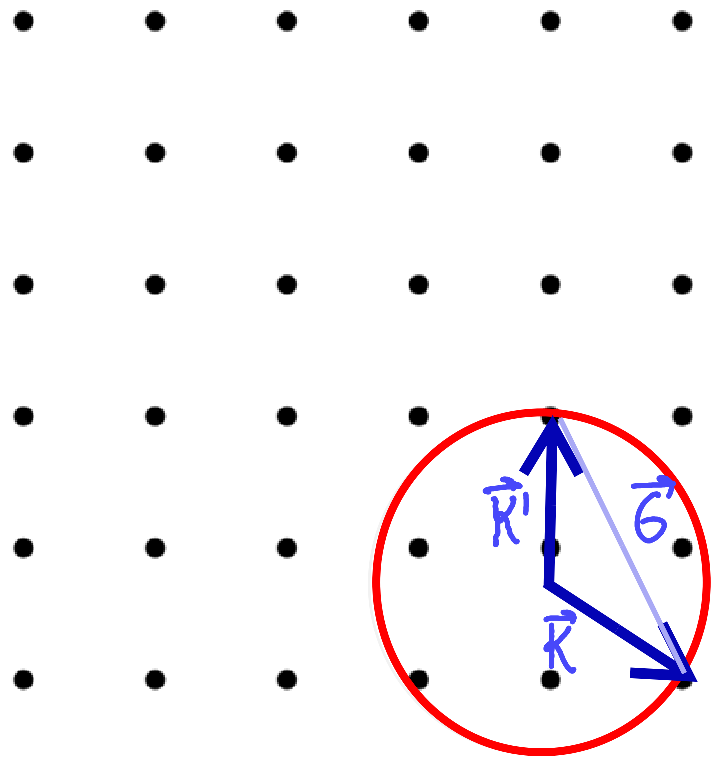
Methods of Scattering experiments

Ewald construction for diffraction

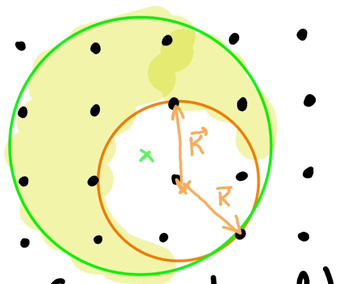


R.L.

$K = \frac{2\pi}{\lambda}$

Diffraction condition $\Delta\vec{K} = \vec{G}$

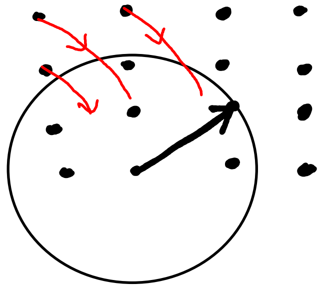
$\Rightarrow$ Probability to obtain a diffraction spot is low



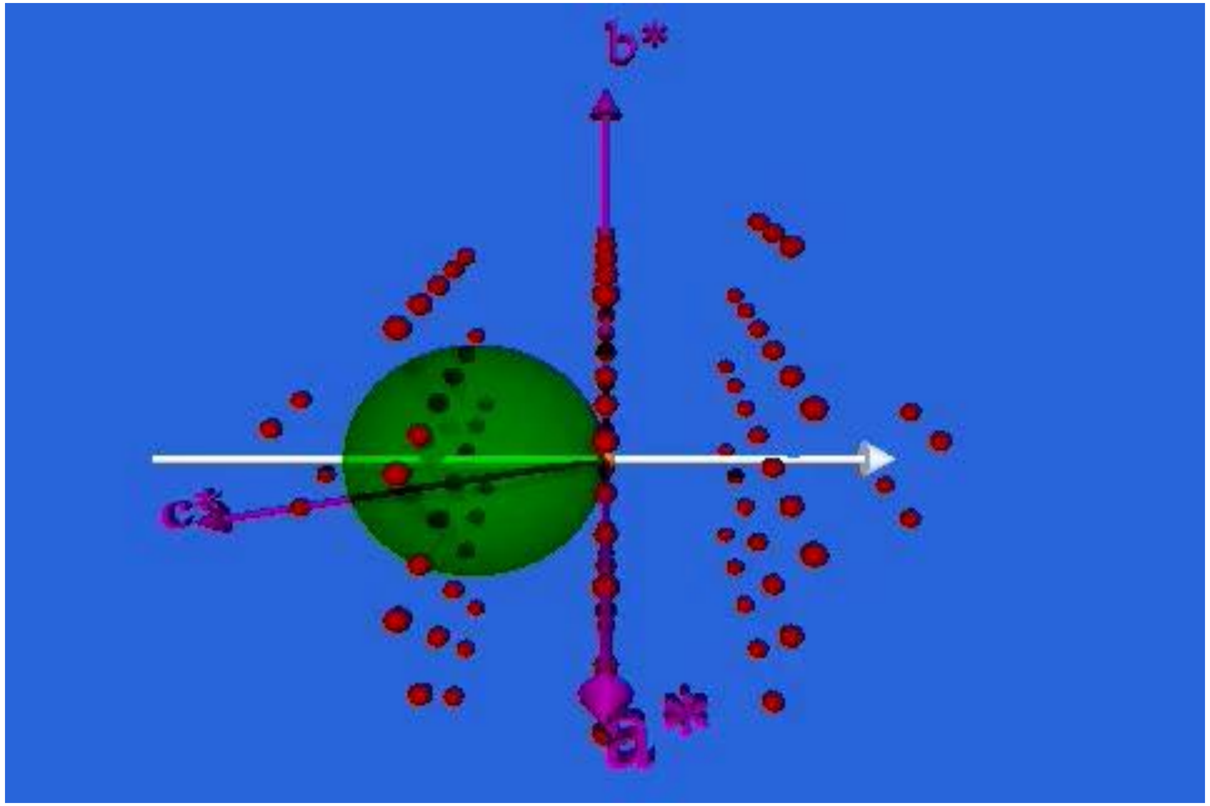
Methods

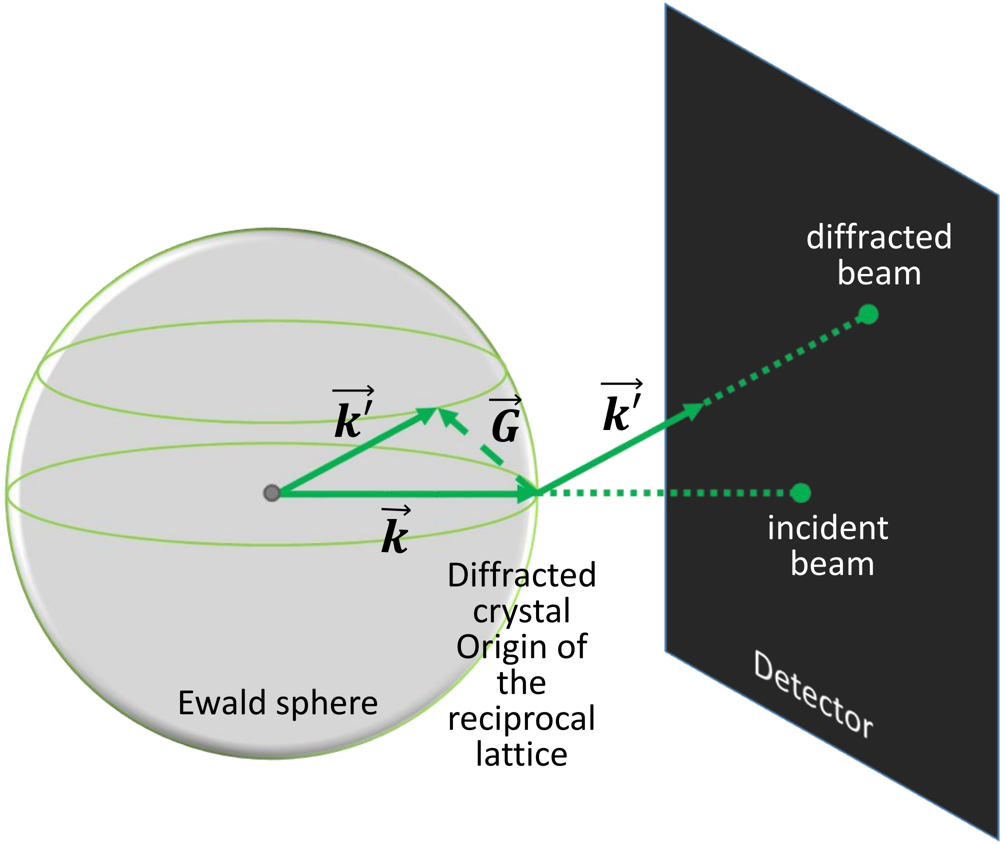
* Laue Method (range of λ instead of a monochromatic incident wave)

* Rotating Crystal Method



Ewald sphere





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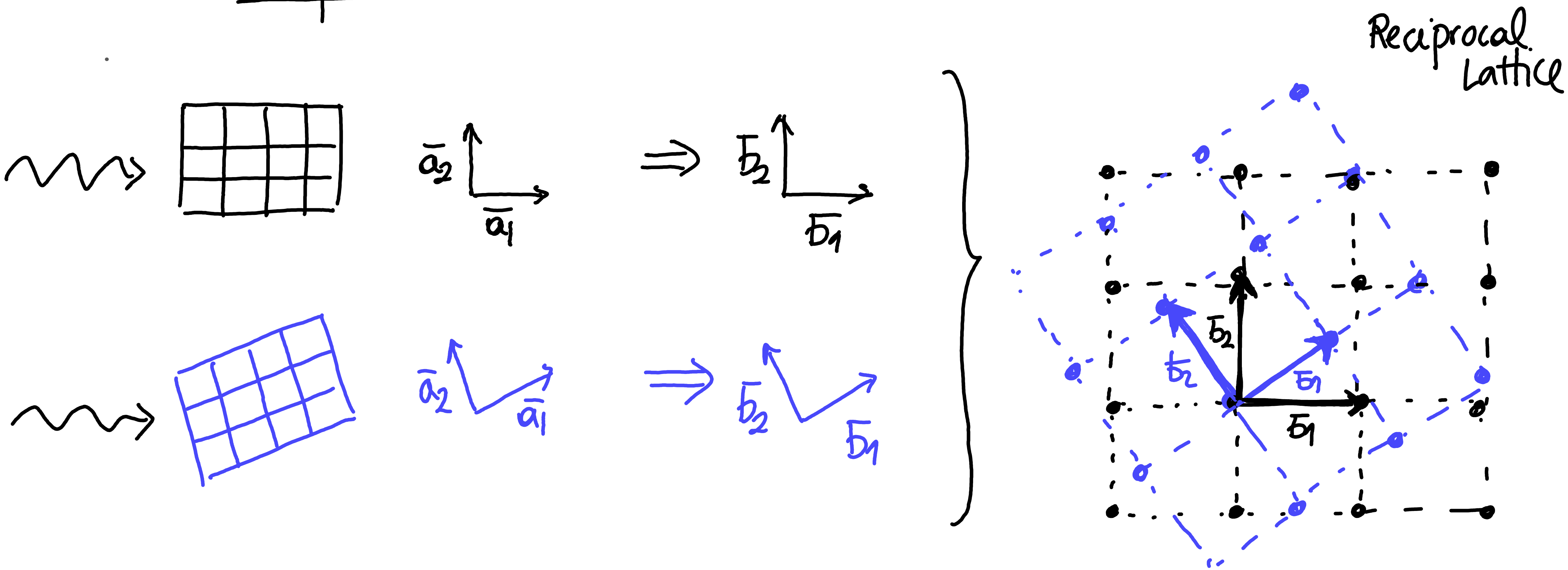
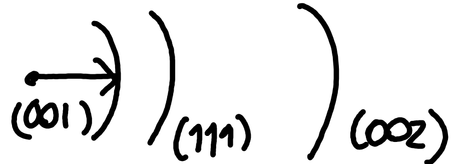
Powder diffraction

(not single crystalline samples)

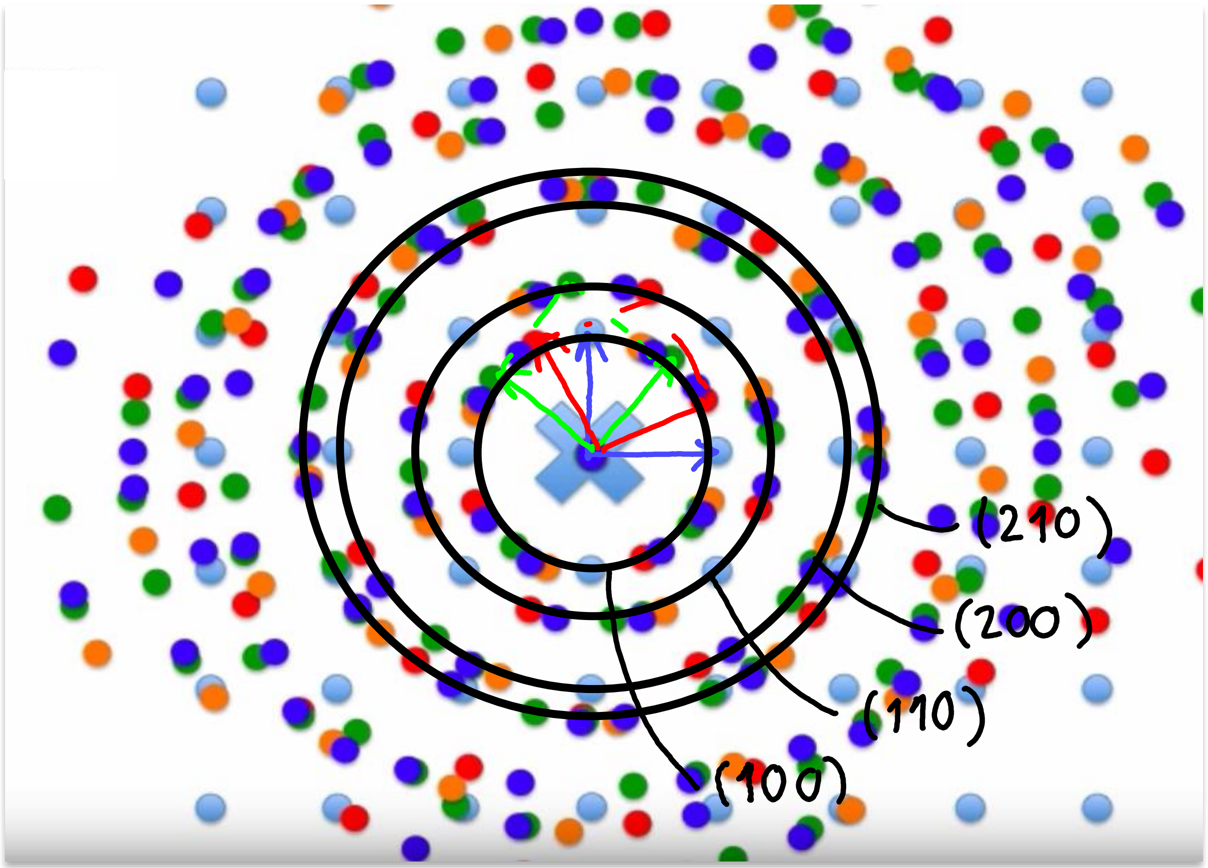
or Debye-Scherrer method

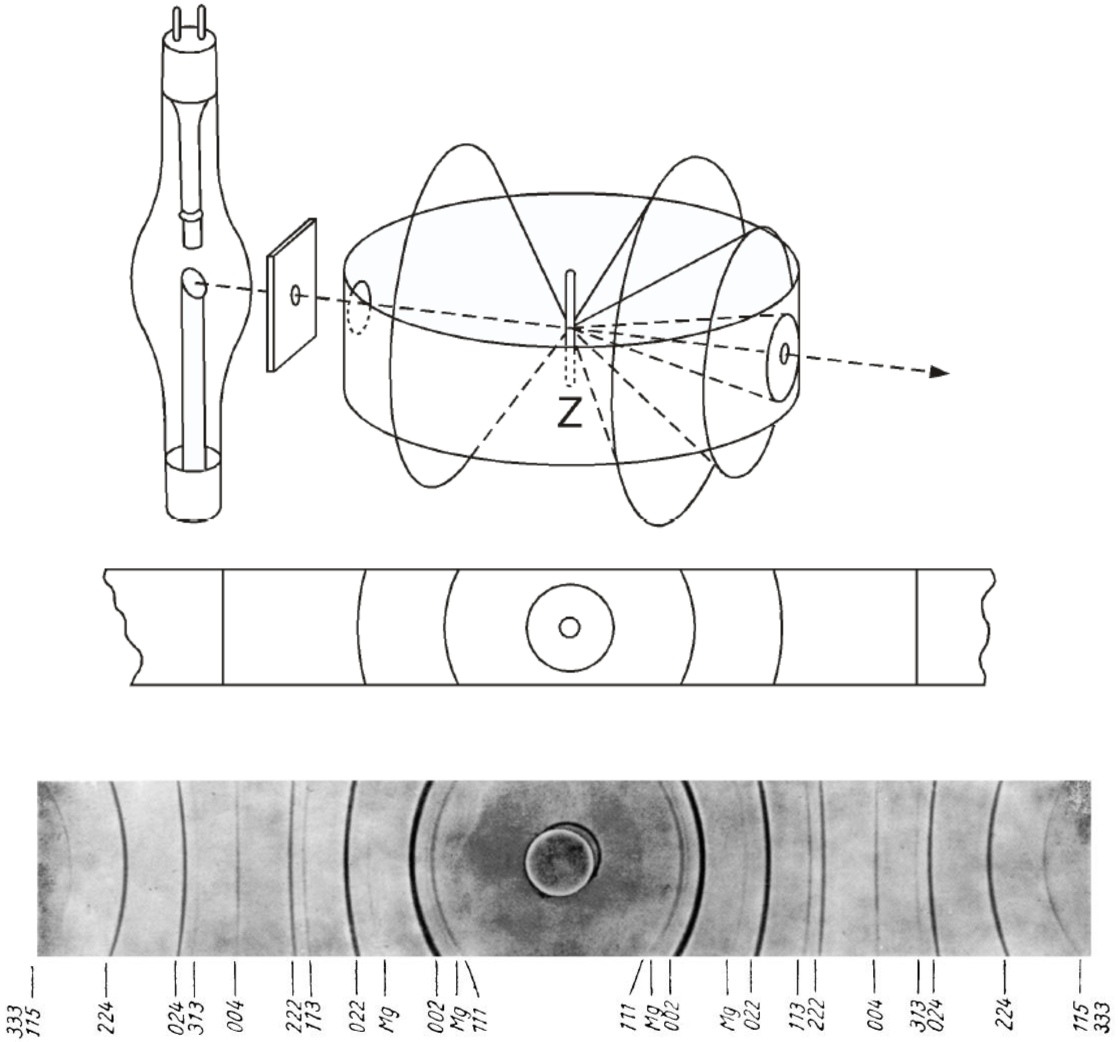


superposition of scattering of many small crystals (which can be oriented in any direction)



Powder diffraction

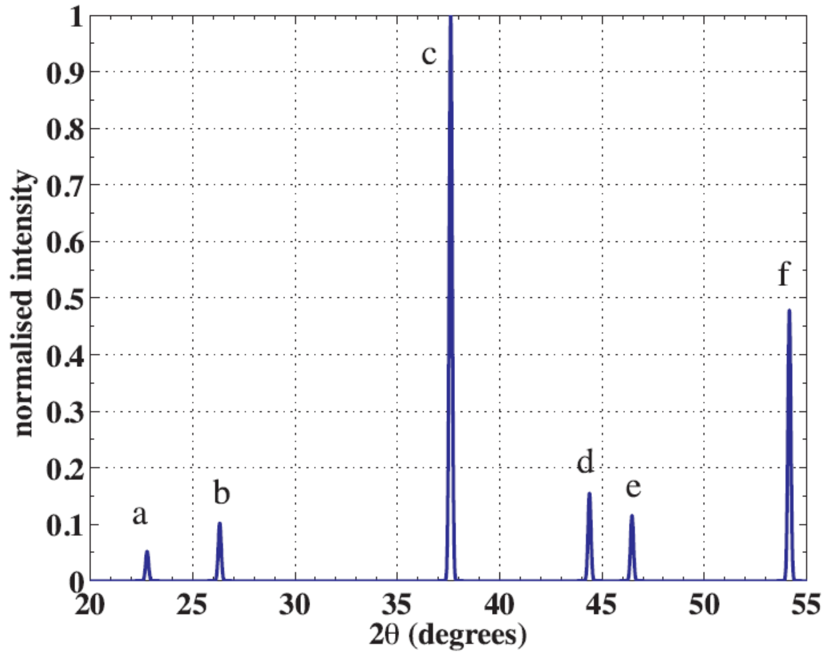




Debye-Scherrer-Diagramm von MgO aus Gerthsen, Kneser, Vogel: *Physik*, 13. Aufl. (Springer, Berlin, Heidelberg, New York 1978) Abb. 12.37

Powder diffraction analysis

(some tips for the exercices...)



From Experiment ⇓

$2d\sin\theta = \lambda \Rightarrow d = \frac{\lambda}{2\sin\theta}$

We Know

* Lattice Plane selection rules : table

{hkl} cubic bcc fcc N

1 0 0

1 1 0

⋮

* Assuming a cubic lattice :

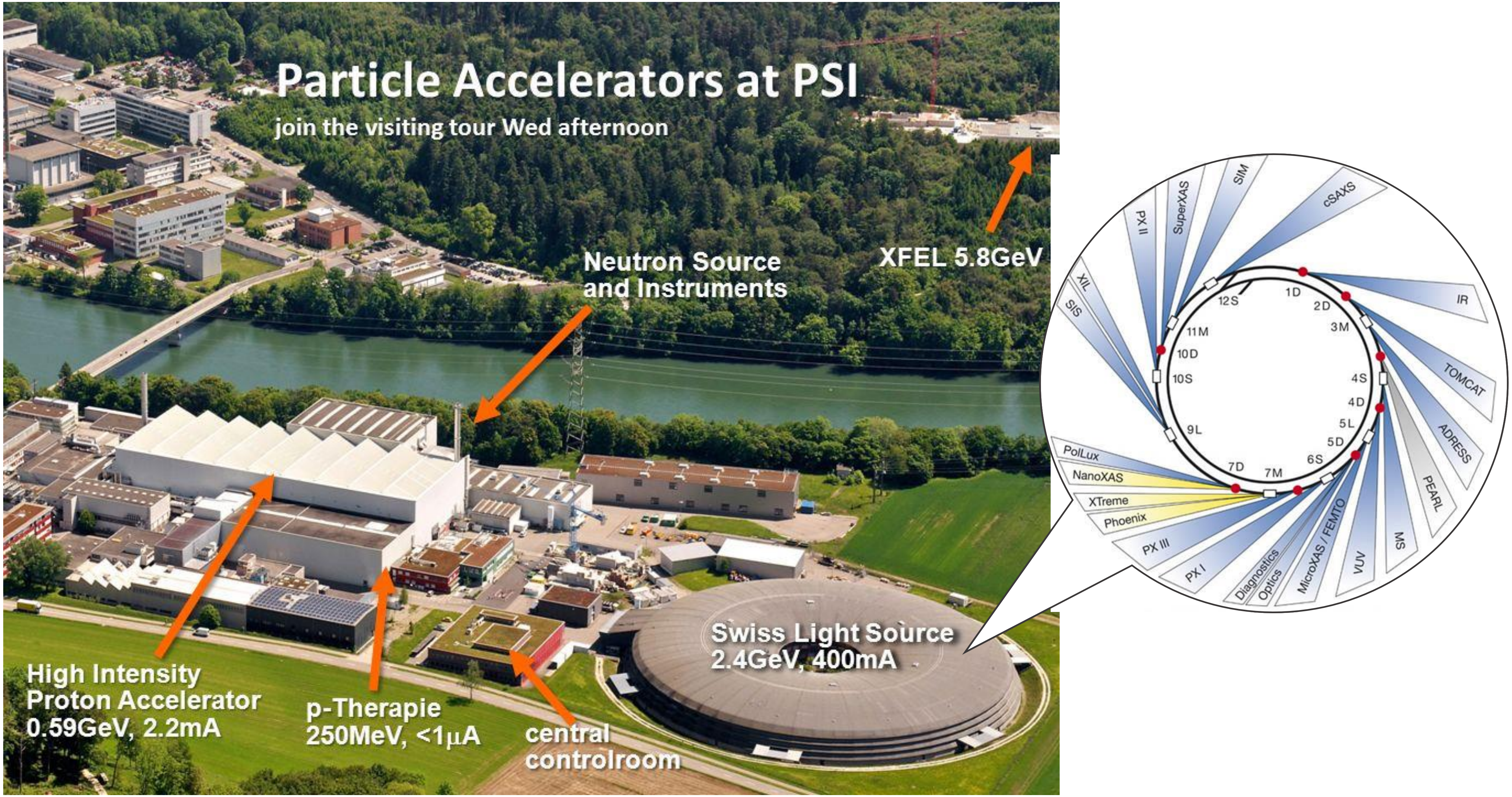
$d(hkl) = \frac{\lambda}{2\sin\theta} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

$\frac{a^2}{d^2} = h^2+k^2+l^2 \equiv N$

* Remember multiplicity :

$I\{hkl\} \propto M\{hkl\} |S_{hkl}|^2$

X-ray diffractometer


Particle Accelerators at PSI
join the visiting tour Wed afternoon
XFEL 5.8GeV
Neutron Source
and Instruments
High Intensity
Proton Accelerator
0.59GeV, 2.2mA
p-Therapie
250MeV, <1μA
central
controlroom
Swiss Light Source
2.4GeV, 400mA
PX II
SuperXAS
SIM
cSAXS
XIL
SIS
IR
TOMCAT
ADRESS
PEARL
MS
VUV
MicroXAS / FEMTO
Optics
Diagnostics
PX I
PX III
Phoenix
XTreme
NanoXAS
PolLux
12S
1D
2D
3M
4S
4D
5L
5D
6S
7M
7D
9L
10S
10D
11M

Learning outcomes - Scattering

- Understand diffraction of waves from crystals in both Laue and Bragg formulations

$$2d\ sin\theta = n\lambda \qquad \Delta\vec{k} = \vec{G}$$

- Brillouin zone and its special role in diffraction
- Structure factor, atomic form factor
- There are systematic absences in diffraction peaks depending on the crystal structure
- Analyze a powder diffraction pattern (see exercises!)