EPFL

Diffraction and Imaging part III

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EPFL-IPHYS-LSME

Diffraction and imaging III program

- Q and A from MOOC week 5 lectures and exercises
- Mini-lecture on:
  - Camera length
  - Structure factor
  - Zone axis SADP indexing
- JEMS tutorial

“Camera length” in TEM diffraction

Camera length in TEM diffraction

- Magnification in diffraction mode is called “camera length”
- Historically refers to virtual distance between diffracting object and screen when assuming Fraunhofer far-field diffraction
- Larger camera length ⟹ magnified diffraction pattern

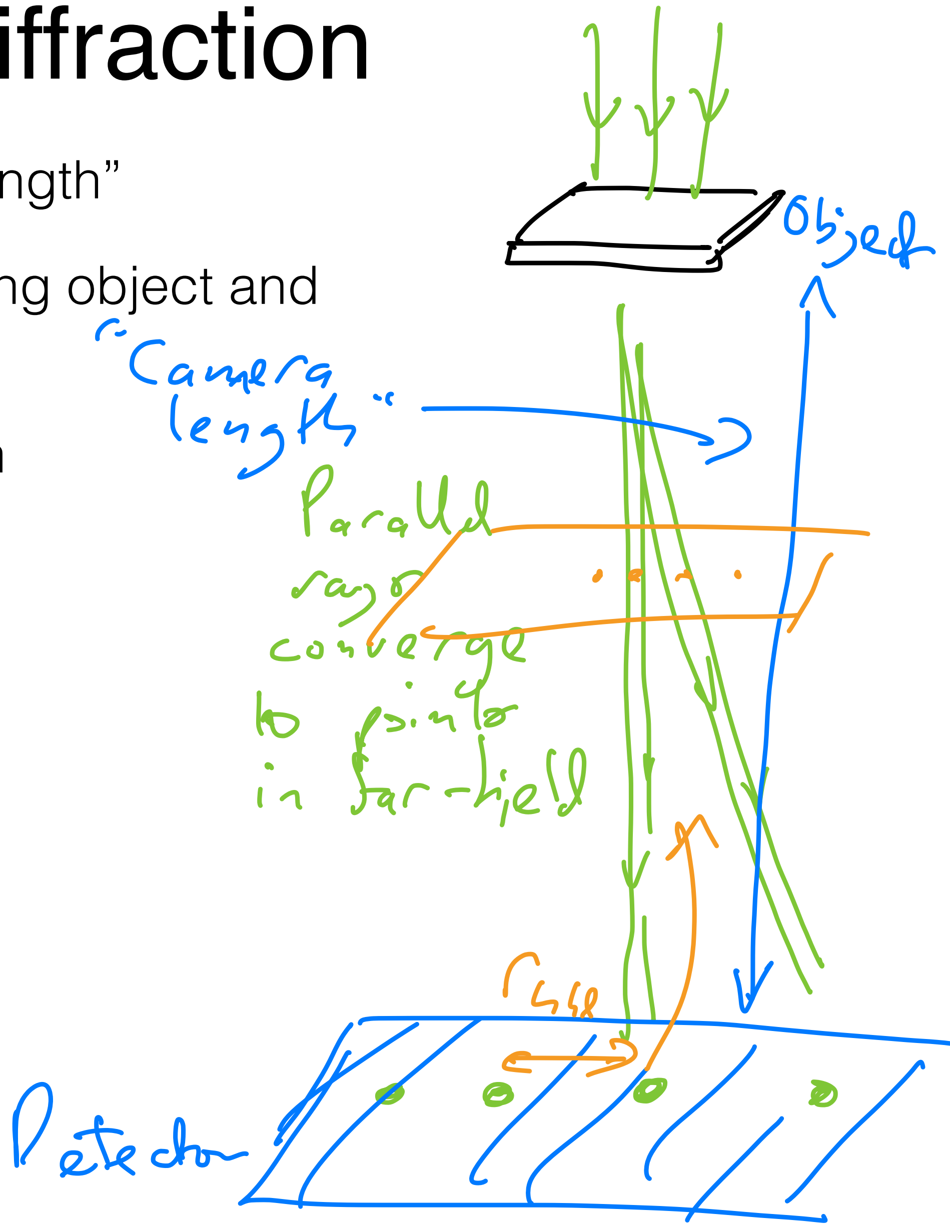
$$\lambda L = d_{hkl}\, r_{hkl}$$

e^- wavelength

Camera length

plane spacing

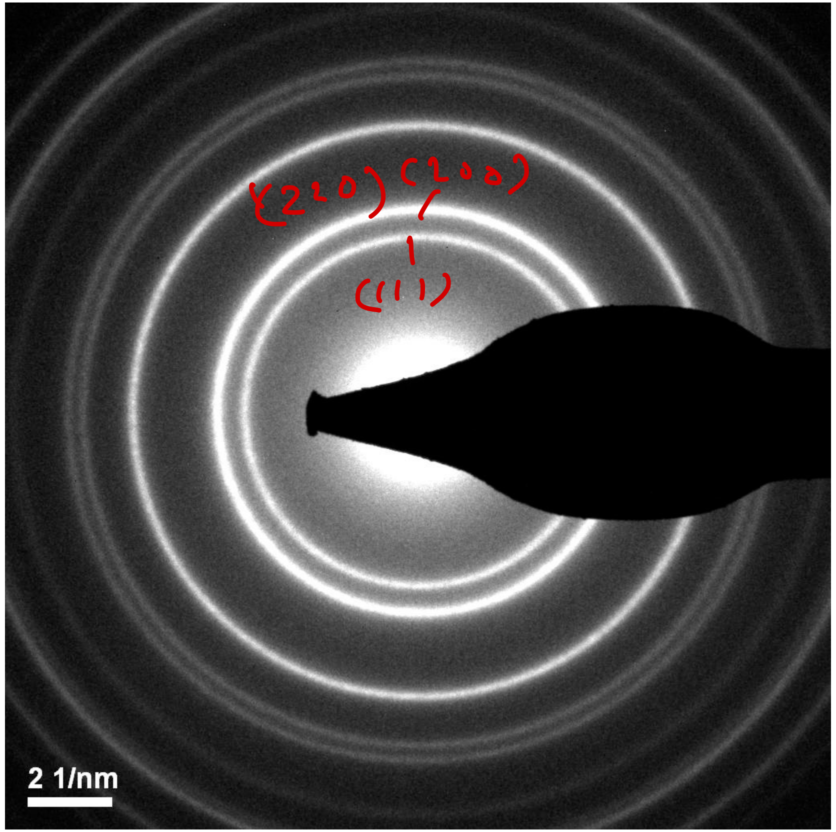
Spot spacing that we measure

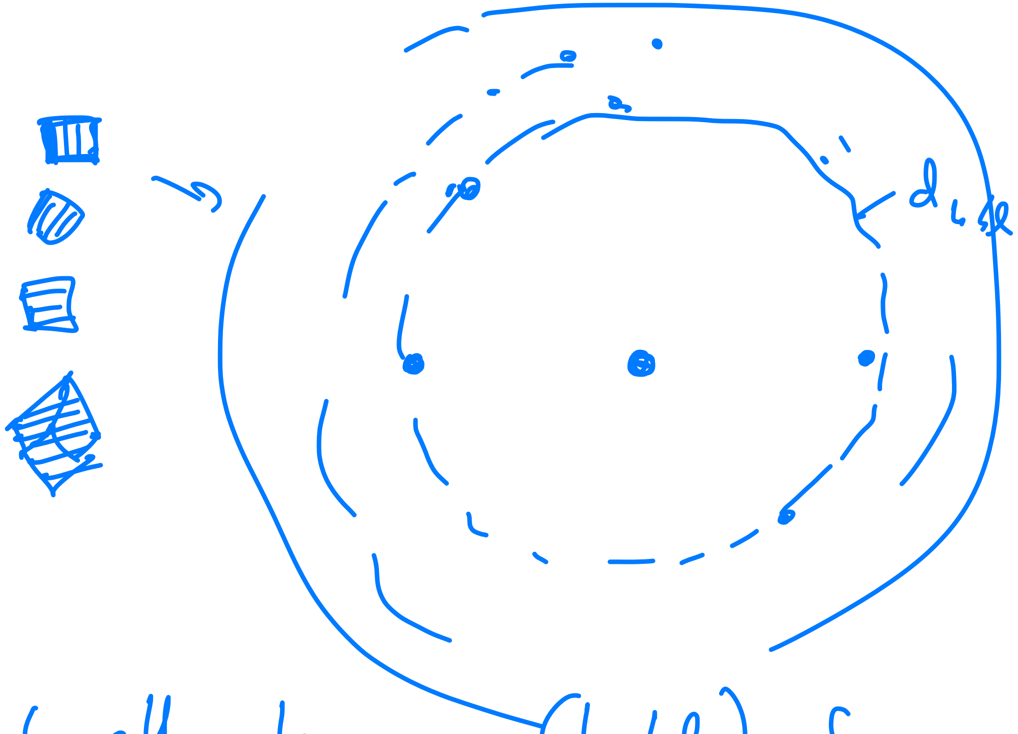


Calibrating camera length

FCC (?)

- Digital camera: pixels calibrated in reciprocal plane spacing (nm^{-1})
- To calibrate: record SADP from a known standard – e.g. NiO_x polycrystalline sample





Sample all planes (hkl) of our xtal → each makes a ring

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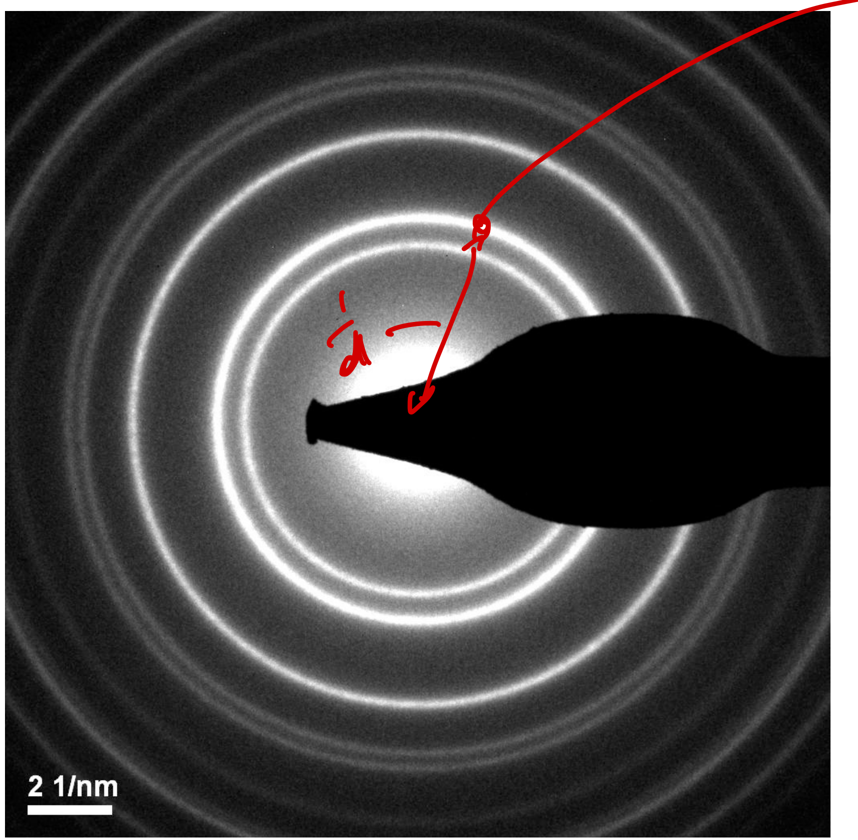
Calibrating camera length

- Digital camera: pixels calibrated in reciprocal plane spacing (nm^{-1})
- To calibrate: record SADP from a known standard – e.g. NiO_x polycrystalline sample

Diameter in terms of θ_B ?
↳ $4\theta_B$

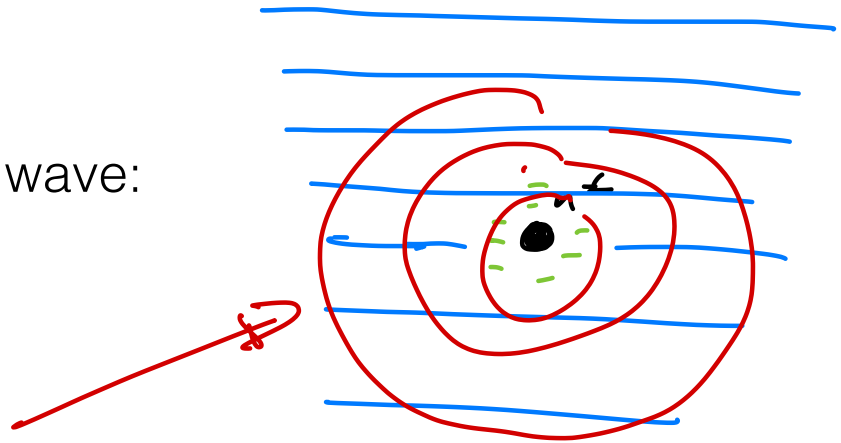


$$(D/2)C = d_{hkl}^{-1}$$

D: diameter of ring (pixels)
C: calibration (nm^{-1} per pixel)
d_{hkl}^{-1}: reciprocal plane spacing (nm^{-1})

The structure factor

Structure factor



- Position dependent wave function for incident plane wave:

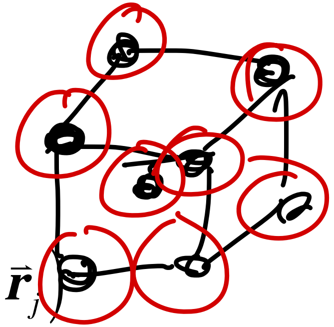
$$\psi(\vec{\boldsymbol{r}}) = \psi_0 \exp\left(-2\pi i \vec{\boldsymbol{k}}.\vec{\boldsymbol{r}}\right)$$

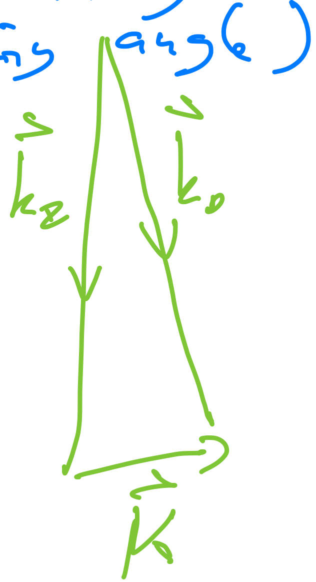
- Scattered by individual atom gives spherical scattered wave:

$$\psi_{\text{atom}}(\vec{\boldsymbol{r}}) = \frac{\exp\{-2\pi i k r\}}{r} f\left(\vec{\boldsymbol{K}}\right)$$

atomic scattering factor
= Amplitude of scattering
(in function of scattering angle)

- Consider assembly of atoms into a unit cell. Total scattered wave is:





$\vec{r}_j$: atom position in unit cell

$$\psi_s(\vec{\boldsymbol{r}}) = \frac{\exp\{-2\pi i k r\}}{r} \underbrace{\sum_j f_j \exp\left(2\pi i \vec{\boldsymbol{K}} \cdot \vec{\boldsymbol{r}}_j\right)}$$

- Define structure factor for unit cell: $F\left(\vec{\boldsymbol{K}}\right) = \sum_j f_j \exp\left(2\pi i \vec{\boldsymbol{K}} \cdot \vec{\boldsymbol{r}}_j\right)$

Structure factor

- Scattered wave given by: $\psi_s(\vec{r}) = \frac{\exp\{-2\pi i k r\}}{r} F(\vec{K})$
- At Bragg condition: $\vec{K} = \vec{g} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$
- Position of each atom in unit cell: $\vec{r}_j = x_j\boldsymbol{a} + y_j\boldsymbol{b} + z_j\boldsymbol{c}$
- Structure factor for reflection $\vec{g}$: $F_g = \sum_j f_j \exp\left[2\pi i\left(hx_j + ky_j + lz_j\right)\right]$
- Add up scattering from all unit cells across a sample of thickness t find intensity of scattered beam:

$$I_g = \left[\frac{\sin(\pi t s)}{\xi_g s}\right]^2 \qquad \text{where:} \qquad \xi_g = \frac{\pi k V_0 \cos\theta_B}{F_g}$$

$\vec{K}\cdot\vec{r}_j$

$= hx_j + ky_j + lz_j$

$I_g \propto |F_g|^2$

Kinematical

Systematic absences

- Depending on symmetry of a structure, certain planes can have structure factor $F_g = 0$
- If so, intensity of diffracted beam $I_g = 0 \implies$ “systematic absence”/“forbidden reflection”
- Example: face-centred cubic lattice (FCC)

Lattice point positions: $x, y, z = \quad 0,0,0; \quad \tfrac{1}{2},\tfrac{1}{2},0; \quad \tfrac{1}{2},0,\tfrac{1}{2}; \quad 0,\tfrac{1}{2},\tfrac{1}{2}$

$$F_g = \sum_j f_j \exp\left[2\pi i\left(hx_j + ky_j + lz_j\right)\right]$$

1 atom per lattice point: $F_g = f\left[1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)}\right]$

h, k, l mixed even, odd : $F_g = 0$ ← Systematic absences

— " — all even / all odd : $F_g = 4f$

Systematic absences

- FCC: planes with indices h,k,l mixed odd and even are *absent*

- How about body centred cubic (BCC), with lattice points: $x,y,z = \quad 0,0,0; \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

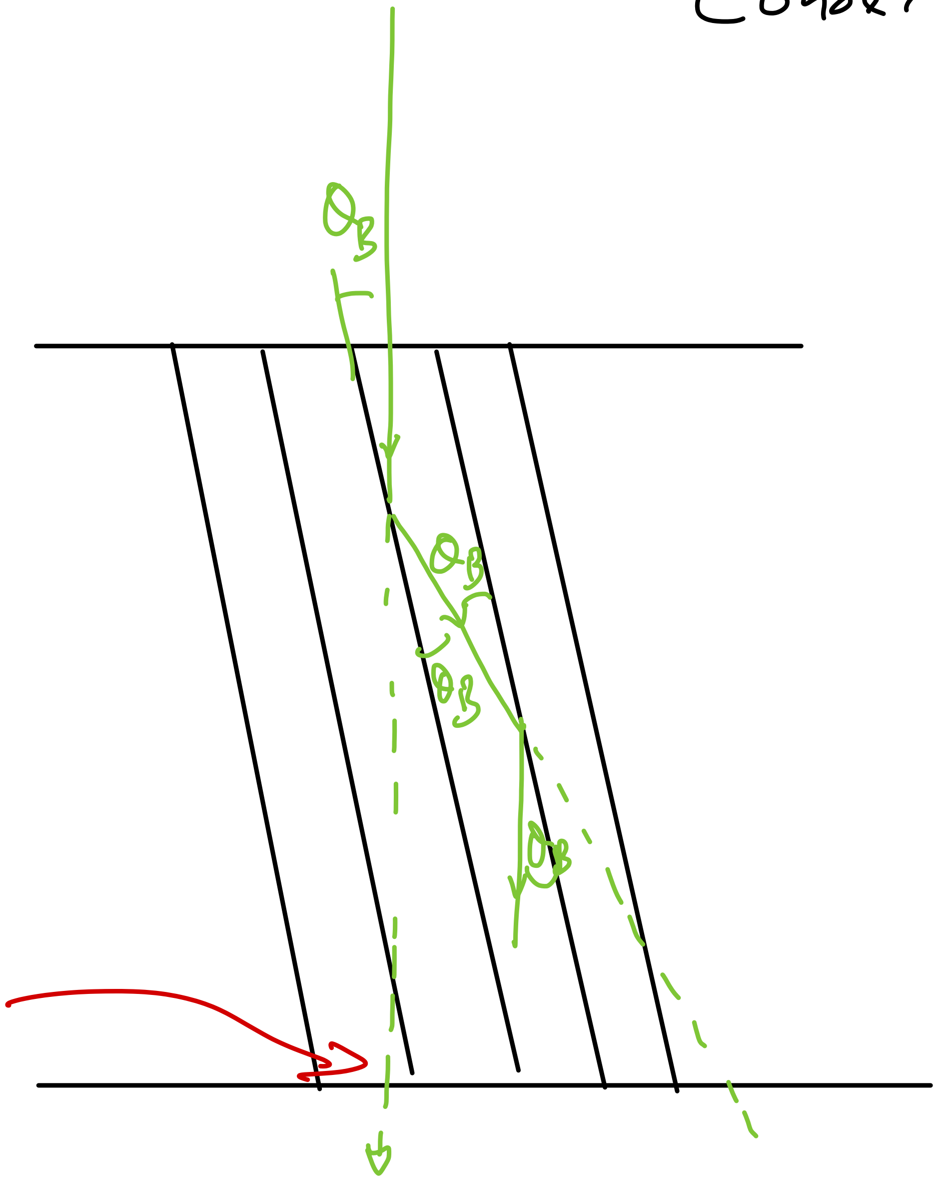
$$F_g = f\left[1 + e^{\pi i(h+k+l)}\right]$$

$h+k+l = \text{even}: \quad F_g = 2f$

$h+k+l = \text{odd}: \quad F_g = 0 \leftarrow$ Systematic absence

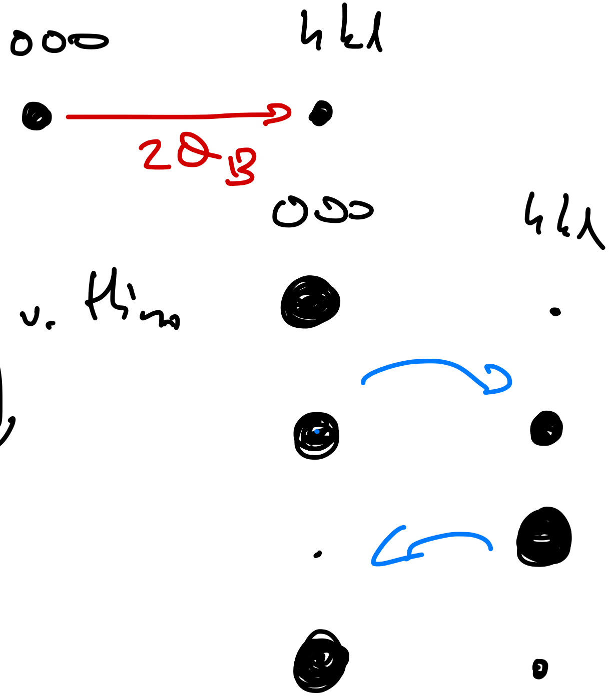
Conservation of intensity

Sample in 2-beam condition



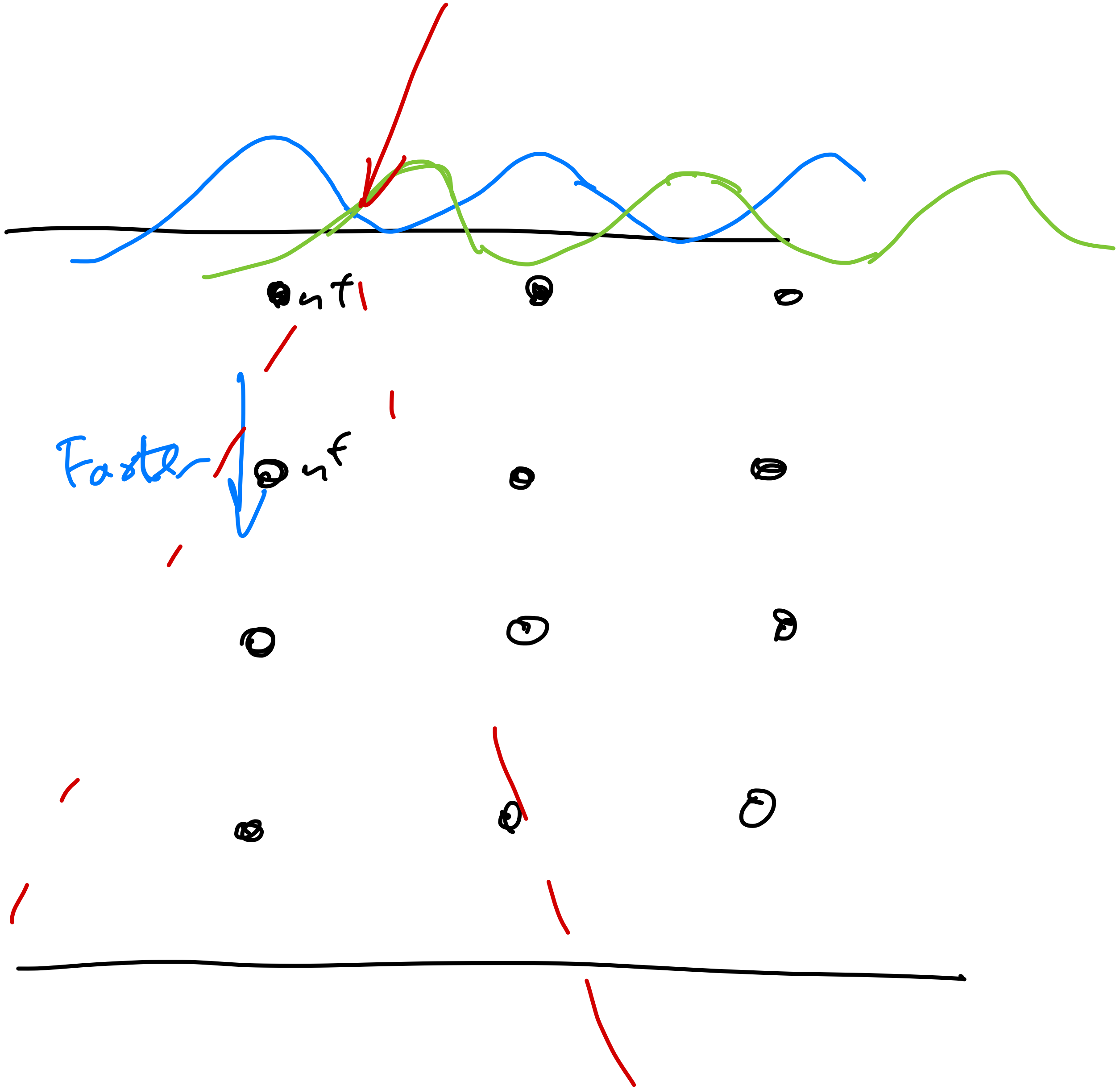
"Direct beam"

Back focal plane



sample v. thin

thicker


Faster

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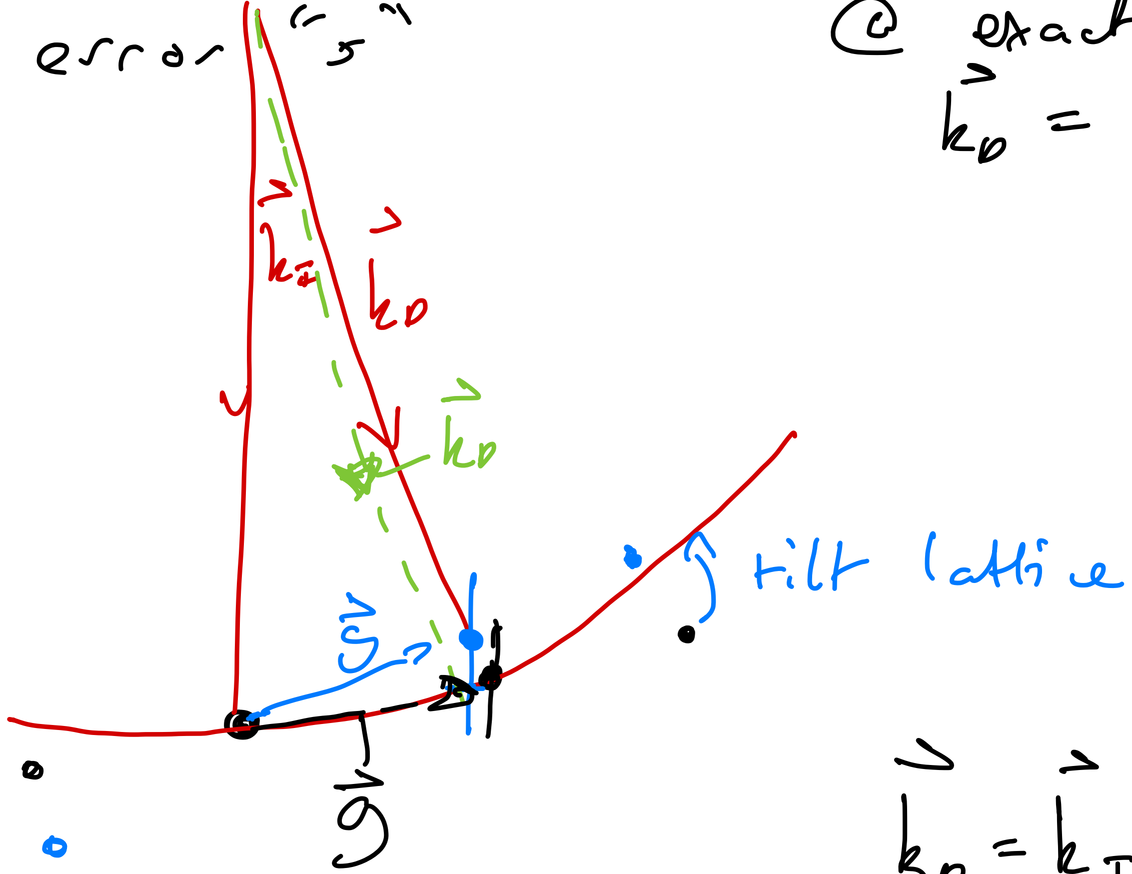
Excitation error "s"



@ exact Bragg

$\vec{k}_D = \vec{k}_I + \vec{g}$

$\vec{k}_D = \vec{k}_I + \vec{g} + \vec{s}$

Deviation from Bragg scattering

s = magnitude of $\vec{s}$

If $\vec{g}$ is inside Ewald sphere: s +ve