Diffraction and Imaging part II

Duncan Alexander
EPFL-IPHYS-LSME

Diffraction and imaging I program

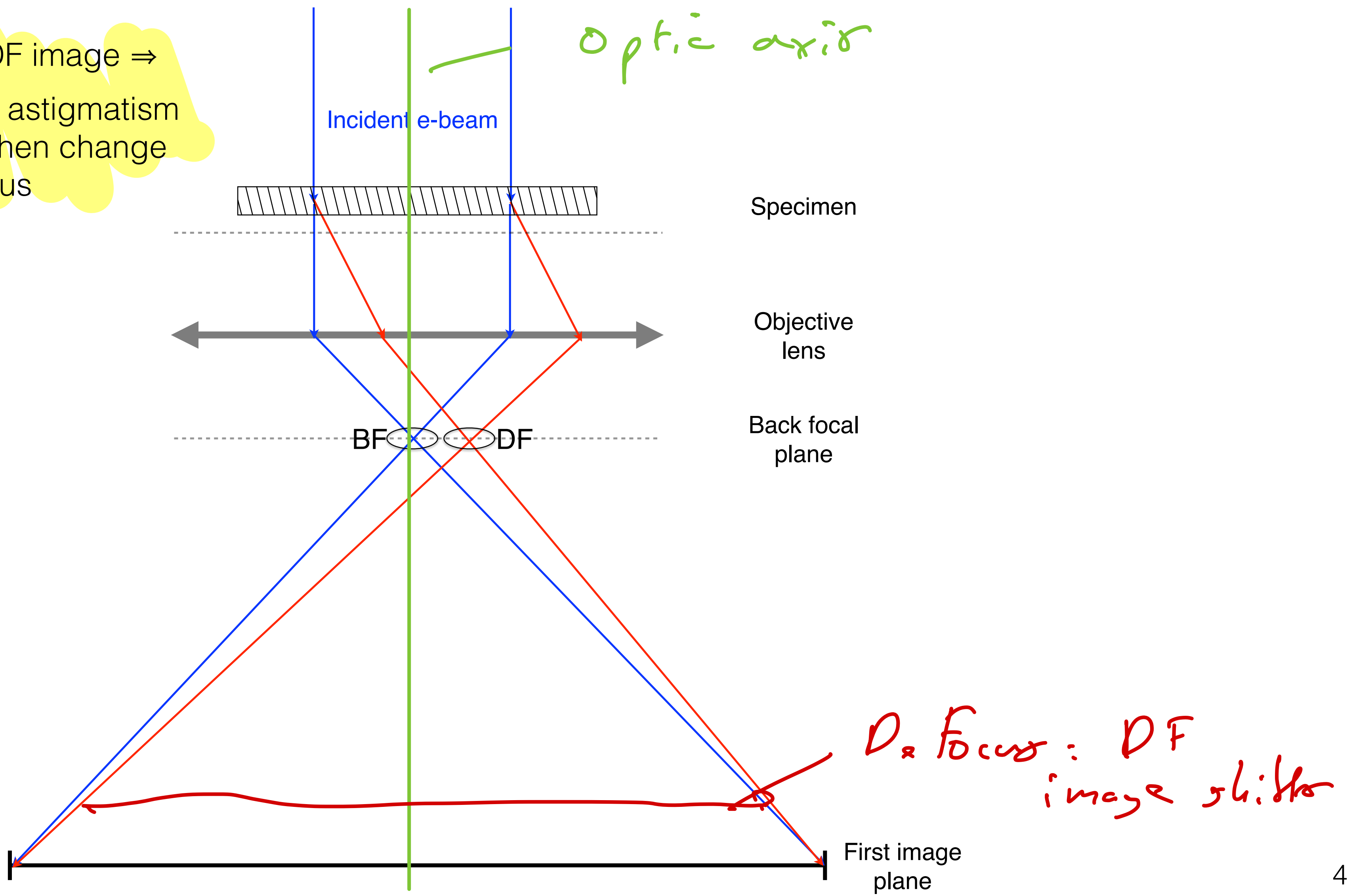
- Q and A from MOOC week 4 lectures and exercises
- Mini-lecture on:
  - Centred dark-field imaging in 2-beam condition
- Demo: 2-beam diffraction and imaging using centred dark-field

Centred aperture dark-field imaging

Displaced aperture dark-field

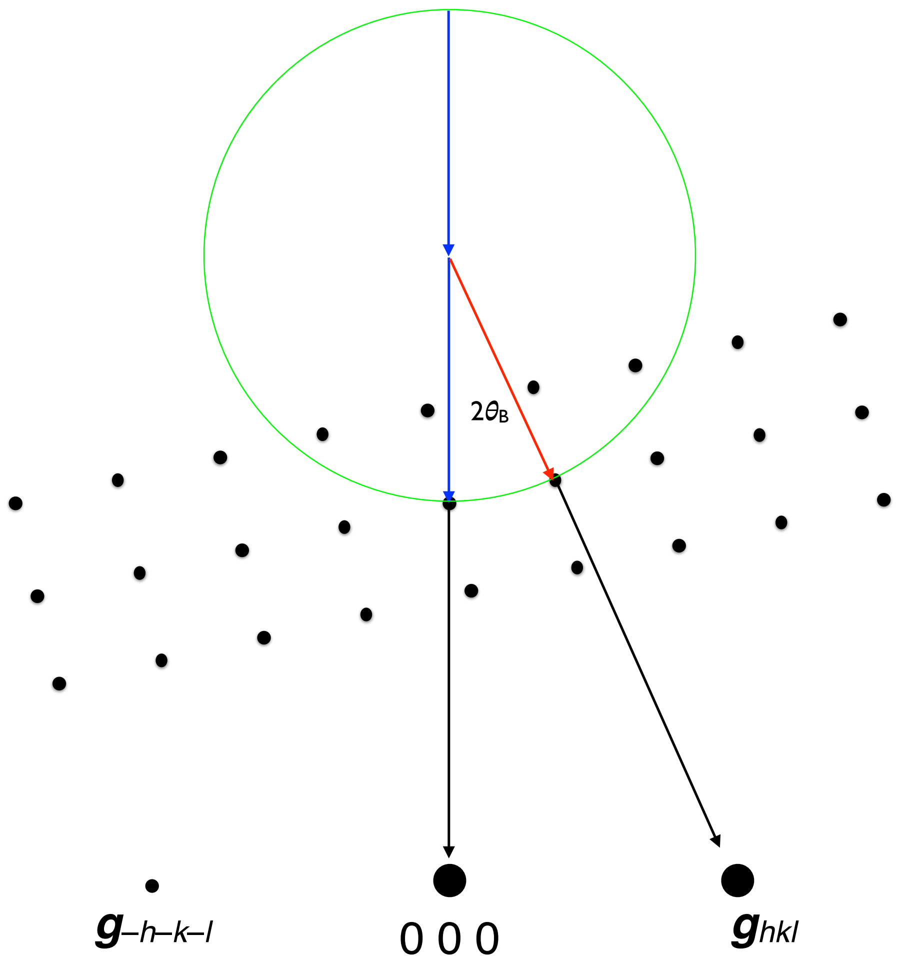
Off-axis rays for DF image ⇒

– aberrations and astigmatism
– image moves when change objective lens focus



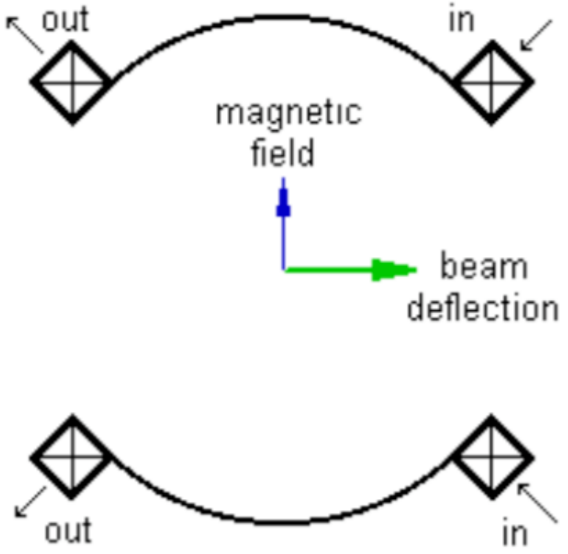
Displaced aperture dark-field

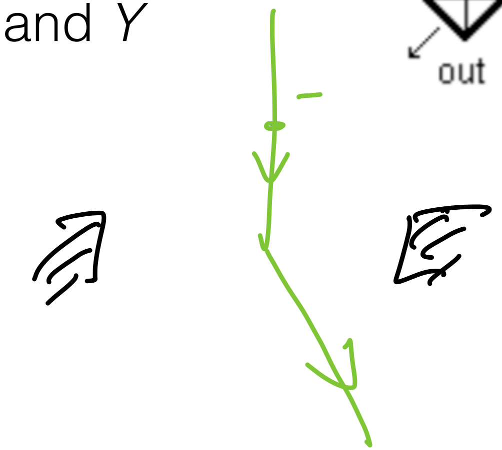
- Ewald sphere cuts reciprocal lattice node exactly
- Off-axis rays form DF image
  ⟹ aberrations and astigmatism
  ⟹ image moves when change objective lens focus



Beam deflection coils

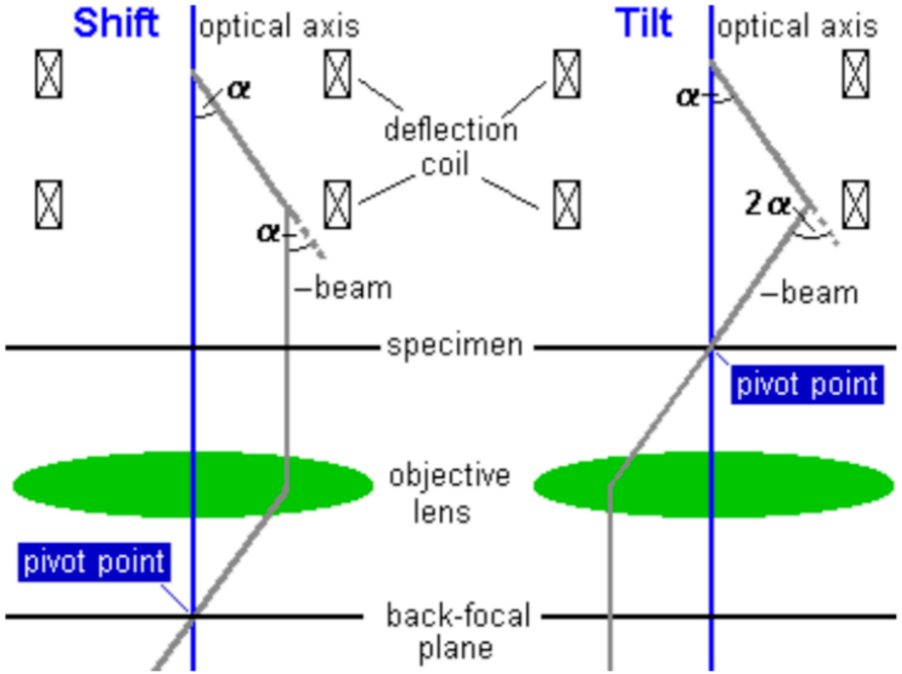
- Deflection coils: set of coils either side of e^- beam
- Apply positive magnetic field to one, negative to the other
  $\Longrightarrow$ Deflection of e^- beam towards positive field
- Arcs used to generate homogeneous magnetic field
- Two perpendicular sets allow deflection in *X* and *Y* directions





Beam deflection coils

- Above objective lens have set of double deflection coils
- Can be used to:
  - Shift incident beam on sample
  - Tilt incident beam on sample

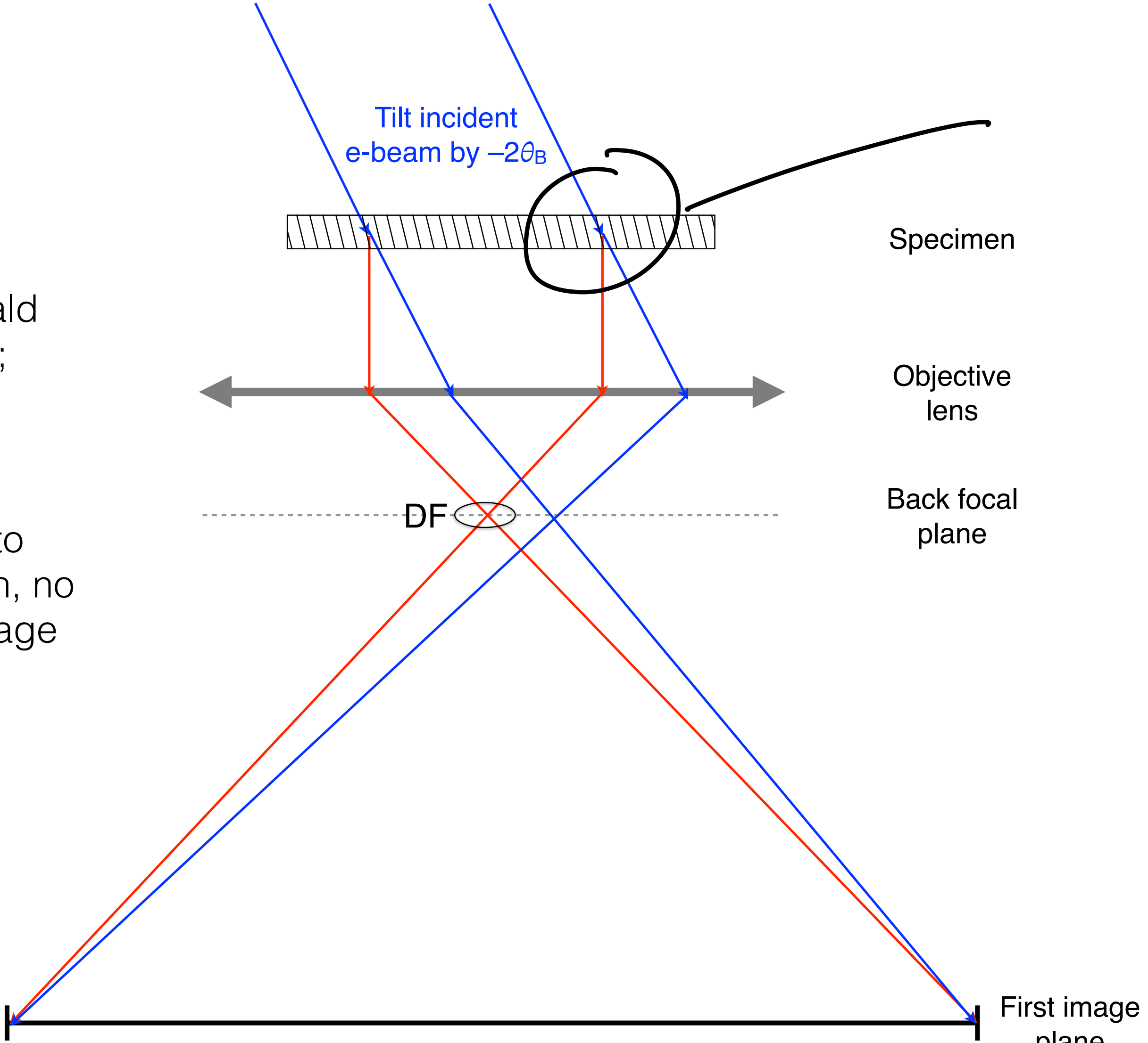


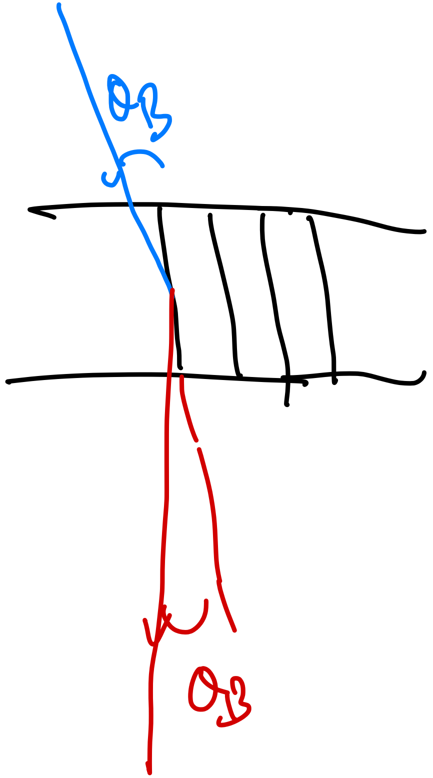
Centred aperture dark-field

Corresponds to tilting of Ewald sphere by $2\theta_B$, excite $\boldsymbol{g}_{-h\,-k\,-l}$;

0 0 0 takes place of $\boldsymbol{g}_{h\,k\,l}$ in SADP

Can now go from BF image to DF image by pressing button, no off-axis aberrations in DF image

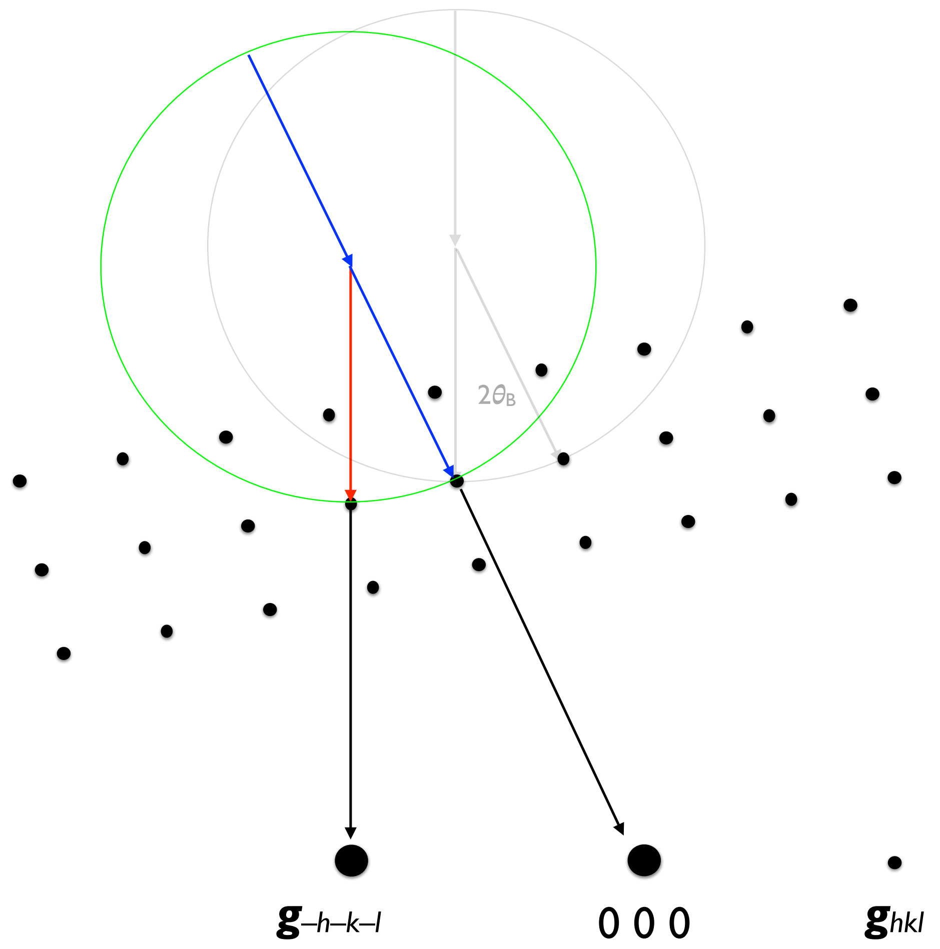




Centred aperture dark-field

- Corresponds to tilting of Ewald sphere by $2\theta_B$, excite $\boldsymbol{g}_{-h-k-l}$;
  0 0 0 takes place of $\boldsymbol{g}_{hkl}$ in SADP
- Can now go from BF image to DF image by pressing button, no off-axis aberrations in DF image

SADP: selected area diffraction pattern



Bragg formula: $n\lambda = 2d\sin\theta_B$

d_{hkl}

$$d_{2h\,2k\,2l} = \frac{d_{hkl}}{2}$$

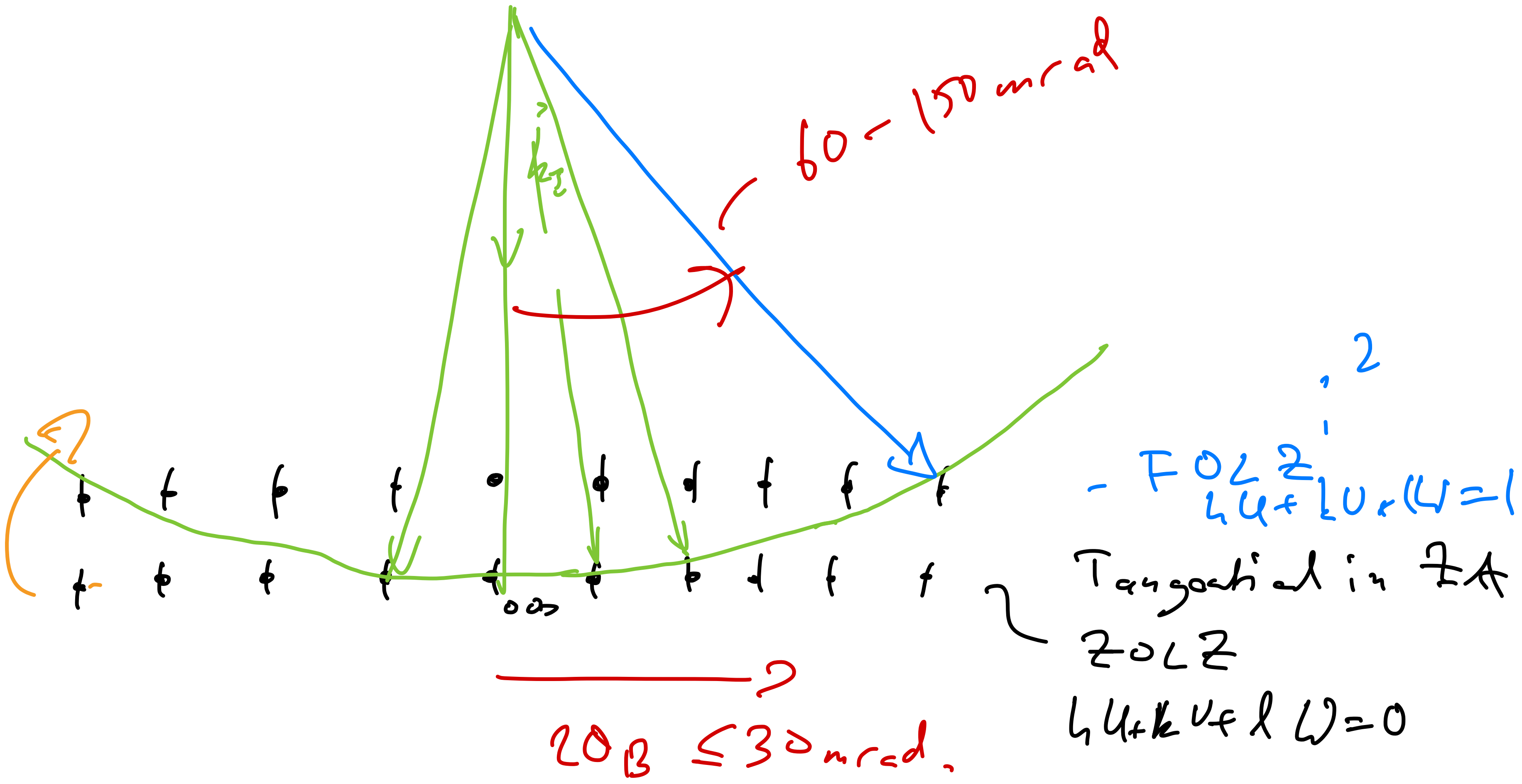
$$\lambda = 2d_{hkl}\sin\theta_B$$

$$2\lambda = 2d_{hkl}\sin\theta_B \Rightarrow \sin\theta_B = \frac{2\lambda}{2d_{hkl}}$$

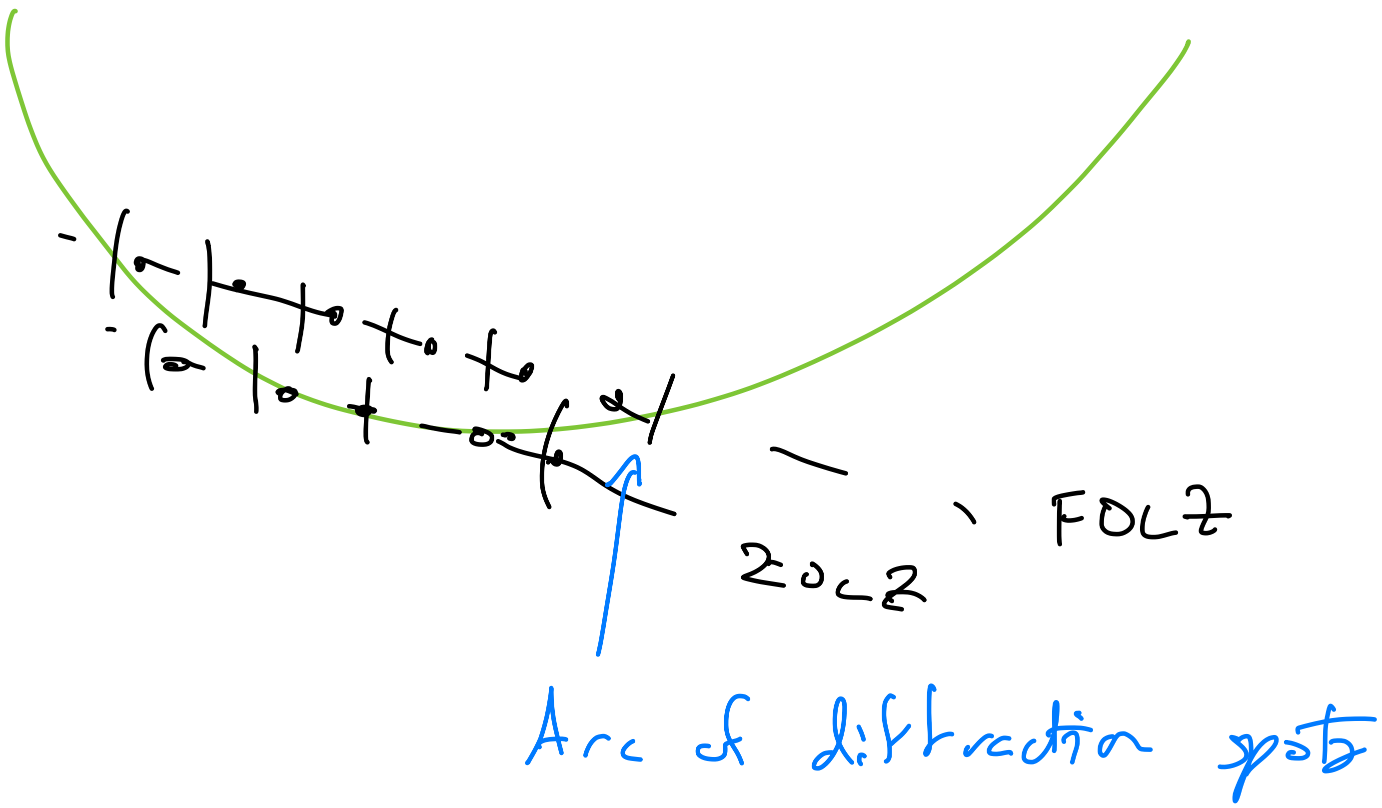
$$\lambda = 2d_{2h\,2k\,2l}\sin\theta_B$$

small angle approx: $2\theta_B \simeq \frac{\lambda}{d}$

Laue zones


60 - 150 mrad
k_I
- FOLZ, 2
$hu+kv+lw=1$
Tangential in ZA
ZOLZ
$hu+kv+lw=0$
$2\theta_B \leq 30$ mrad.

Tilt crystal



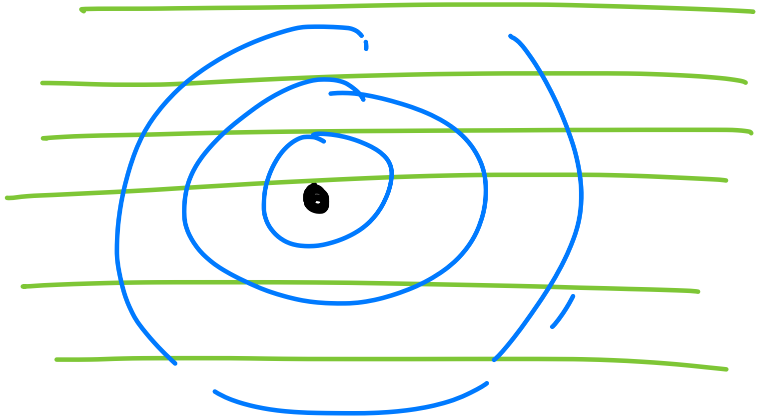
Structure factor for diffraction

$$F_g = \sum_i f_i \exp\left[2\pi i (h x_i + k y_i + l z_i)\right]$$

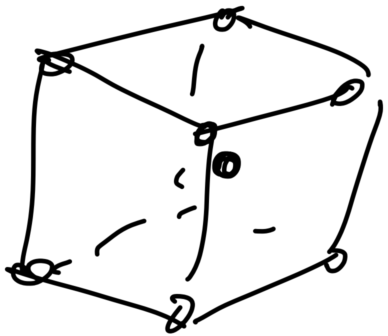
Amplitude of scattering from unit cell →

f_i : atomic scattering factor

Relates to scattering of spherical wave by atom



Unit cell



Add scattering

$$I_{hkl} \propto |F_{hkl}|^2 \qquad \text{(kinematical)}$$

$$F_{hkl} = \sum_i f_i \exp[2\pi i(hx_i + ky_i + lz_i)]$$

Suppose FCC Al: atoms x, y, z:

0, 0, 0
$\frac{1}{2}, \frac{1}{2}, 0$
$\frac{1}{2}, 0, \frac{1}{2}$
$0, \frac{1}{2}, \frac{1}{2}$

$$F_{hkl} = f_{Al}\left[\exp[2\pi i(0)] + \exp(\pi i(h+k)) + \exp(\pi i(h+l)) + \exp(\pi i(k+l))\right]$$

$(h\,k\,l) = (100) \rightarrow F_{100} = f_{Al}[1 - 1 - 1 + 1] = 0$

$(200) \rightarrow F_{200} = f_{Al}[1 + 1 + 1 + 1] = 4 f_{Al}$

EPFL

$\Rightarrow F_{hkl} = 4f$ for h,k,l all even or all odd

$'' = 0$ for h,k,l mixed odd and even

Si : FCC with 2 atom motif : 0, 0, 0
1/4, 1/4, 1/4

$\Rightarrow$ (200) also forbidden !