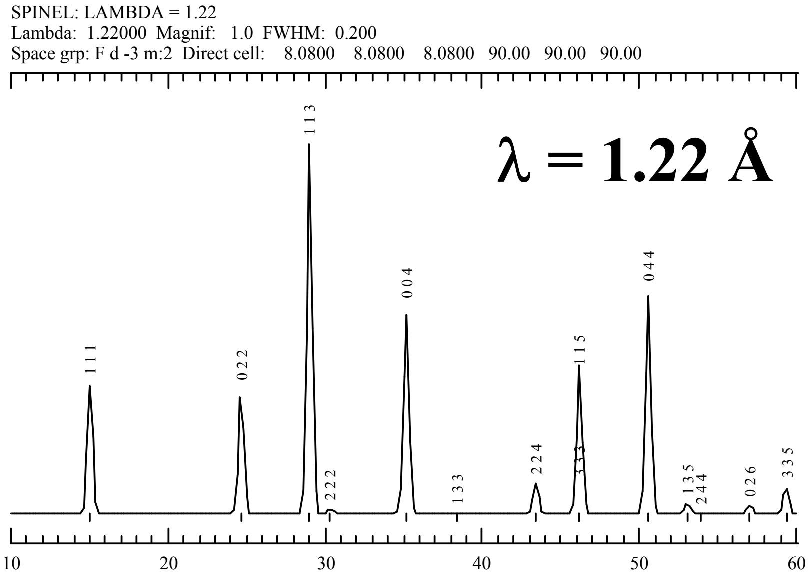
Some consequences:
how many lines = reciprocal lattice point will we see

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

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

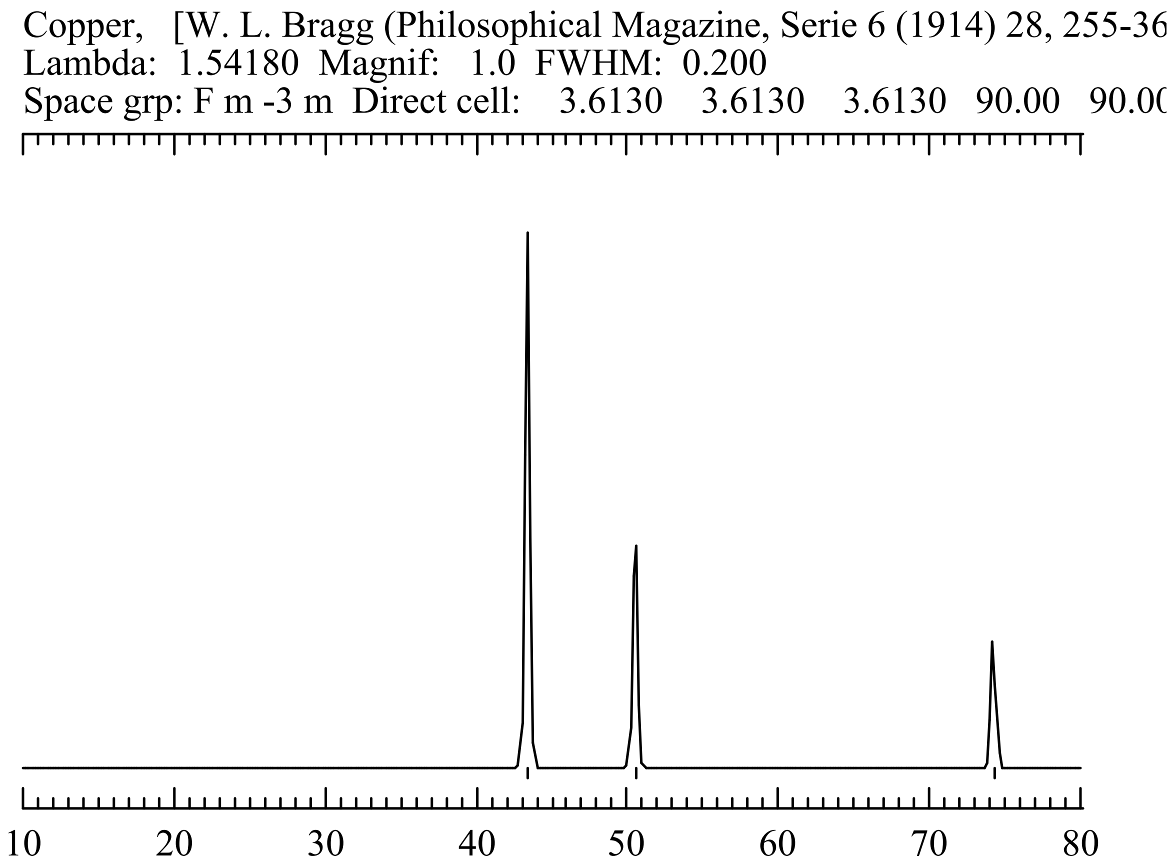
Let's take an example: The unit cell of copper is 3.613 Å. What is the Bragg angle for the (100) reflection with Cu Kα radiation (λ = 1.5418 Å)?

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

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

θ= 12.32°, so 2θ = 24.64°

BUT….



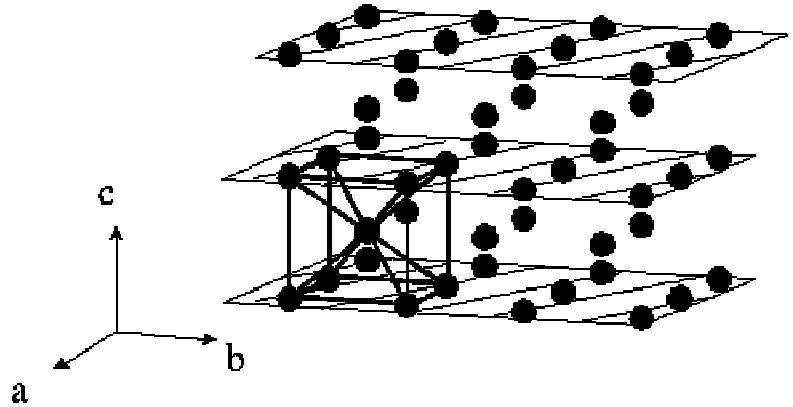
Some consequences:
how many lines = reciprocal lattice point will we see

- 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.

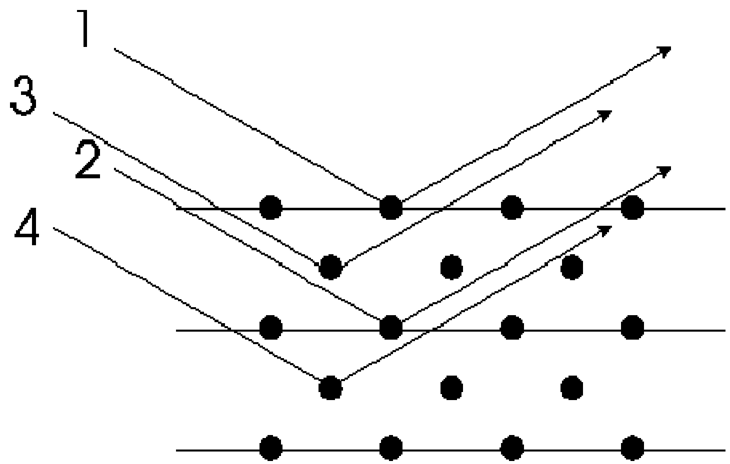
e.g. the (001) reflection in a BCC lattice is absent.



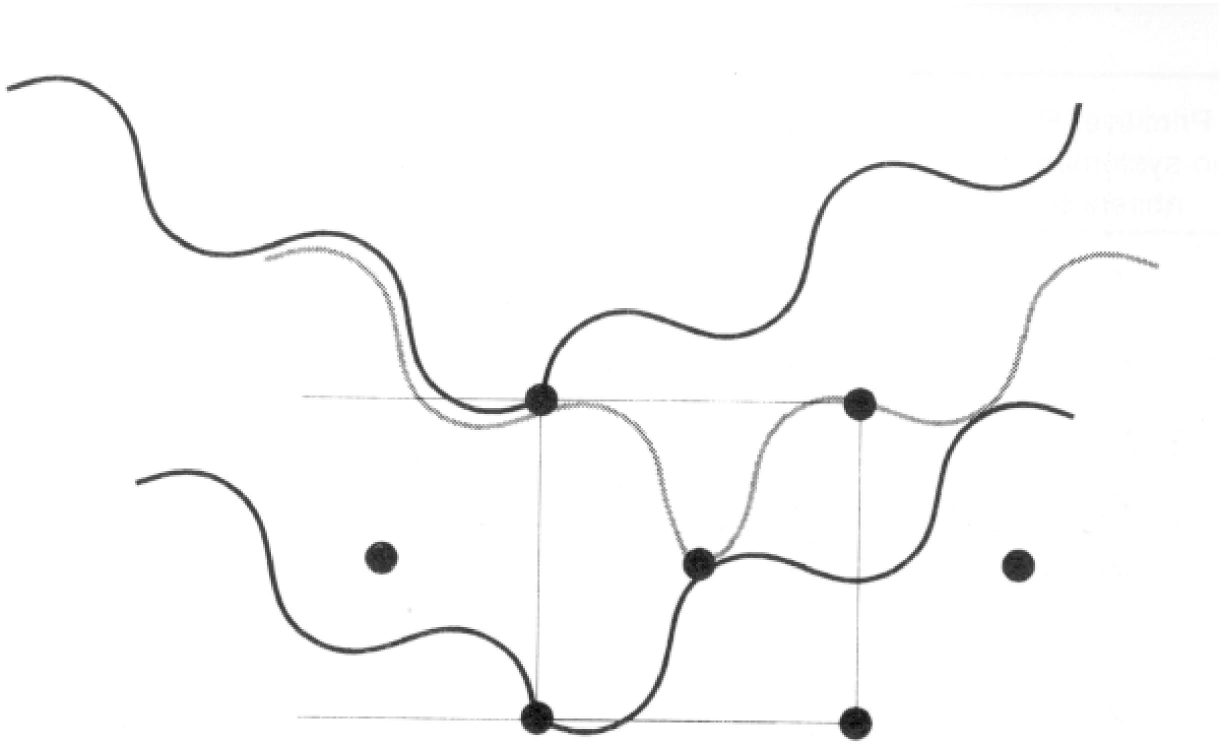
Consider the additional path lengths vs. beam "1":

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:

$h^2 + k^2 + l^2$	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