Advanced Topics in Condensed Matter

Lecture 3: Reciprocal lattice

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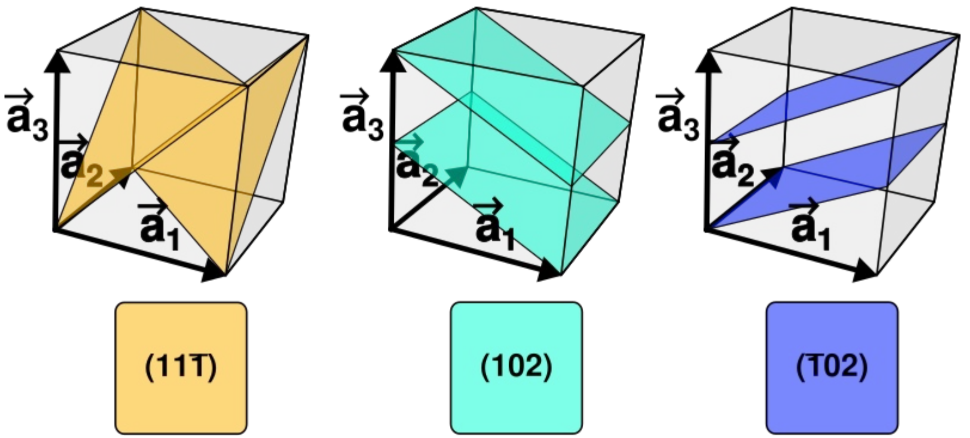
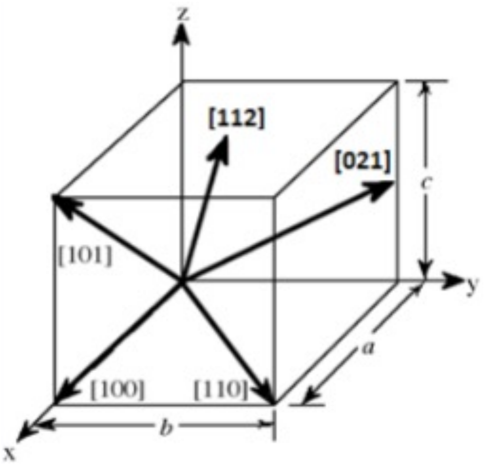
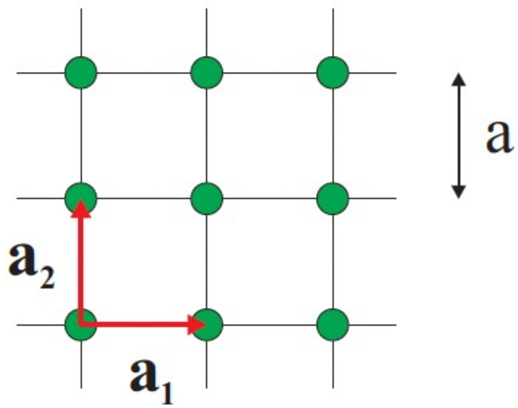
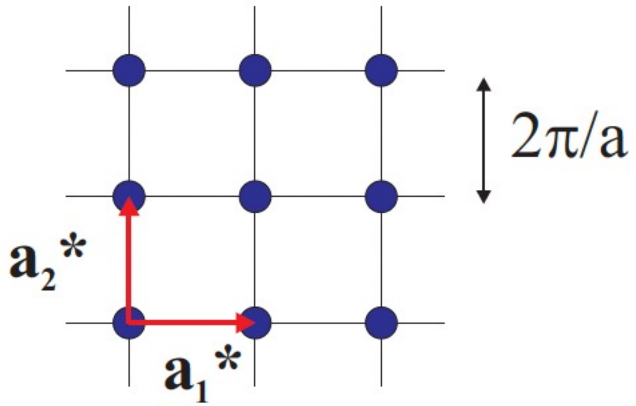
Recap

- Crystal lattice and unit cell
- Crystallographic directions $[uwv]$
- Crystallographic planes (hkl)
- Fourier transform of a discrete lattice







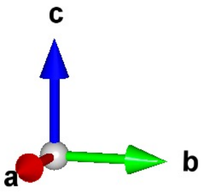


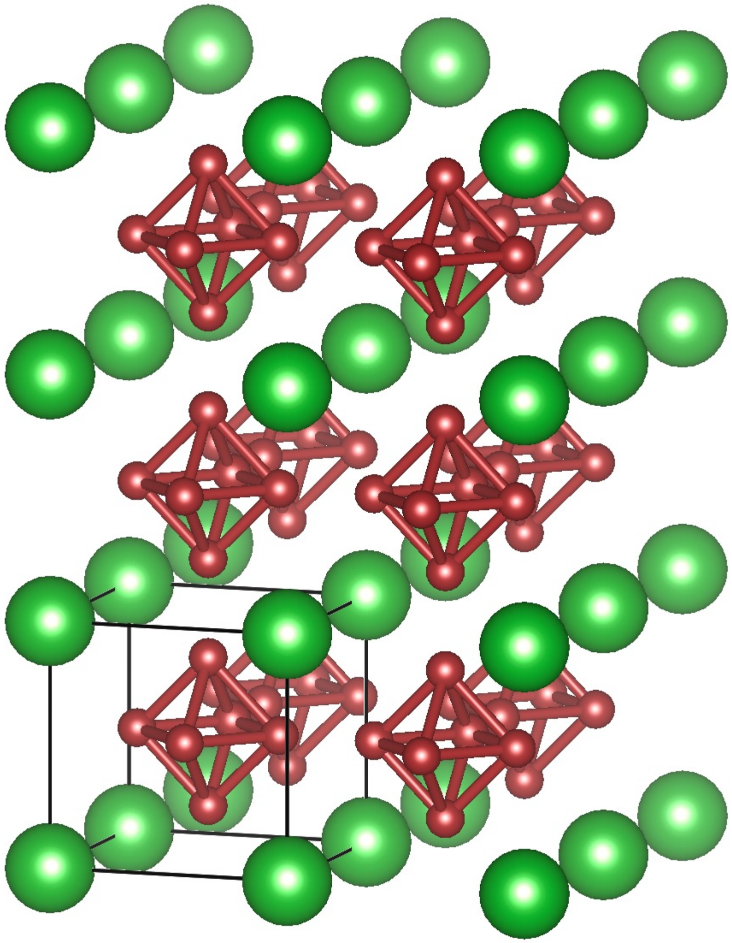
Scattering from a crystal

Position of any atom inside a crystal:

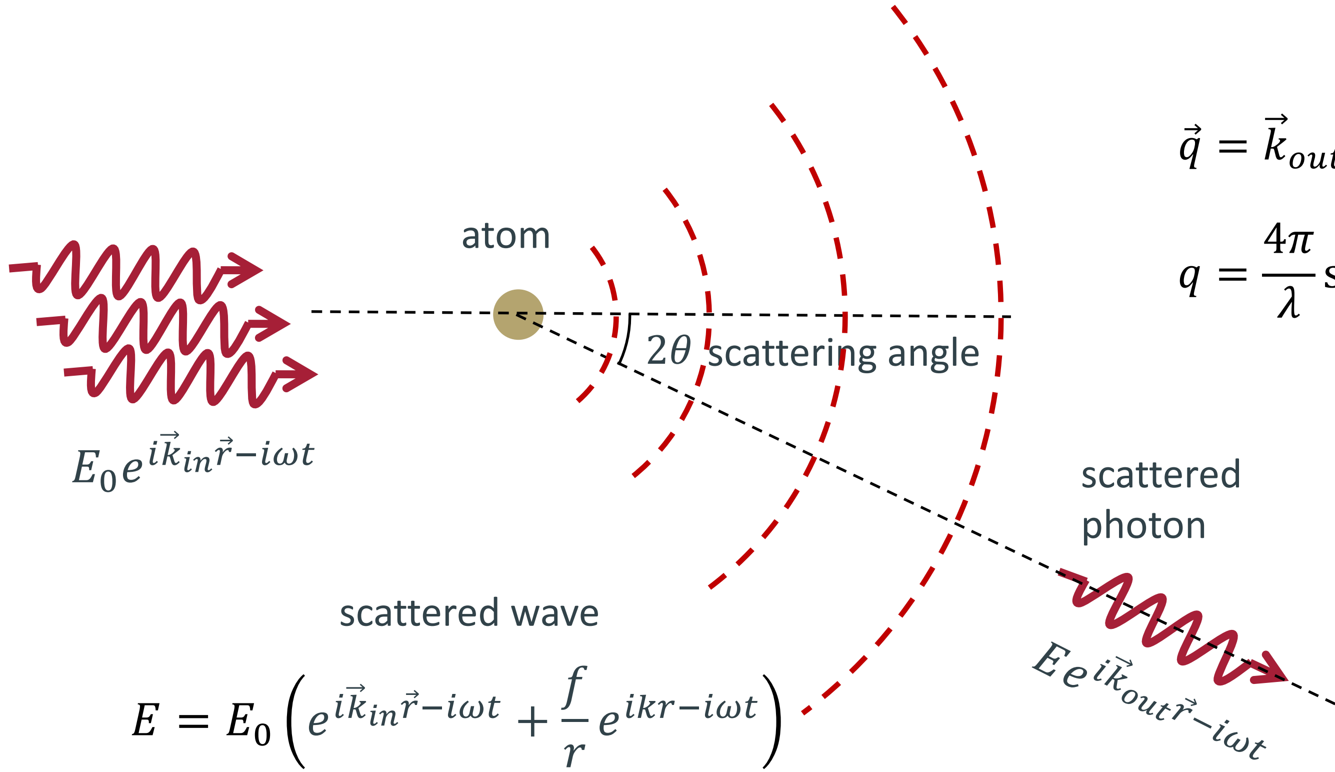
$$\vec{r} = \underbrace{n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3}_{\vec{R}_n} + \underbrace{x\vec{a}_1 + y\vec{a}_2 + z\vec{a}_3}_{\vec{r}_j}$$

Crystal lattice — basis





Scattering by an atom



$$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$$

$$q = \frac{4\pi}{\lambda}\sin\theta$$

$$E = E_0\left(e^{i\vec{k}_{in}\vec{r}-i\omega t} + \frac{f}{r}e^{ikr-i\omega t}\right)$$

X-rays

$$f = r_e \int \rho_{el}(\vec{r})e^{-i\vec{q}\vec{r}}d\vec{r}$$

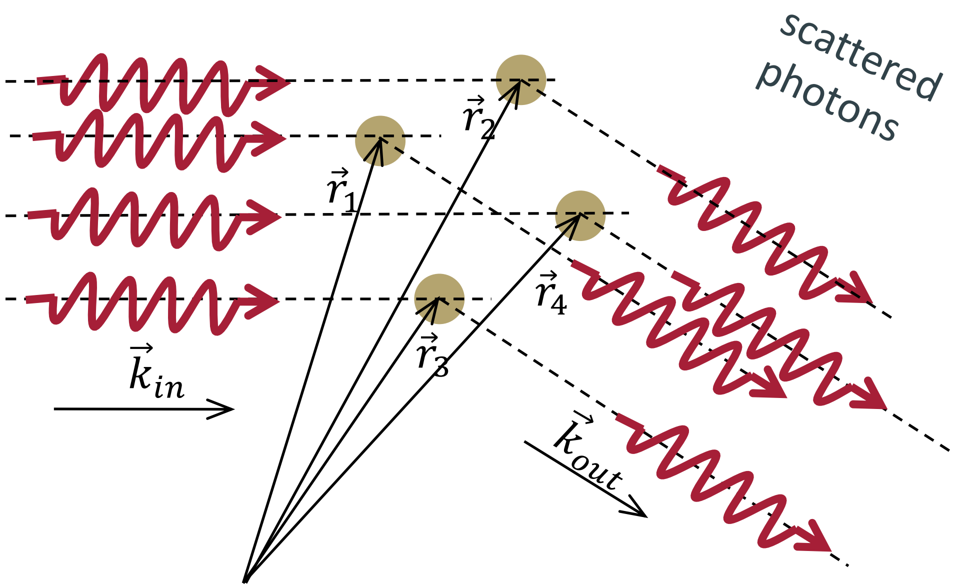
neutrons

$$f = -b = const$$

electrons

$$f = \frac{2}{a_0}\cdot\frac{Z - f_{X-ray}(\vec{q})}{q^2}$$

Scattering from a crystal



$$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$$

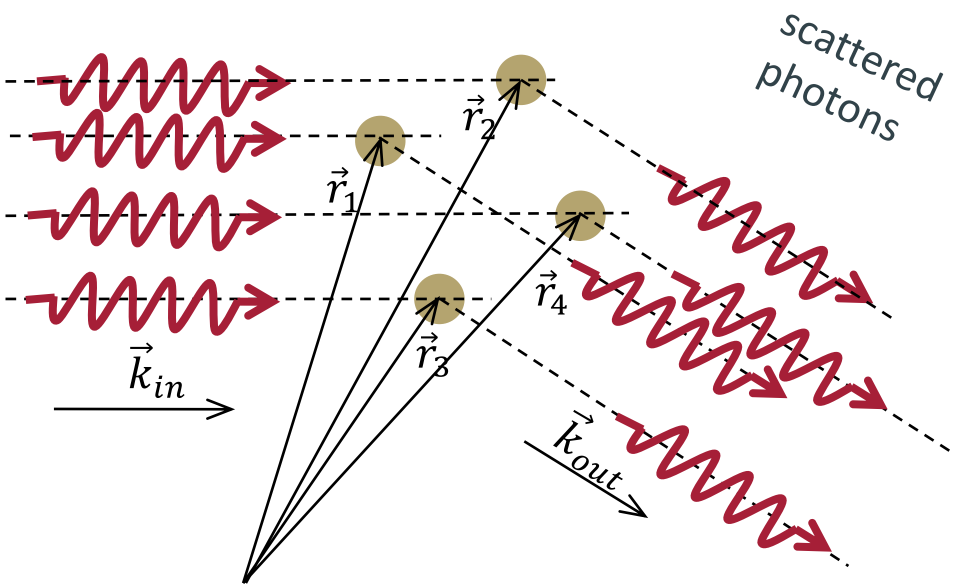
Single scattering approximation:

$$E = E_0 \sum_i \frac{f_i}{|\vec{r} - \vec{r}_i|} e^{ik|\vec{r}-\vec{r}_i|-i\omega t} \cdot e^{i\vec{k}_{in}\vec{r}_i}$$

Far-field approximation:

$$k|\vec{r} - \vec{r}_i| \approx kr - k\frac{\vec{r}}{r}\vec{r}_i = kr - \vec{k}_{out}\vec{r}_i$$

Scattering from a crystal



$$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$$

Single scattering approximation:

$$E = E_0 \sum_i \frac{f_i}{|\vec{r} - \vec{r}_i|} e^{ik|\vec{r} - \vec{r}_i| - i\omega t} \cdot e^{i\vec{k}_{in}\vec{r}_i}$$

$$E \approx E_0 \frac{e^{ikr - i\omega t}}{r} \sum_i f_i \cdot e^{-i(\vec{k}_{out} - \vec{k}_{in})\vec{r}_i}$$

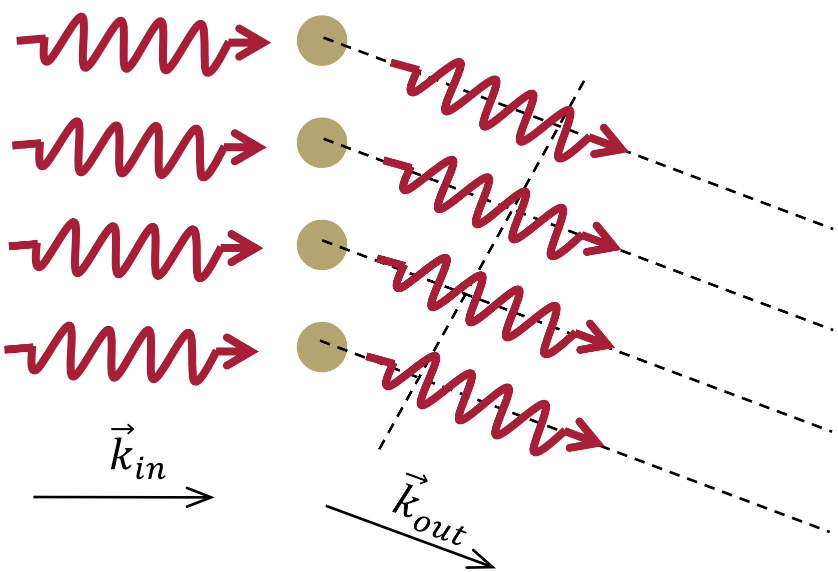
$$E \propto \sum_i f_i \cdot e^{-i\vec{q}\vec{r}_i}$$

Far-field approximation:

$$k|\vec{r} - \vec{r}_i| \approx kr - k\frac{\vec{r}}{r}\vec{r}_i = kr - \vec{k}_{out}\vec{r}_i$$

Scattering from a 1D periodic array of atoms

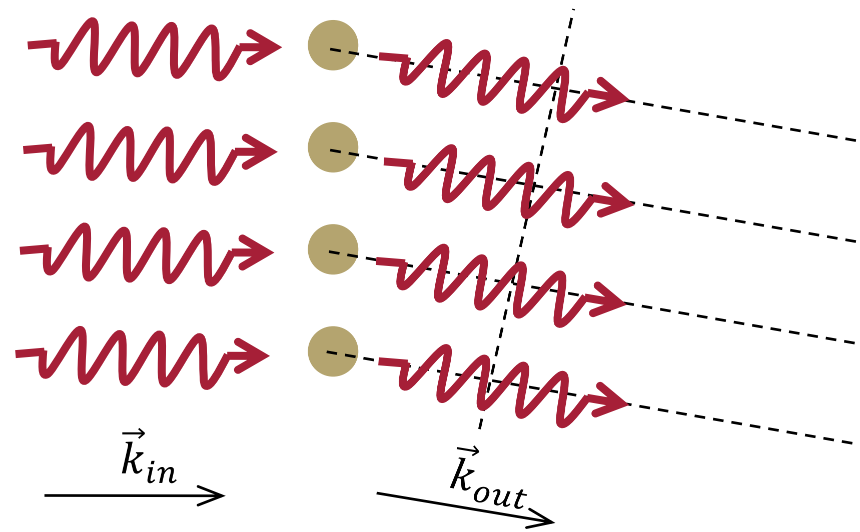
Scattering in phase:



$$E \propto f(q) \sum_{n=1}^{N} e^{-i\vec{q}\vec{r}_n} = f(q) \sum_{n=1}^{N} 1 \propto N \cdot f(q)$$

If for all atoms, $\vec{q}\vec{r}_n = 2\pi \cdot m$

Scattering out of phase:

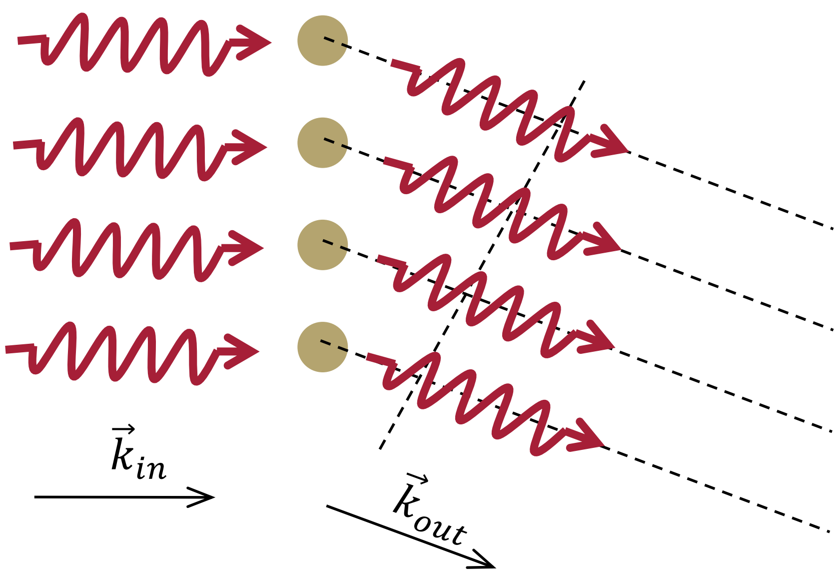


$$E \propto f(q) \sum_{n=1}^{N} e^{-i\vec{q}\vec{r}_n} = f(q) \sum_{n=1}^{N} (\pm 1) = 0$$

If for all atoms, $\vec{q}\vec{r}_n = \pi \cdot m$

Scattering from a 1D perioic array of atoms

Scattering in phase:



$$E \propto f(q) \sum_{n=1}^{N} e^{-i\vec{q}\vec{r}_n} = f(q) \sum_{n=1}^{N} 1 \propto N \cdot f(q)$$

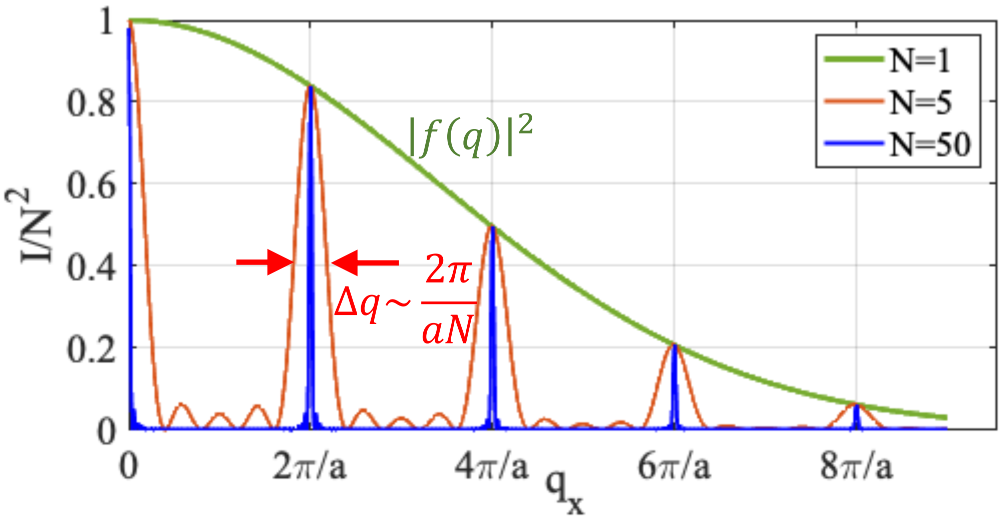
If for all atoms, $\vec{q}\vec{r}_n = 2\pi \cdot m$

For a periodic array of atoms: $x_n = n \cdot a$

$$E \propto f(q) \sum_{n=1}^{N} e^{-iq_x x_n} = f(q) \sum_{n=1}^{N} e^{-iq_x a \cdot n}$$

$$= f(q) e^{-iq_x a} \frac{1 - e^{-iq_x a \cdot N}}{1 - e^{-iq_x a}}$$

$$I \propto |E|^2 \propto |f(q)|^2 \cdot \left| \frac{\sin\left(\frac{q_x a}{2} \cdot N\right)}{\sin\left(\frac{q_x a}{2}\right)} \right|^2$$



Scattering by a 3D crystal

Position of any atom inside a crystal:

$$\vec{r} = \underbrace{n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3}_{\vec{R}_n} + \underbrace{x\vec{a}_1 + y\vec{a}_2 + z\vec{a}_3}_{\vec{r}_j}$$

Crystal lattice — basis

General equation for the scattered amplitude:

$$E \propto \sum_i f_i\,(q) \cdot e^{-i\vec{q}\vec{r}_i}$$

$$E \propto \underbrace{\sum_n e^{-i\vec{q}(n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3)}}_{\text{sum over all unit cells (lattice sum)}} \underbrace{\sum_i f_i\,(q) \cdot e^{-i\vec{q}(x\vec{a}_1+y\vec{a}_2+z\vec{a}_3)}}_{\text{sum over all atoms within a unit cells (structure factor)}}$$

sum over all unit cells
(lattice sum)

sum over all atoms
within a unit cells
(structure factor)

Lattice sum

$$E \propto \underbrace{\sum_n e^{-i\vec{q}\vec{R}_n} = \sum_n e^{-i\vec{q}(n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3)}}_{\text{sum over all unit cells (lattice sum)}}$$

Constructive interference only if all phases are the same:

$$\vec{q}\vec{R}_n = 2\pi \cdot m$$

Condition for the scattering vector $\vec{q}$:

$$\vec{q} = \vec{G}_{hkl} = h \cdot \vec{a}_1^* + k \cdot \vec{a}_2^* + l \cdot \vec{a}_3^*$$

where $\quad \vec{a}_i^* \cdot \vec{a}_j = 2\pi\delta_{ij}$

Reciprocal lattice

Real space

three unit vectors

$$\vec{a}_1, \vec{a}_2, \vec{a}_3$$

define crystal lattice

$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

Reciprocal space

three reciprocal unit vectors

$$\vec{a}_1^* = \frac{2\pi[\vec{a}_2 \times \vec{a}_3]}{\vec{a}_1 \cdot [\vec{a}_2 \times \vec{a}_3]}$$

$$\vec{a}_2^* = \frac{2\pi[\vec{a}_3 \times \vec{a}_1]}{\vec{a}_2 \cdot [\vec{a}_3 \times \vec{a}_1]}$$

$$\vec{a}_3^* = \frac{2\pi[\vec{a}_1 \times \vec{a}_2]}{\vec{a}_3 \cdot [\vec{a}_1 \times \vec{a}_2]}$$

define reciprocal lattice

$$\vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$$

$$\vec{a}_i^* \cdot \vec{a}_j = 2\pi\delta_{ij}$$

$$\vec{q}\vec{R}_n = 2\pi \cdot m$$

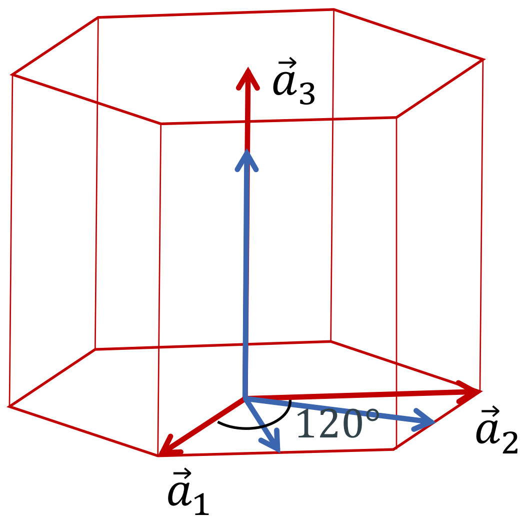
$$\sum_n e^{-i\vec{q}\vec{R}_n} = \begin{cases} 0, if\ \vec{q} \neq \vec{G}_{hkl} \\ N, if\,\vec{q} = \vec{G}_{hkl} \end{cases}$$

Reciprocal lattice

Real space

three unit vectors

$$\vec{a}_1, \vec{a}_2, \vec{a}_3$$



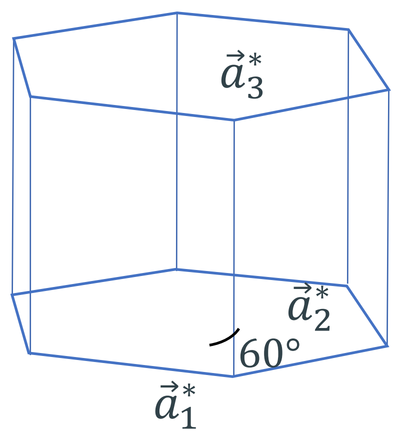
Reciprocal space

three reciprocal unit vectors

$$\vec{a}_1^* = \frac{2\pi[\vec{a}_2 \times \vec{a}_3]}{\vec{a}_1 \cdot [\vec{a}_2 \times \vec{a}_3]}$$

$$\vec{a}_2^* = \frac{2\pi[\vec{a}_3 \times \vec{a}_1]}{\vec{a}_2 \cdot [\vec{a}_3 \times \vec{a}_1]}$$

$$\vec{a}_3^* = \frac{2\pi[\vec{a}_1 \times \vec{a}_2]}{\vec{a}_3 \cdot [\vec{a}_1 \times \vec{a}_2]}$$



$$a_1^* = \frac{4\pi}{a\sqrt{3}}$$

$$a_2^* = \frac{4\pi}{a\sqrt{3}}$$

$$a_3^* = \frac{2\pi}{c}$$

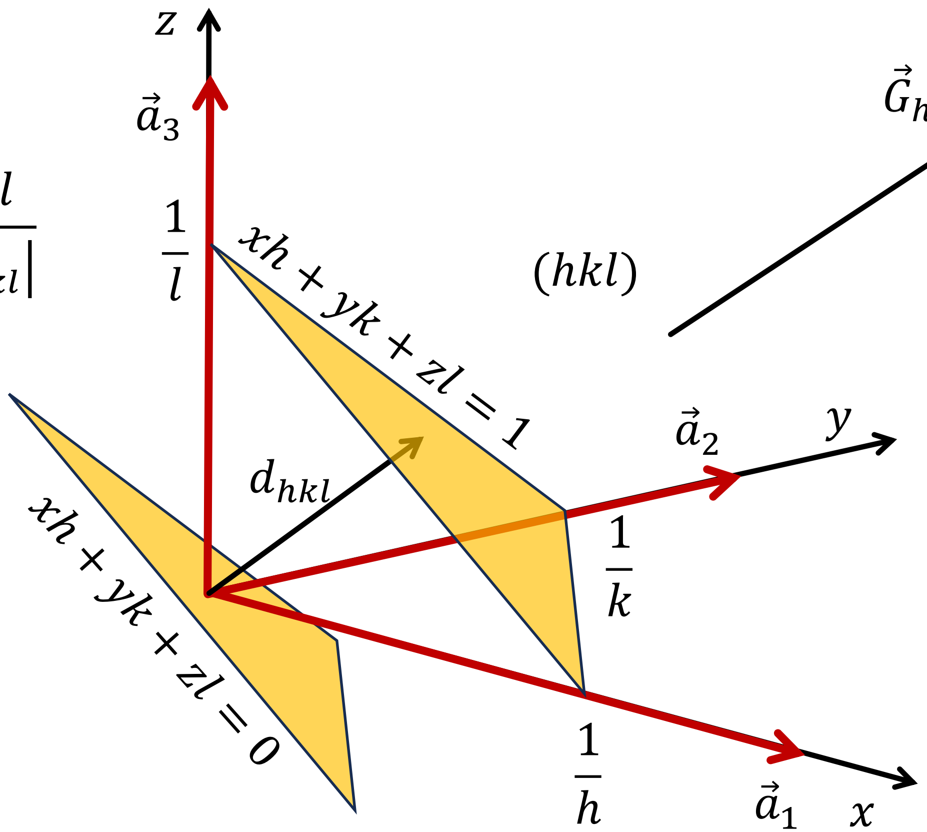
Reciprocal lattice and lattice planes

Let us look at all radius-vectors $\vec{R} = x\vec{a}_1 + y\vec{a}_2 + z\vec{a}_3$ which are perpendicular to the reciprocal lattice vector $\vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$:

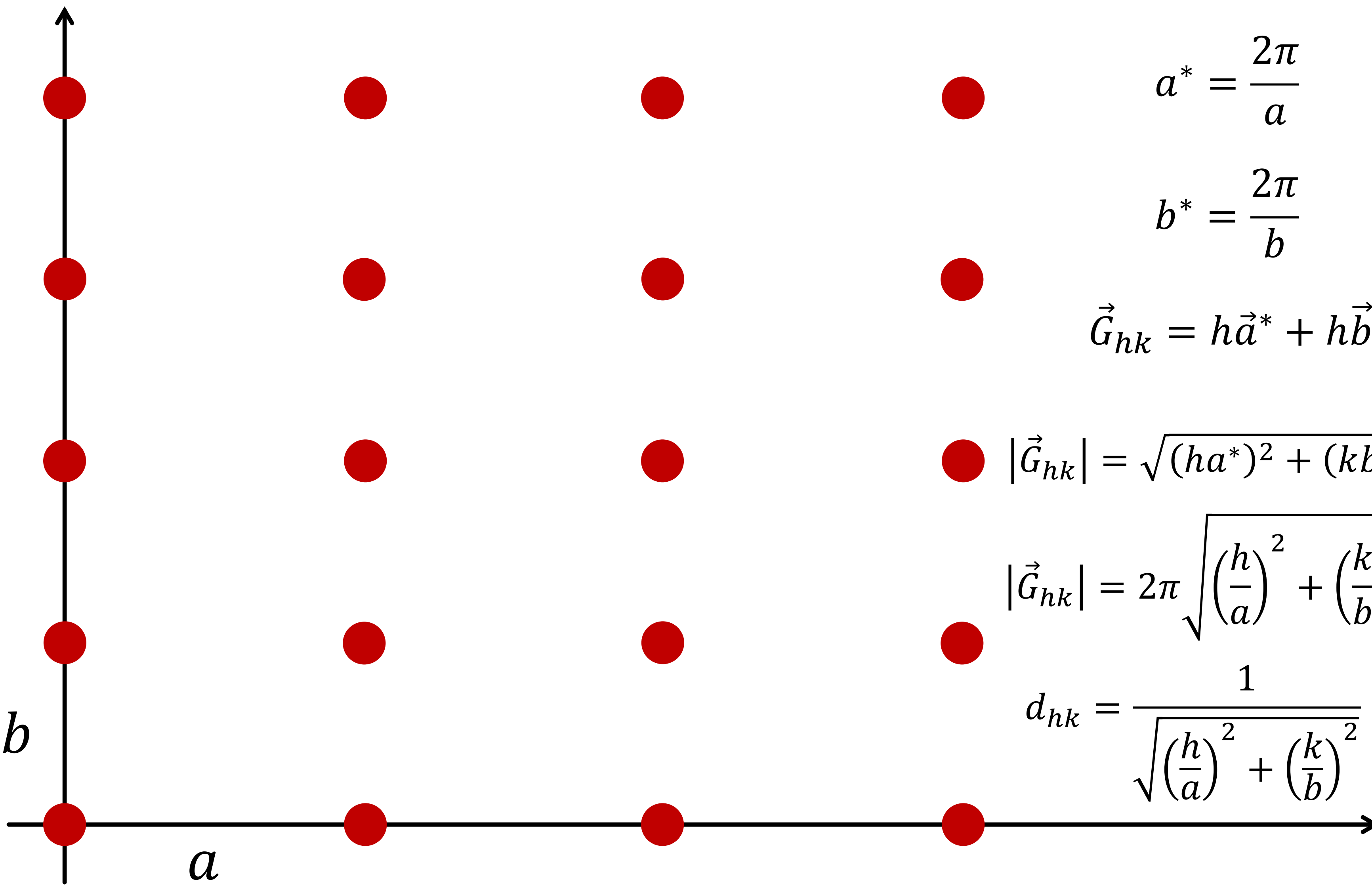
$$\vec{R}\vec{G}_{hkl} = 2\pi(xh + yk + zl) = 0$$

$$d_{hkl} = \frac{1}{l}\vec{a}_3 \cdot \vec{n} = \frac{1}{l}\vec{a}_3 \cdot \frac{\vec{G}_{hkl}}{|\vec{G}_{hkl}|} = \frac{1}{l}\frac{2\pi l}{|\vec{G}_{hkl}|}$$

$$\boxed{d_{hkl} = \frac{2\pi}{|\vec{G}_{hkl}|}}$$



Example



$$a^* = \frac{2\pi}{a}$$

$$b^* = \frac{2\pi}{b}$$

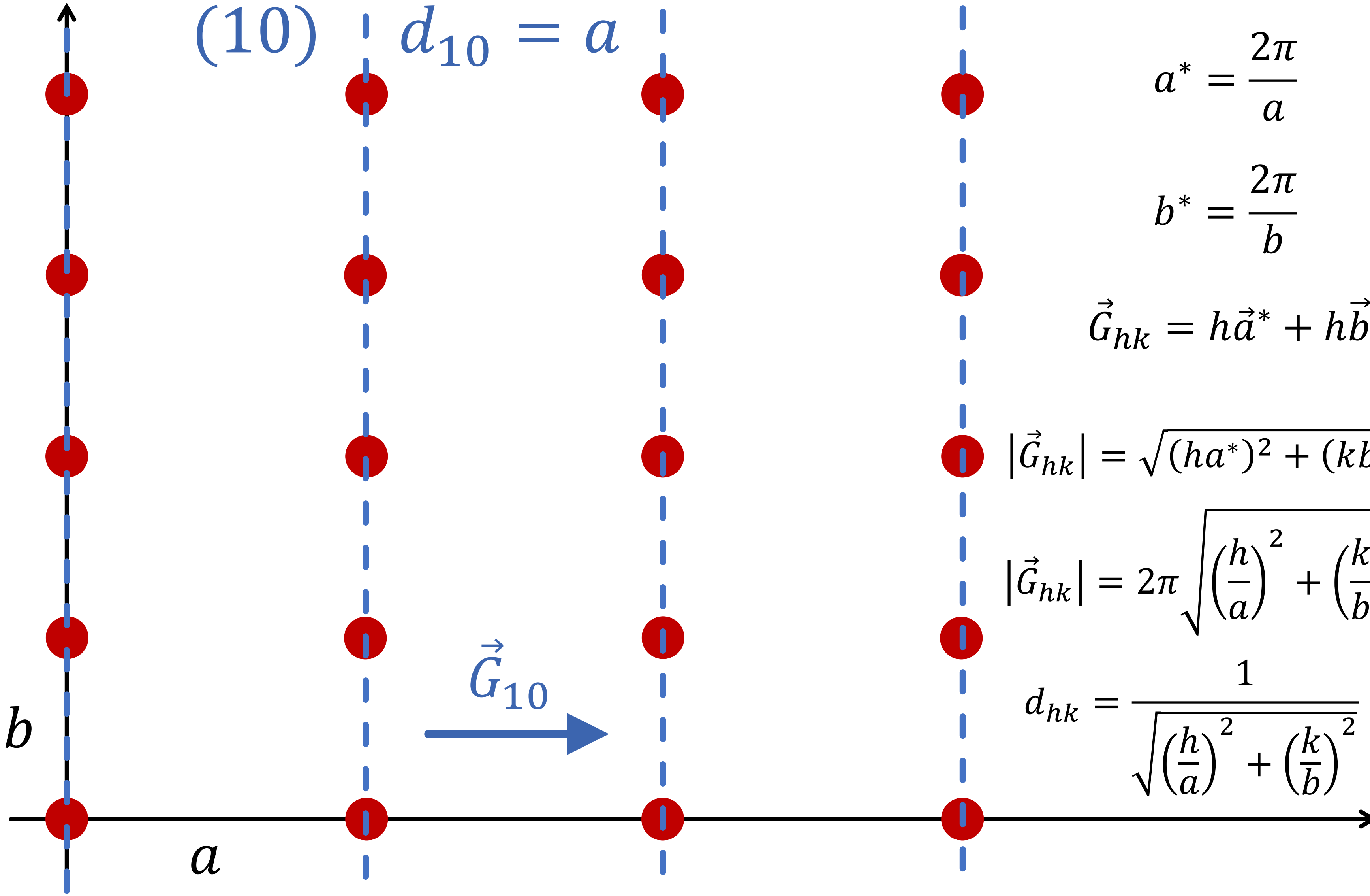
$$\vec{G}_{hk} = h\vec{a}^* + h\vec{b}^*$$

$$|\vec{G}_{hk}| = \sqrt{(ha^*)^2 + (kb^*)^2}$$

$$|\vec{G}_{hk}| = 2\pi\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2}$$

$$d_{hk} = \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2}}$$

Example



$$a^* = \frac{2\pi}{a}$$

$$b^* = \frac{2\pi}{b}$$

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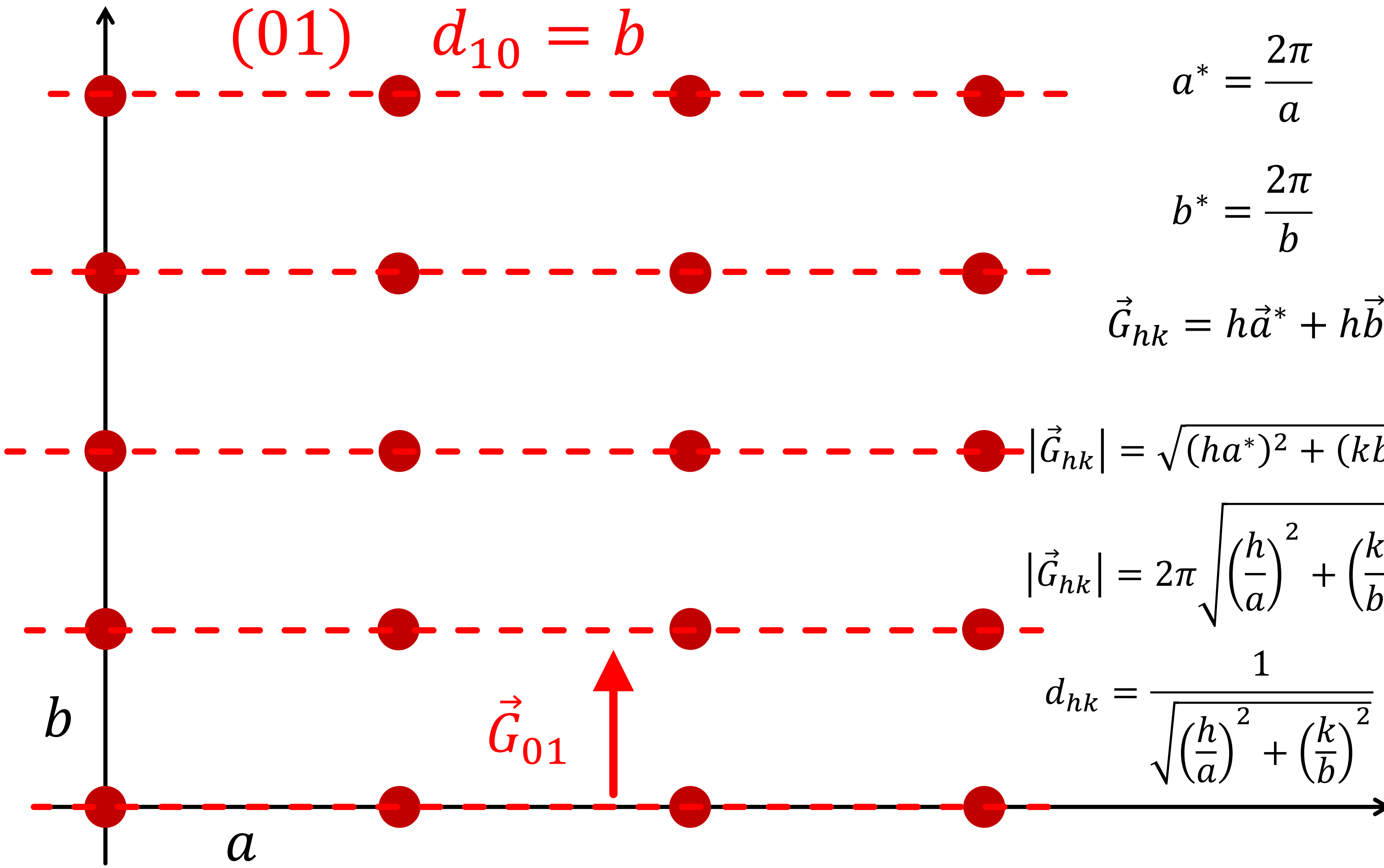
Example



$$a^* = \frac{2\pi}{a}$$

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$$|\vec{G}_{hk}| = \sqrt{(ha^*)^2 + (kb^*)^2}$$

$$|\vec{G}_{hk}| = 2\pi\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2}$$

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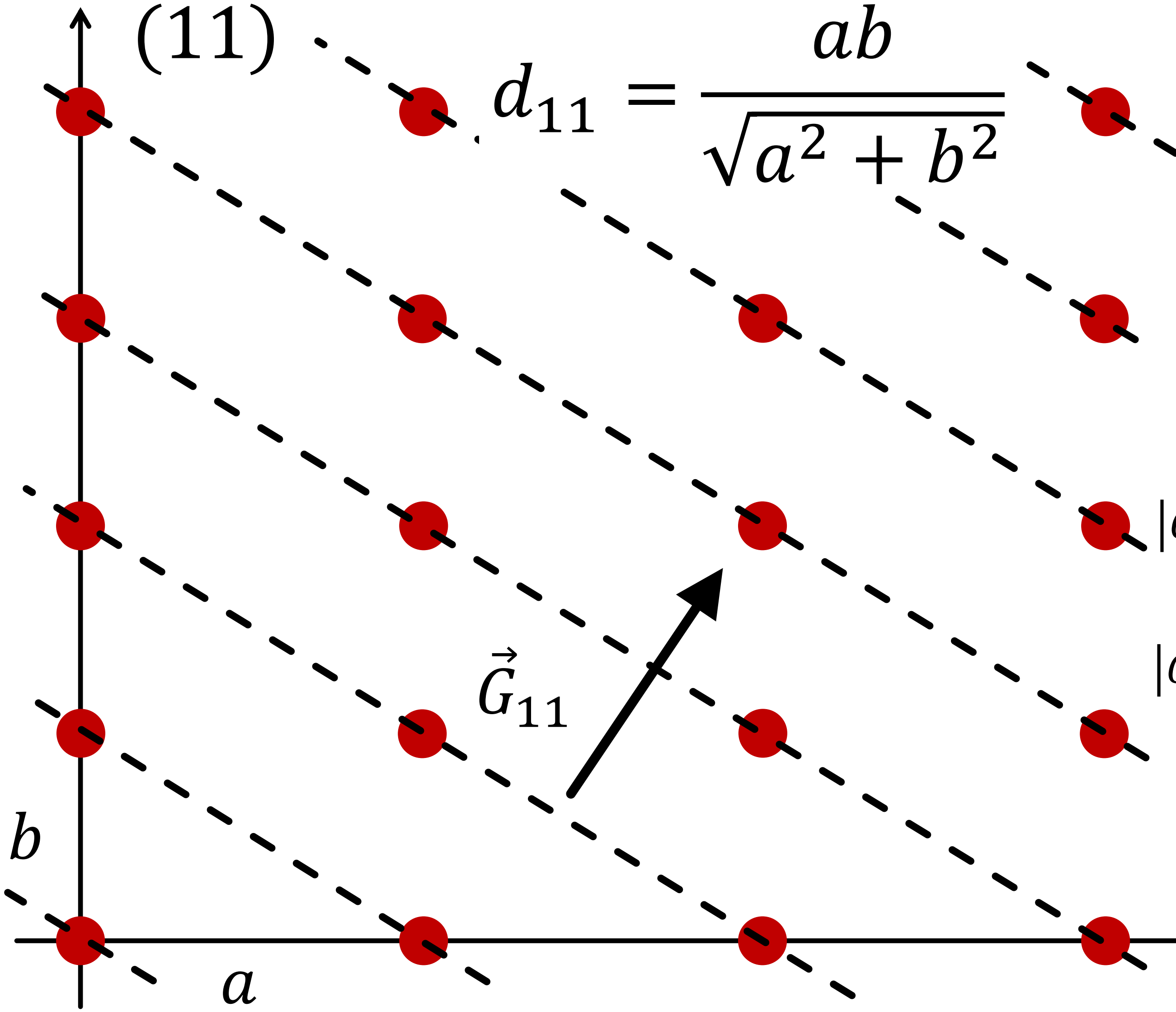
Example



$$d_{11} = \frac{ab}{\sqrt{a^2 + b^2}}$$

$$a^* = \frac{2\pi}{a}$$

$$b^* = \frac{2\pi}{b}$$

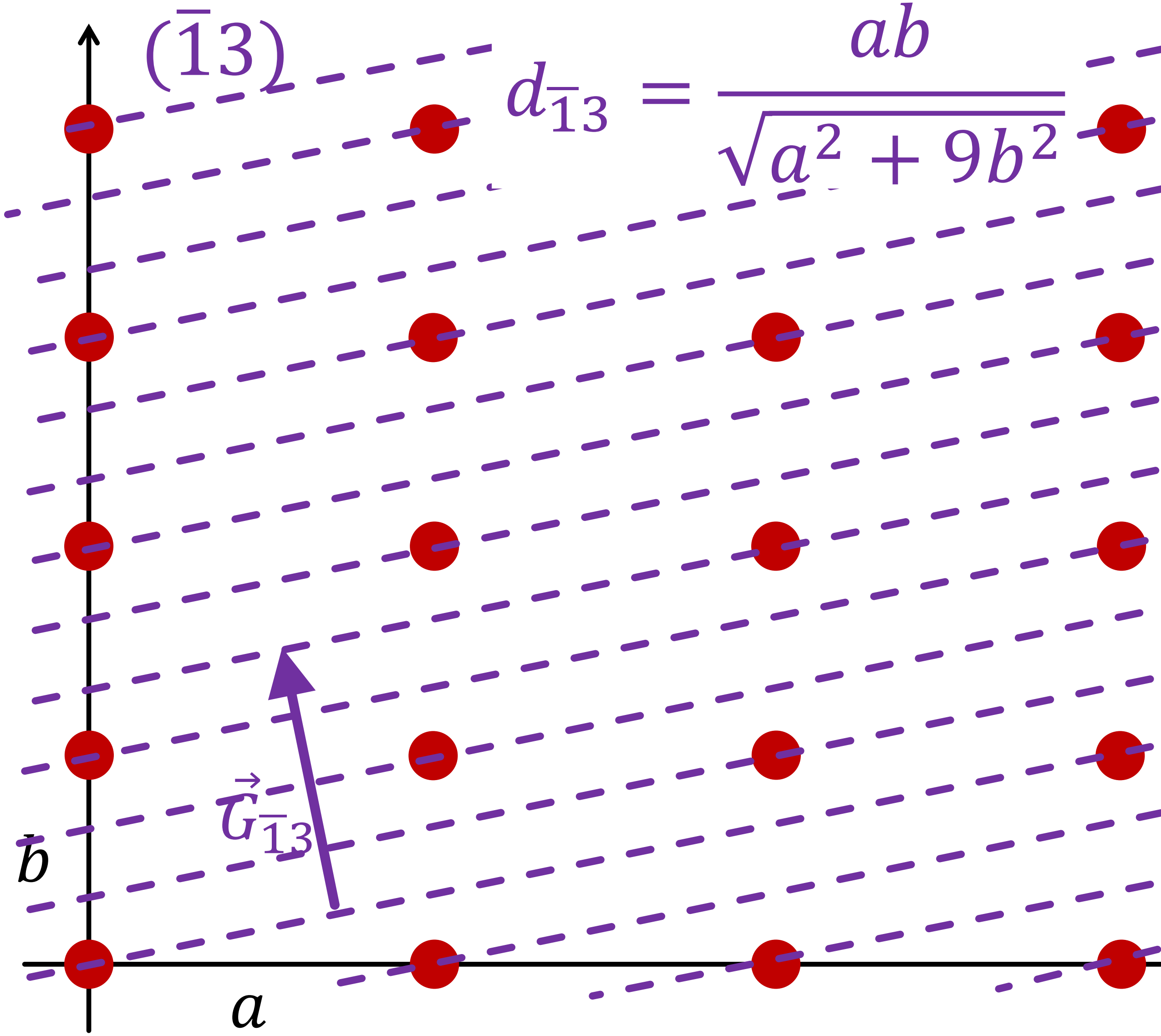
$$\vec{G}_{hk} = h\vec{a}^* + h\vec{b}^*$$

$$|\vec{G}_{hk}| = \sqrt{(ha^*)^2 + (kb^*)^2}$$

$$|\vec{G}_{hk}| = 2\pi\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2}$$

$$d_{hk} = \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2}}$$

Example



$$a^* = \frac{2\pi}{a}$$

$$b^* = \frac{2\pi}{b}$$

$$\vec{G}_{hk} = h\vec{a}^* + h\vec{b}^*$$

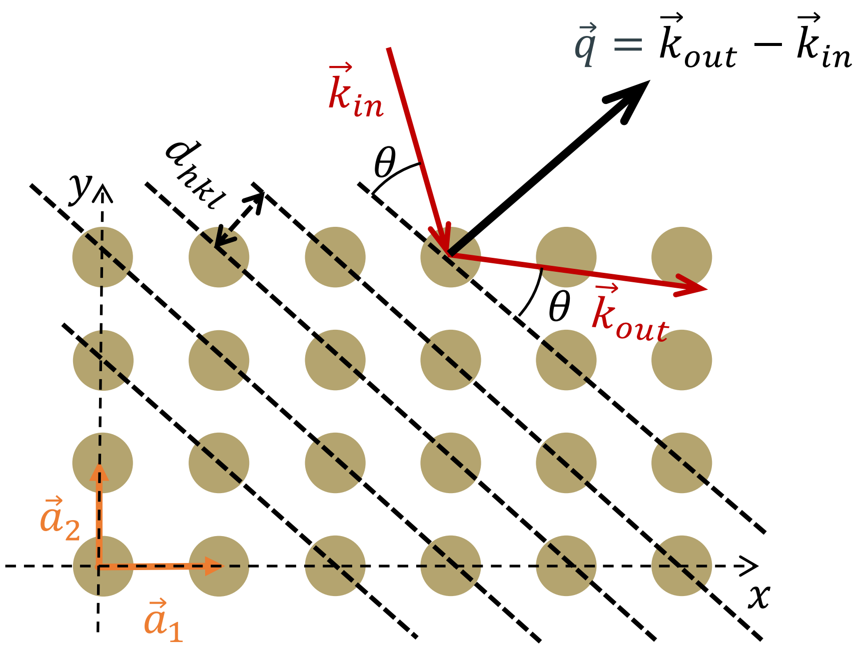
$$|\vec{G}_{hk}| = \sqrt{(ha^*)^2 + (kb^*)^2}$$

$$|\vec{G}_{hk}| = 2\pi\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2}$$

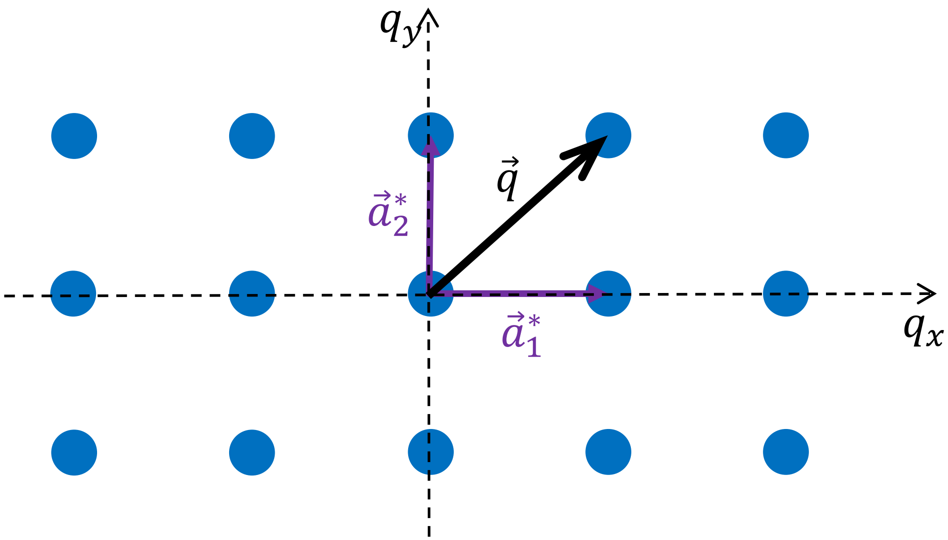
$$d_{hk} = \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2}}$$

Real space and reciprocal space

Scattering in real space



Scattering in reciprocal space



$$\vec{q} = \vec{a}_1^* + \vec{a}_2^* = \vec{G}_{hkl}$$

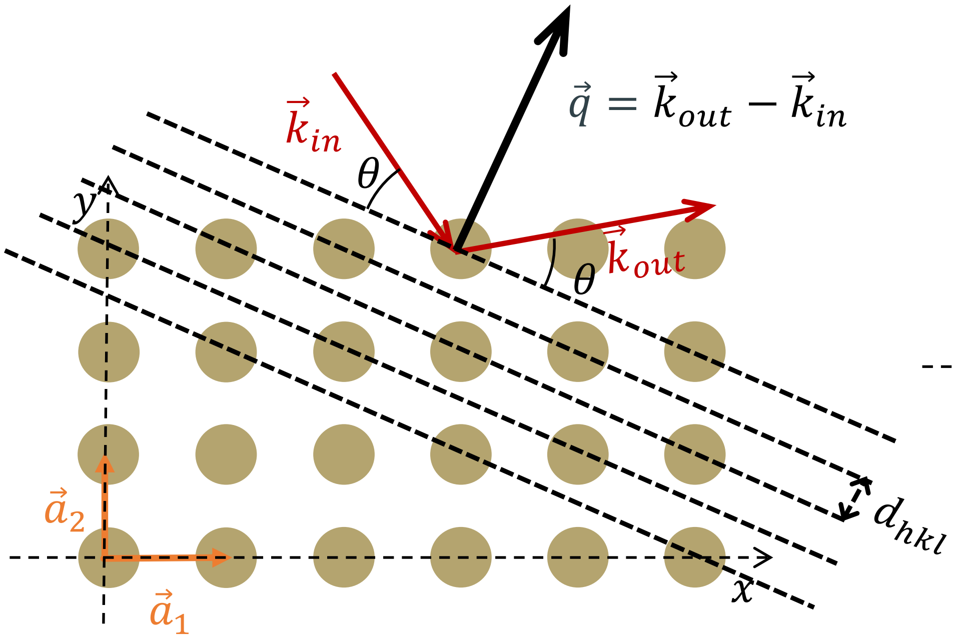
The scattering can be seen as specular reflection from a set of parallel atomic planes. The interference between the photons scattered from different planes will be constructive if the Bragg condition is satisfied:

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

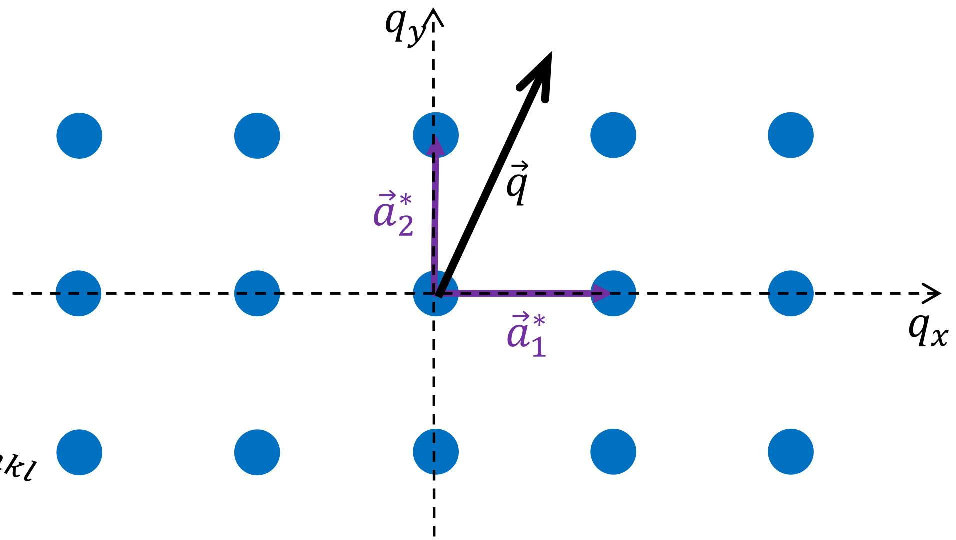
Laue condition is satisfied, so we will see a diffraction peak in this experiment.

Real space and reciprocal space

Scattering in real space



Scattering in reciprocal space



$$\vec{q} \neq \vec{G}_{hkl}$$

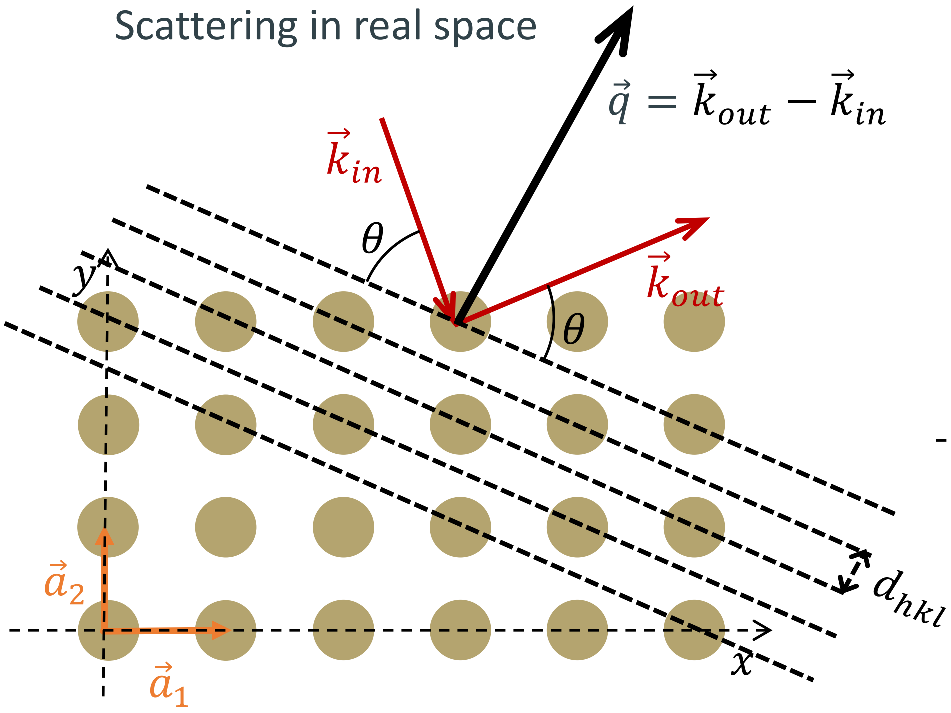
Bragg condition is not satisfied:

$$2d_{hkl} \sin\theta \neq \lambda$$

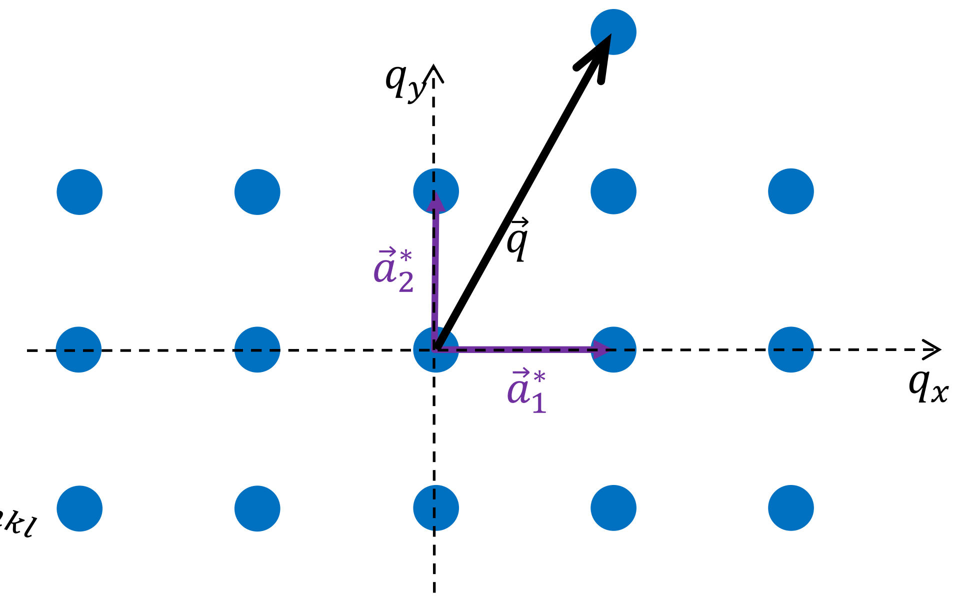
Laue condition is not satisfied, so we will not see a diffraction peak in this experiment.

Real space and reciprocal space

Scattering in real space



Scattering in reciprocal space



$$\vec{q} = \vec{a}_1^* + 2\vec{a}_2^* = \vec{G}_{hkl}$$

Laue condition is satisfied

By adjusting the incidence angle, Bragg condition is satisfied again, so we can see the diffraction peak

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

Intensity of Bragg peaks

$$E \propto \sum_n e^{-i\vec{q}(n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3)} \sum_j f_j(q)\cdot e^{-i\vec{q}(x\vec{a}_1+y\vec{a}_2+z\vec{a}_3)}$$

sum over all unit cells (lattice sum)

sum over all atoms within a unit cells (structure factor F_{hkl})

B:

$\vec{r}_1 = (\frac{1}{5},\frac{1}{2},\frac{1}{2}) = (\frac{1}{2},\frac{1}{2},\frac{1}{2}) - (\frac{3}{10},0,0)$

$\vec{r}_2 = (\frac{4}{5},\frac{1}{2},\frac{1}{2}) = (\frac{1}{2},\frac{1}{2},\frac{1}{2}) + (\frac{3}{10},0,0)$

$\vec{r}_3 = (\frac{1}{2},\frac{1}{5},\frac{1}{2}) = (\frac{1}{2},\frac{1}{2},\frac{1}{2}) - (0,\frac{3}{10},0)$

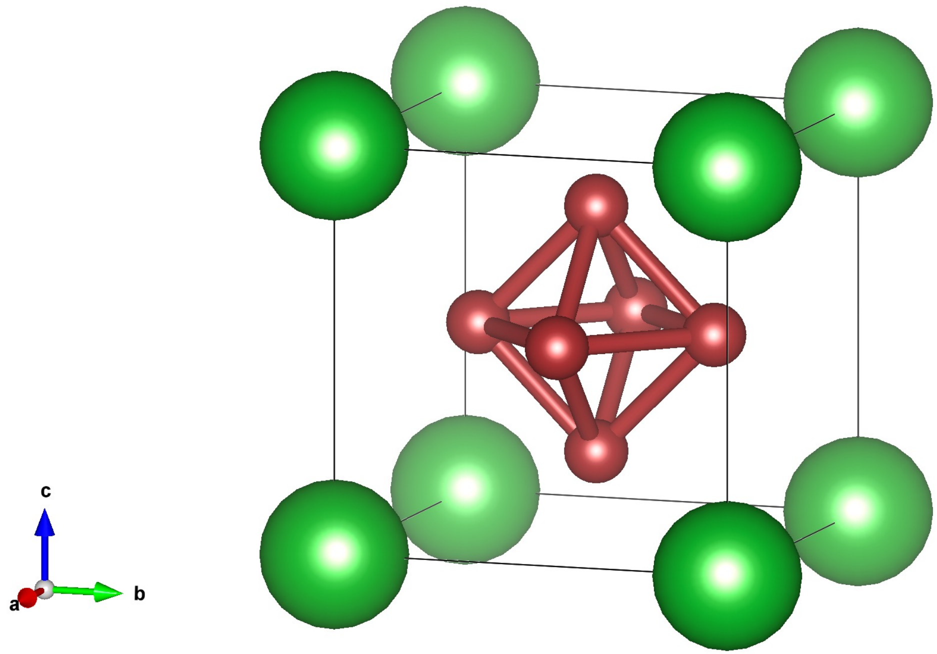
$\vec{r}_4 = (\frac{1}{2},\frac{4}{5},\frac{1}{2}) = (\frac{1}{2},\frac{1}{2},\frac{1}{2}) + (0,\frac{3}{10},0)$

$\vec{r}_5 = (\frac{1}{2},\frac{1}{2},\frac{1}{5}) = (\frac{1}{2},\frac{1}{2},\frac{1}{2}) - (0,0,\frac{3}{10})$

$\vec{r}_6 = (\frac{1}{2},\frac{1}{2},\frac{4}{5}) = (\frac{1}{2},\frac{1}{2},\frac{1}{2}) + (0,0,\frac{3}{10})$

La:

$\vec{r}_7 = (0,0,0)$



Intensity of Bragg peaks

$$F_{hkl} = \sum_j f_j\,(q) \cdot e^{-i\vec{q}\vec{r}_j} = f_{La} + f_B \sum_{j=1}^{6} \exp[-i\vec{q}\vec{r}_j] \;= f_{La} + f_B \exp\left[-i\boldsymbol{q}\frac{1}{2}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)\right] \cdot$$

$$(\exp[-i\boldsymbol{q}(-0.3\vec{a}_1)] + \exp[-i\boldsymbol{q}(0.3\vec{a}_1)]$$

$$+\exp[-i\boldsymbol{q}(-0.3\vec{a}_2)] + \exp[-i\boldsymbol{q}(0.3\vec{a}_2)]$$

$$+\exp[-i\boldsymbol{q}(-0.3\vec{a}_3)] + \exp[-i\boldsymbol{q}(0.3\vec{a}_3)])$$

$$\vec{q} = \vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$$

B:

$$\vec{r}_1 = (\tfrac{1}{5}, \tfrac{1}{2}, \tfrac{1}{2}) = \left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right) - (\tfrac{3}{10}, 0, 0)$$

$$\vec{r}_2 = (\tfrac{4}{5}, \tfrac{1}{2}, \tfrac{1}{2}) = \left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right) + (\tfrac{3}{10}, 0, 0)$$

$$\vec{r}_3 = (\tfrac{1}{2}, \tfrac{1}{5}, \tfrac{1}{2}) = \left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right) - (0, \tfrac{3}{10}, 0)$$

$$\vec{r}_4 = (\tfrac{1}{2}, \tfrac{4}{5}, \tfrac{1}{2}) = \left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right) + (0, \tfrac{3}{10}, 0)$$

$$\vec{r}_5 = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{5}) = \left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right) - (0, 0, \tfrac{3}{10})$$

$$\vec{r}_6 = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{4}{5}) = \left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right) + (0, 0, \tfrac{3}{10})$$

La:

$$\vec{r}_7 = (0,0,0)$$

Intensity of Bragg peaks

$$F_{hkl} = \sum_j f_j\,(q) \cdot e^{-i\vec{q}\vec{r}_j} = f_{La} + f_B \sum_{j=1}^{6} \exp[-i\vec{q}\vec{r}_j] = f_{La} + f_B \exp\left[-i\boldsymbol{q}\frac{1}{2}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)\right] \cdot$$

$$(\exp[-i\boldsymbol{q}(-0.3\vec{a}_1)] + \exp[-i\boldsymbol{q}(0.3\vec{a}_1)]$$

$$+\exp[-i\boldsymbol{q}(-0.3\vec{a}_2)] + \exp[-i\boldsymbol{q}(0.3\vec{a}_2)]$$

$$+\exp[-i\boldsymbol{q}(-0.3\vec{a}_3)] + \exp[-i\boldsymbol{q}(0.3\vec{a}_3)])$$

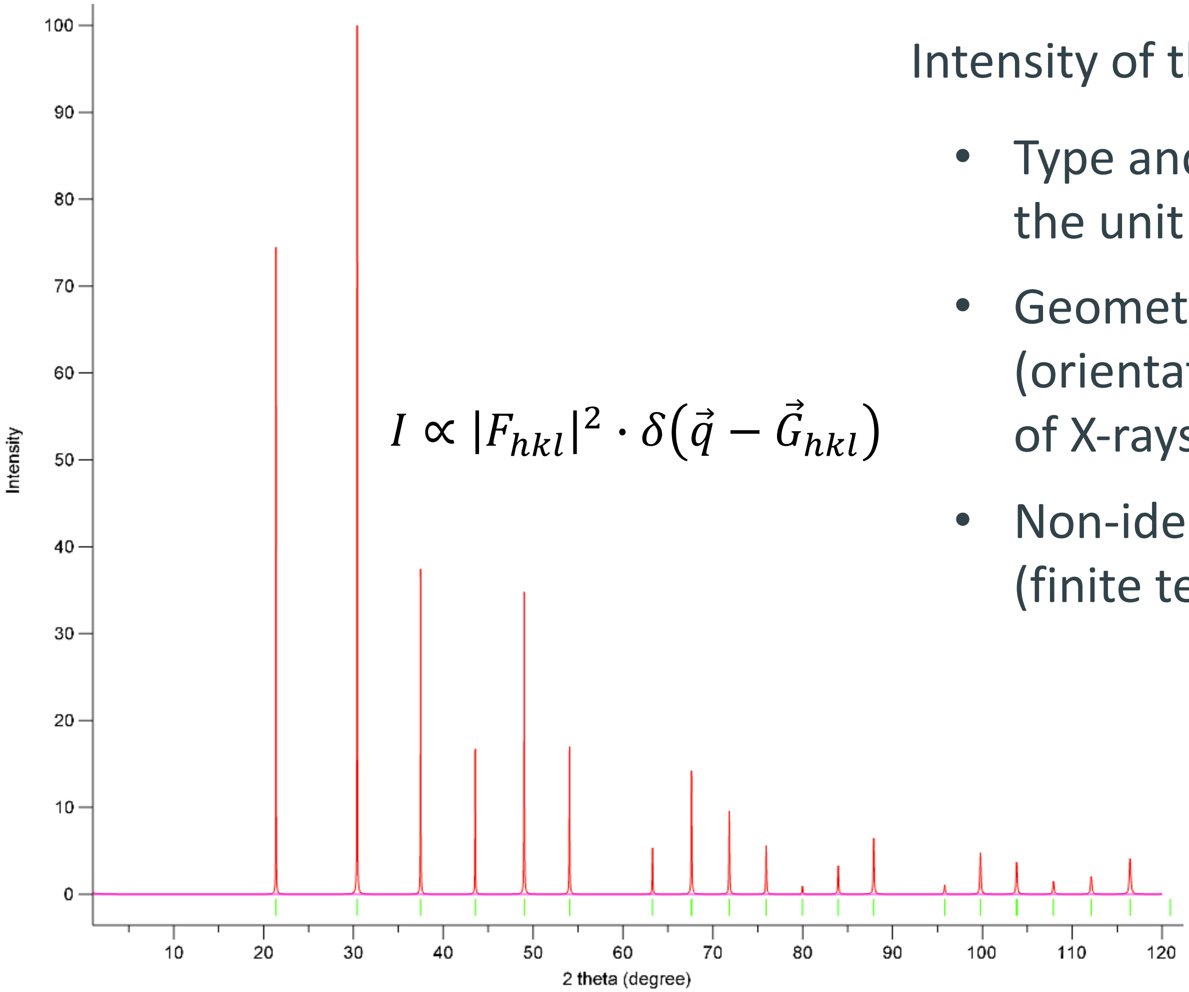
$$\vec{q} = \vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$$

$$= f_{La} + f_B \exp[-i\pi(h + k + l)] \cdot 2 \cdot (\cos(2\pi \cdot 0.3h) + \cos(2\pi \cdot 0.3k) + \cos(2\pi \cdot 0.3l))$$

$$= f_{La} + 2f_B \cdot (-1)^{h+k+l} \cdot (\cos(0.6\pi h) + \cos(0.6\pi k) + \cos(0.6\pi l))$$

Intensity of Bragg peaks

$$F_{hkl} = \sum_j f_j(q) \cdot e^{-i\vec{q}\vec{r}_j} = f_{La} + 2f_B \cdot (-1)^{h+k+l} \cdot (\cos(0.6\pi h) + \cos(0.6\pi k) + \cos(0.6\pi l))$$

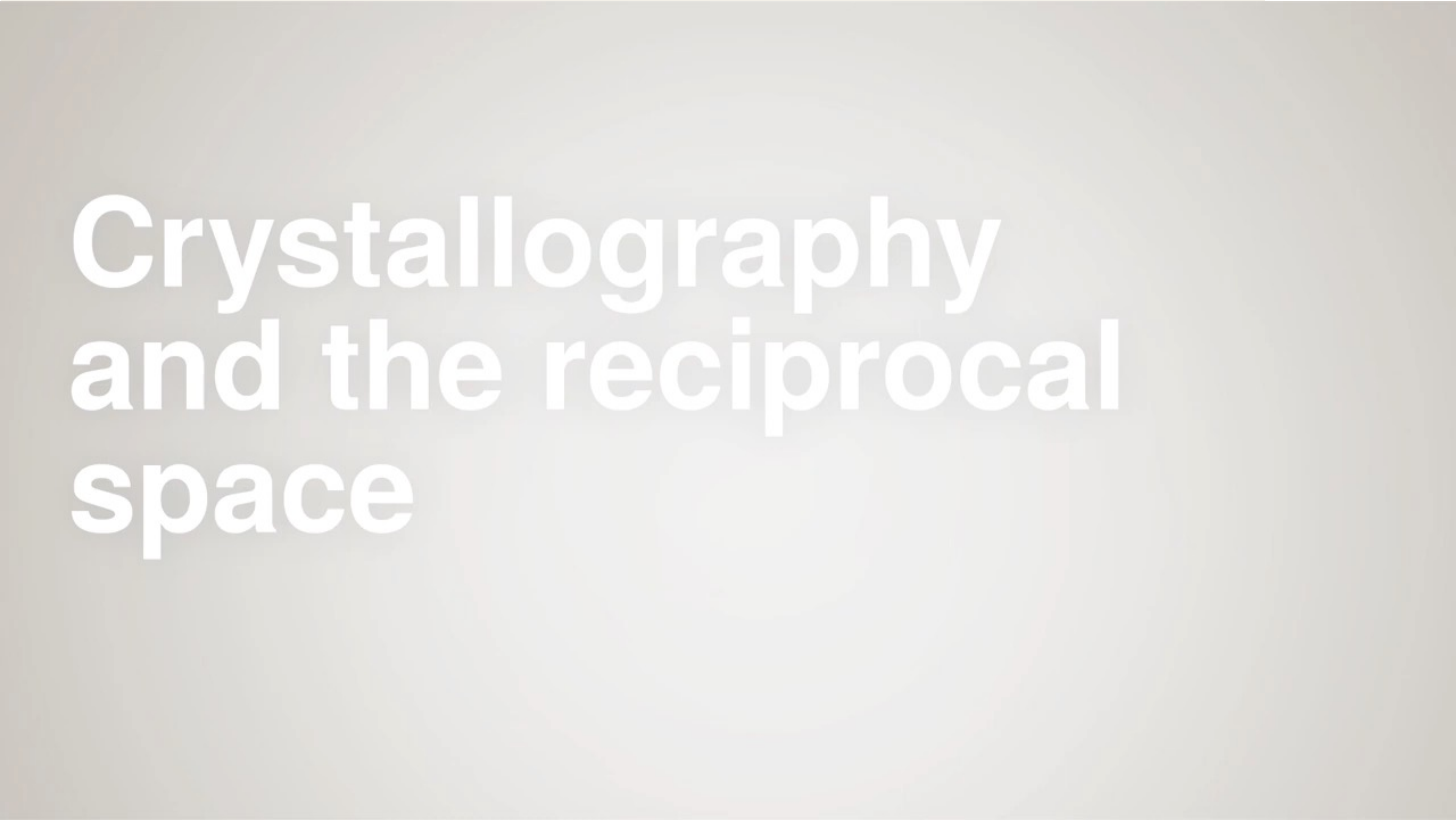


$$I \propto |F_{hkl}|^2 \cdot \delta(\vec{q} - \vec{G}_{hkl})$$

Intensity of the Bragg peaks is determined by:

- Type and position of the atoms within the unit cell (basis)
- Geometry of the experiment (orientation of the sample, polarization of X-rays, crystallinity of the sample etc.)
- Non-ideality of the crystal structure (finite temperature, defects, etc.)

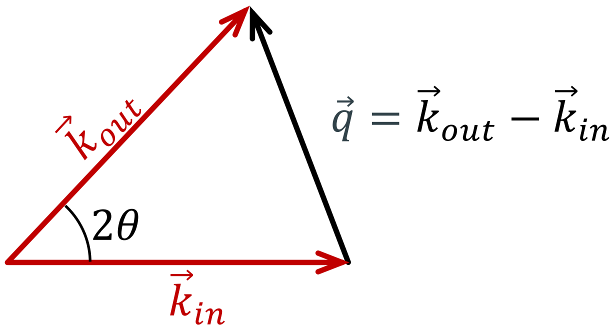
One more illustration



https://toutestquantique.fr/en/

The Ewald sphere

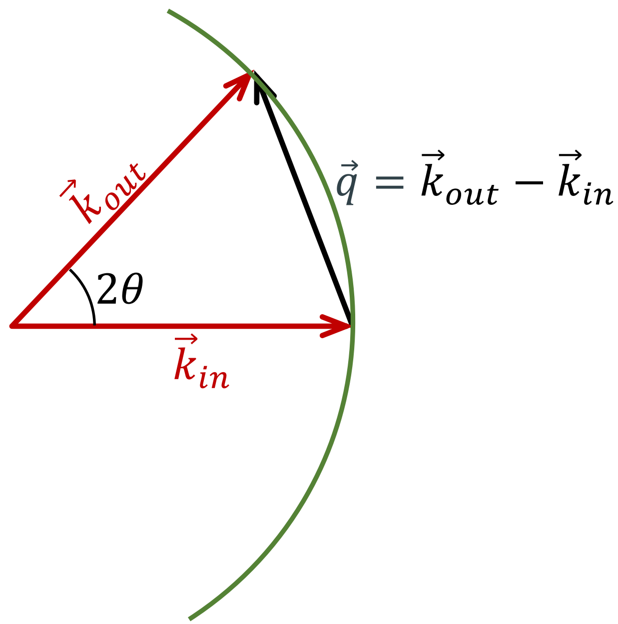
For elastic scattering, $|\vec{k}_{in}| = |\vec{k}_{out}| = \frac{2\pi}{\lambda}$. It means, that all possible scattering vectors $\vec{q} = \vec{k}_{out} - \vec{k}_{in}$ form a sphere of radius $\frac{2\pi}{\lambda}$ in reciprocal space. A diffraction pattern, measured with a 2D detector, is a cross section of reciprocal space with the Ewald sphere.



$$q = \frac{4\pi}{\lambda}\sin\theta$$

The Ewald sphere

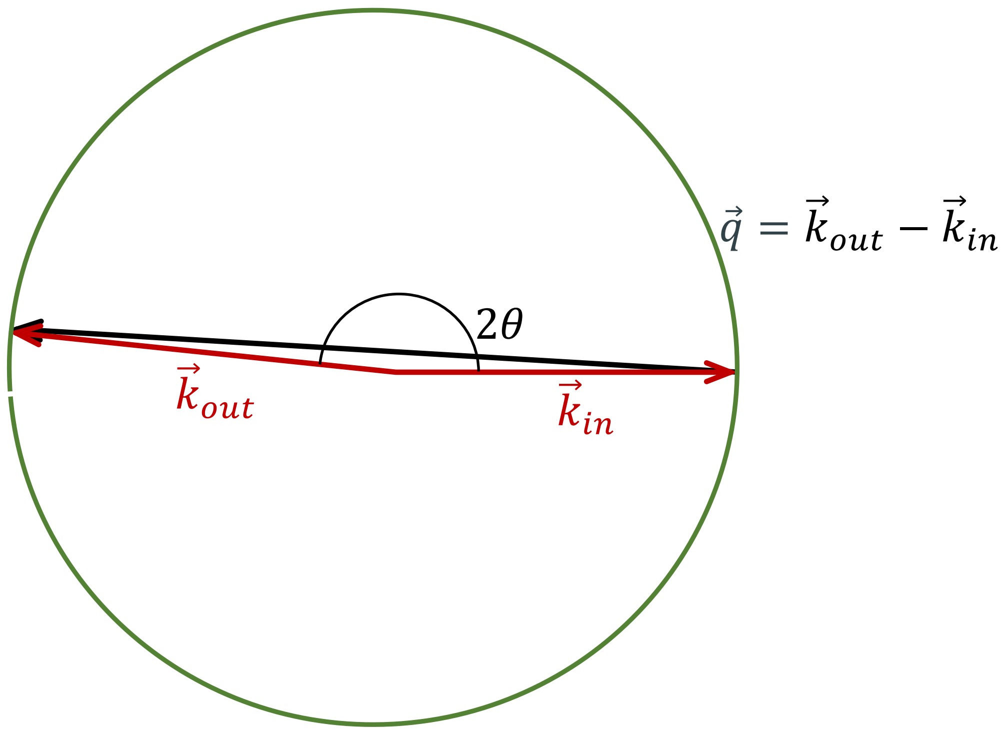
For elastic scattering, $|\vec{k}_{in}| = |\vec{k}_{out}| = \frac{2\pi}{\lambda}$. It means, that all possible scattering vectors $\vec{q} = \vec{k}_{out} - \vec{k}_{in}$ form a sphere of radius $\frac{2\pi}{\lambda}$ in reciprocal space. A diffraction pattern, measured with a 2D detector, is a cross section of reciprocal space with the Ewald sphere.



$$q = \frac{4\pi}{\lambda} \sin\theta$$

The Ewald sphere

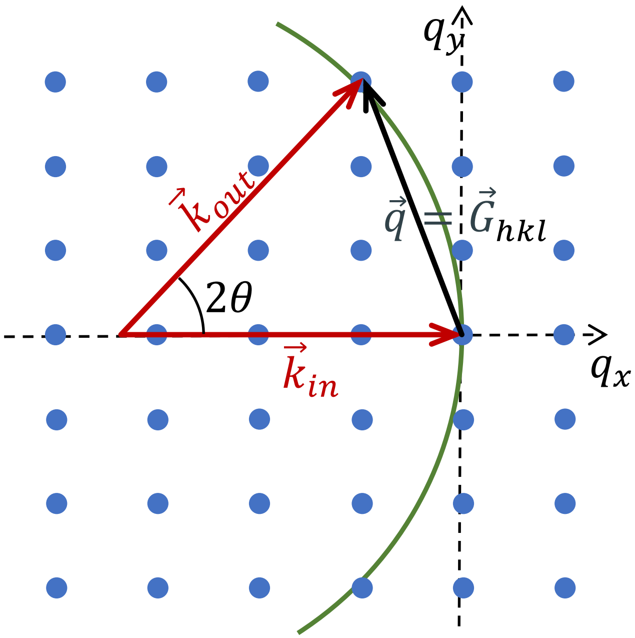
For elastic scattering, $|\vec{k}_{in}| = |\vec{k}_{out}| = \frac{2\pi}{\lambda}$. It means, that all possible scattering vectors $\vec{q} = \vec{k}_{out} - \vec{k}_{in}$ form a sphere of radius $\frac{2\pi}{\lambda}$ in reciprocal space. A diffraction pattern, measured with a 2D detector, is a cross section of reciprocal space with the Ewald sphere.



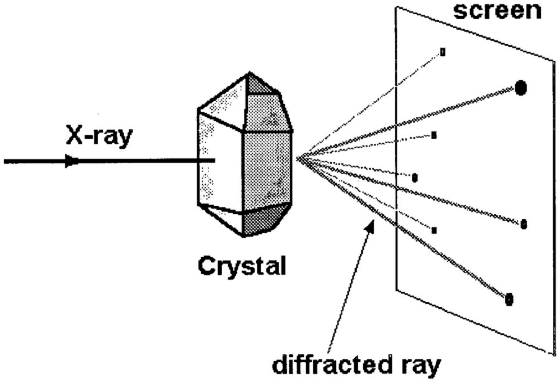
$$q = \frac{4\pi}{\lambda}\sin\theta$$

$$q_{max} = \frac{4\pi}{\lambda}$$

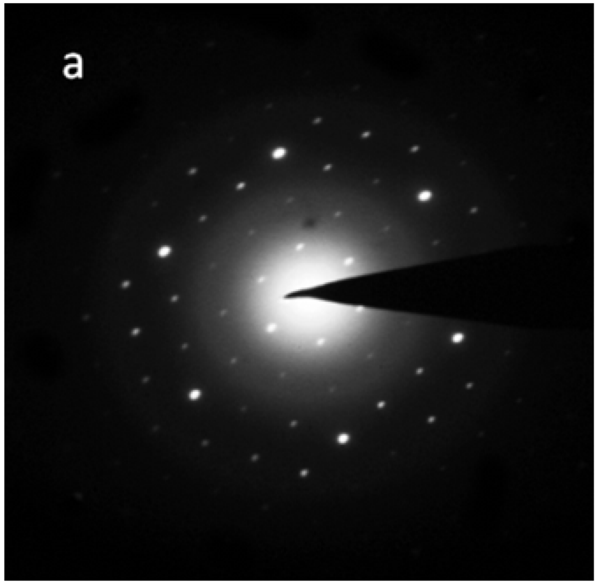
The Ewald sphere



Ewald's sphere in reciprocal space



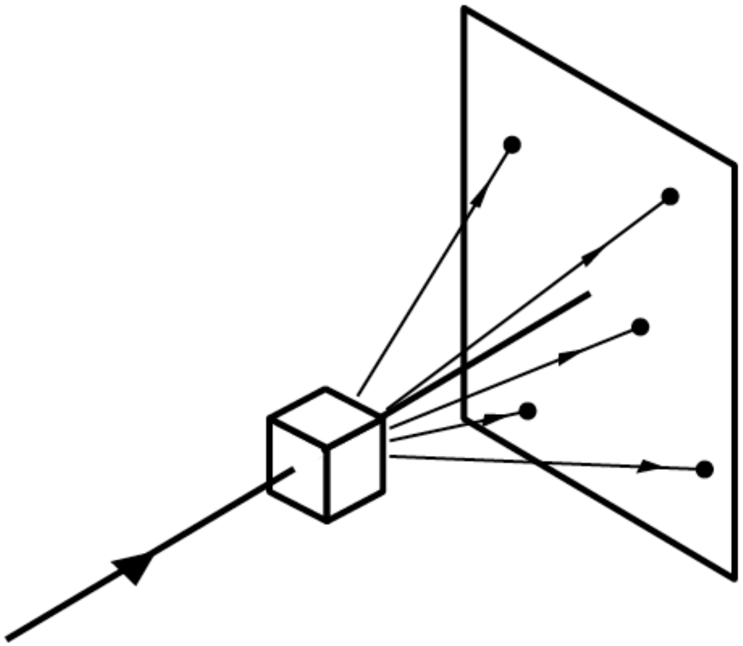
Single crystal diffraction experiment

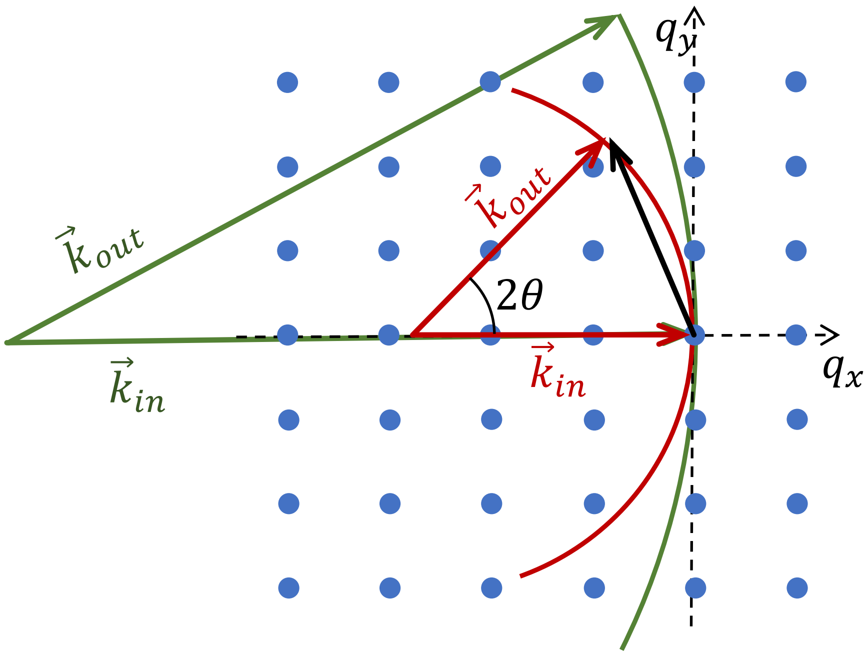


Diffraction pattern

Laue method

- Polychromatic X-ray beam, $k_{min} \leq k \leq k_{max}$ ($\lambda_{min} \leq \lambda \leq \lambda_{max}$)
- Allows to determine orientation of a crystal
- Cannot be used for polycrystals

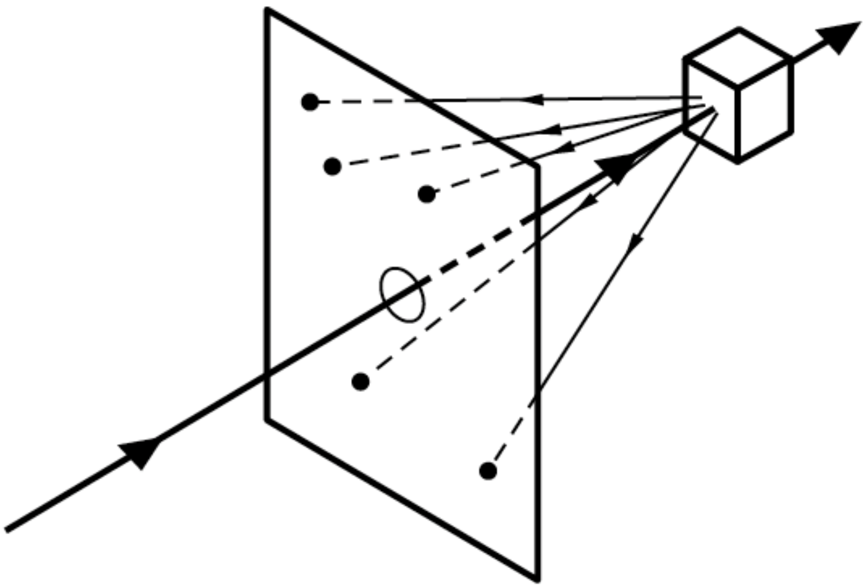


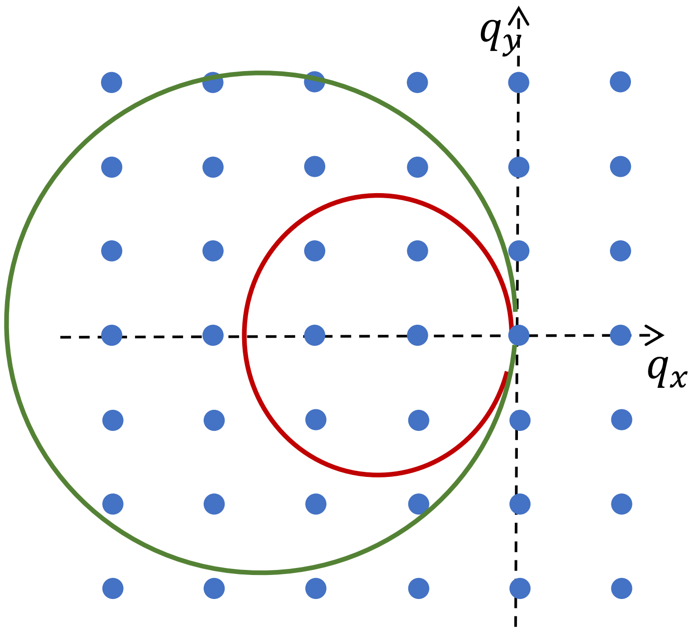


B.D. Cullity & S.R. Strock "Elements of X-ray Diffraction" (2014)

Laue method

- Polychromatic X-ray beam, $k_{min} \leq k \leq k_{max}$ $(\lambda_{min} \leq \lambda \leq \lambda_{max})$
- Allows to determine orientation of a crystal
- Cannot be used for polycrystals

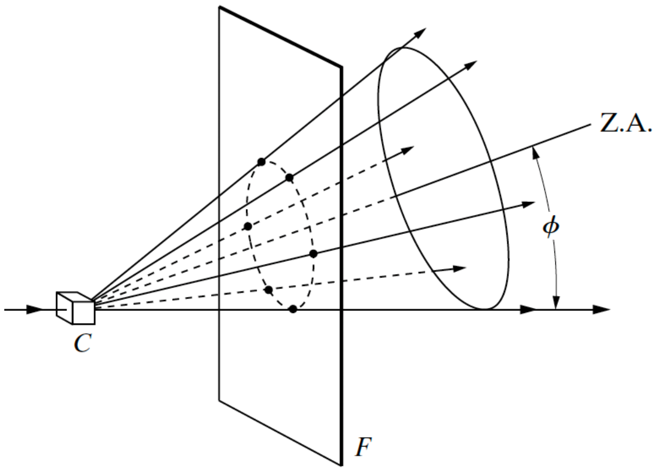


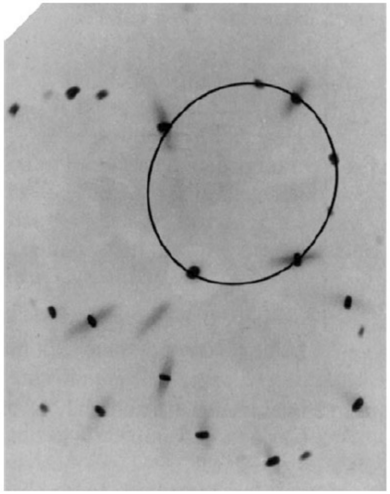


B.D. Cullity & S.R. Strock "Elements of X-ray Diffraction" (2014)

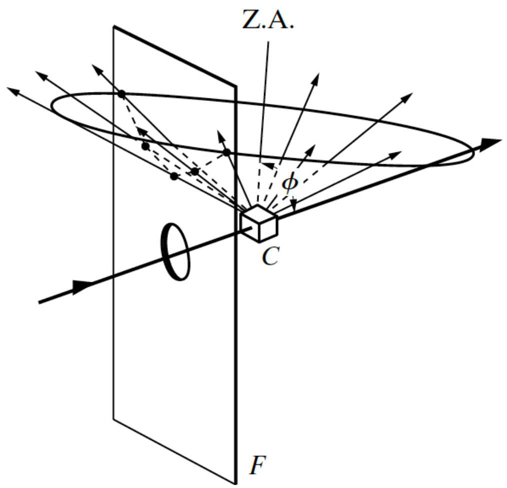
Laue method

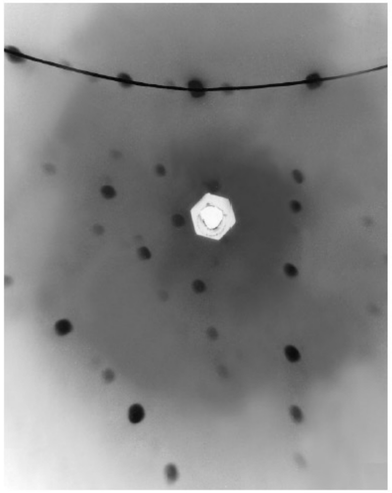
- Reflections from planes belonging to one zone lie on one ellipse or hyperbola





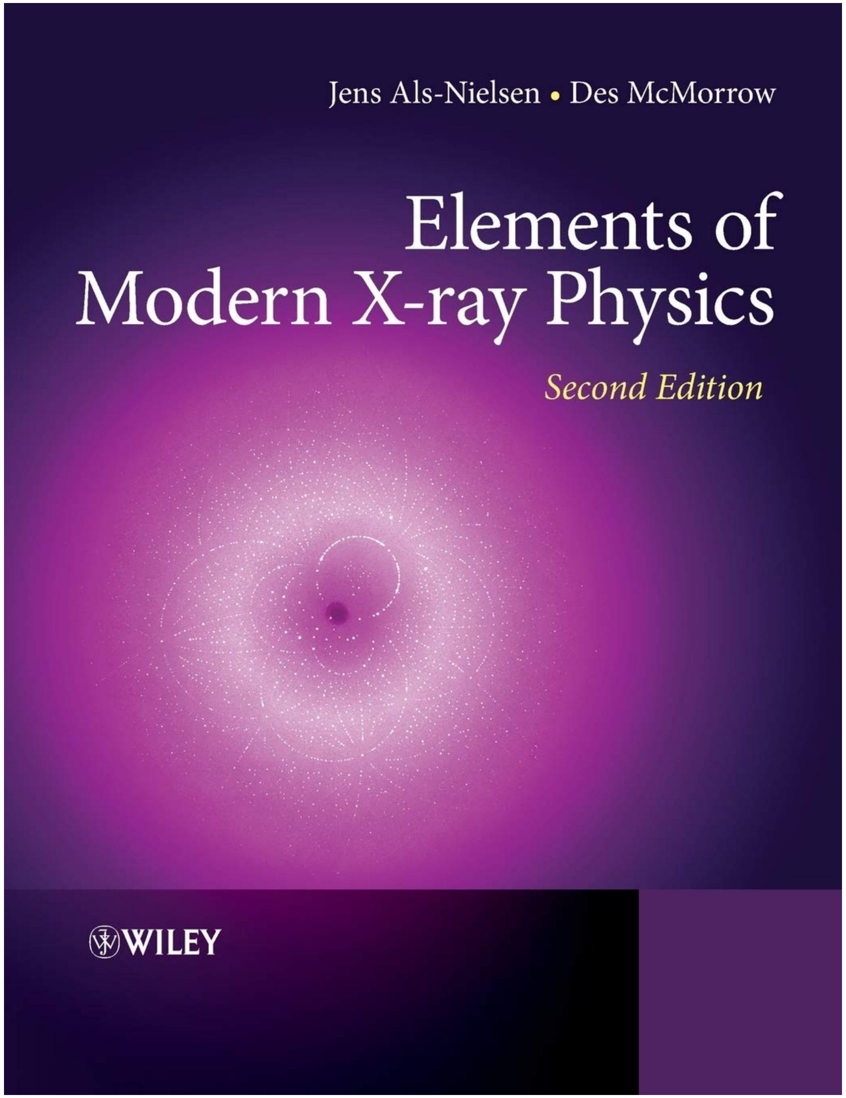
Transmission Laue pattern of an aluminum crystal.

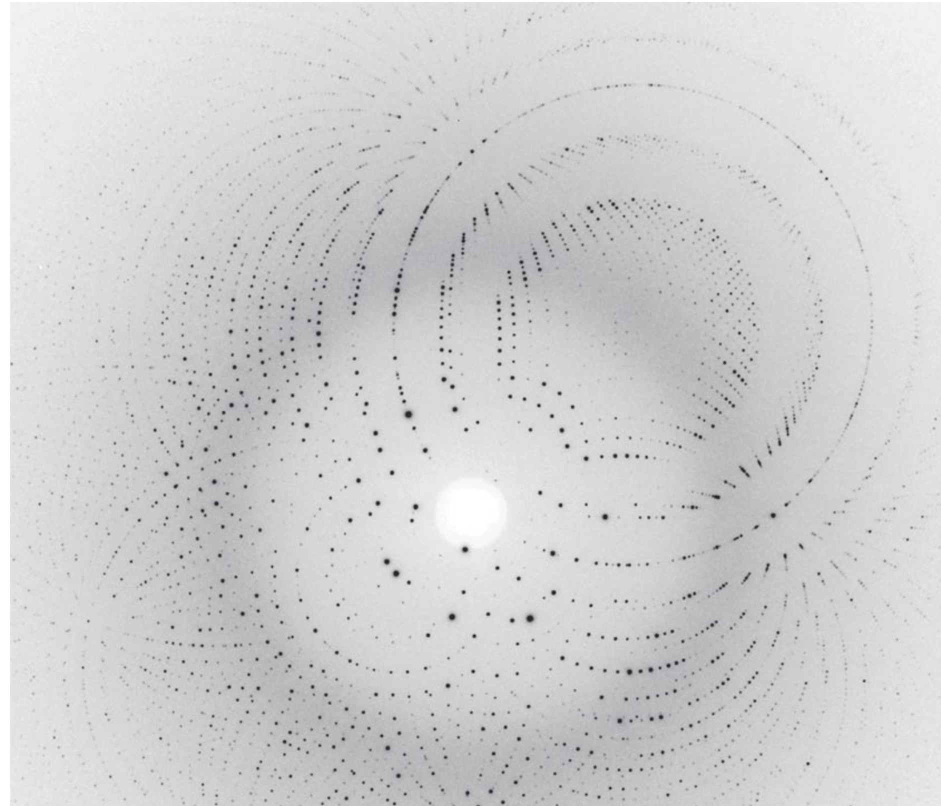




Back-reflection Laue pattern of an aluminum crystal.

B.D. Cullity & S.R. Strock "Elements of X-ray Diffraction" (2014)





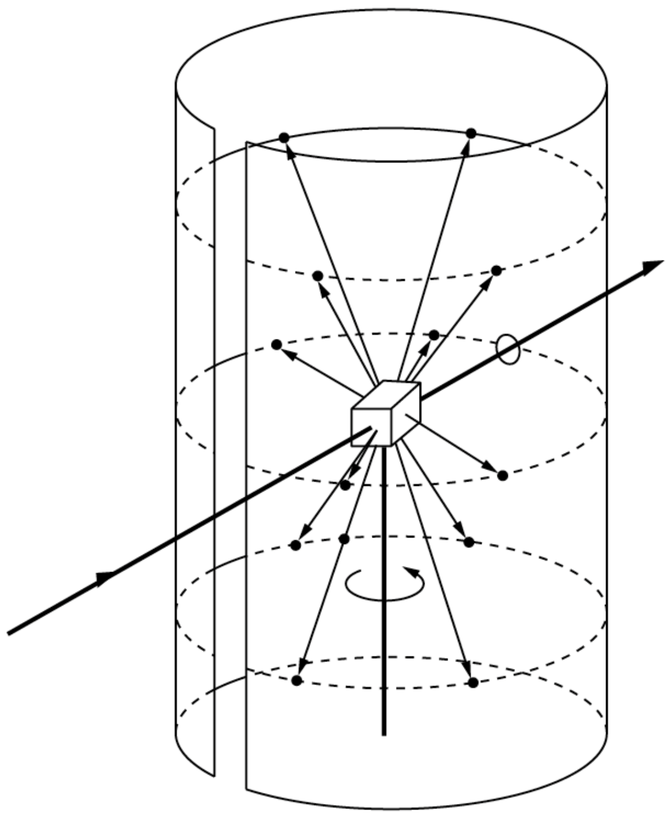
A Laue diffraction image from a protein crystal collected on the MAR345 image plate detector at the APS 14-ID beamline.

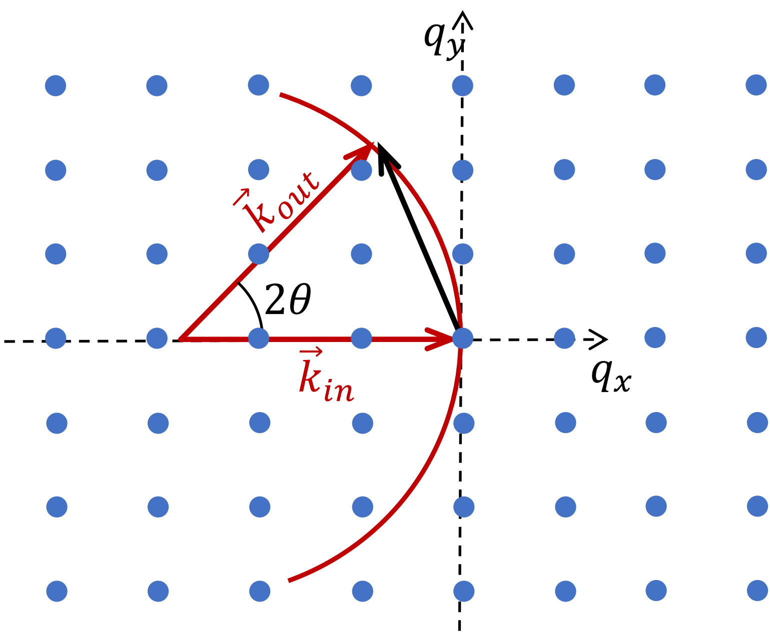
G. Ulrich Nienhaus "Protein-Ligand interactions" (2005)

J. Als-Nielsen & D. McMorrow"Elements of Modern X-ray Physics" (2011)

Rotating crystal method

- Monochromatic X-ray beam, $k = 2\pi/\lambda$
- Single crystal is rotated





B.D. Cullity & S.R. Strock "Elements of X-ray Diffraction" (2014)

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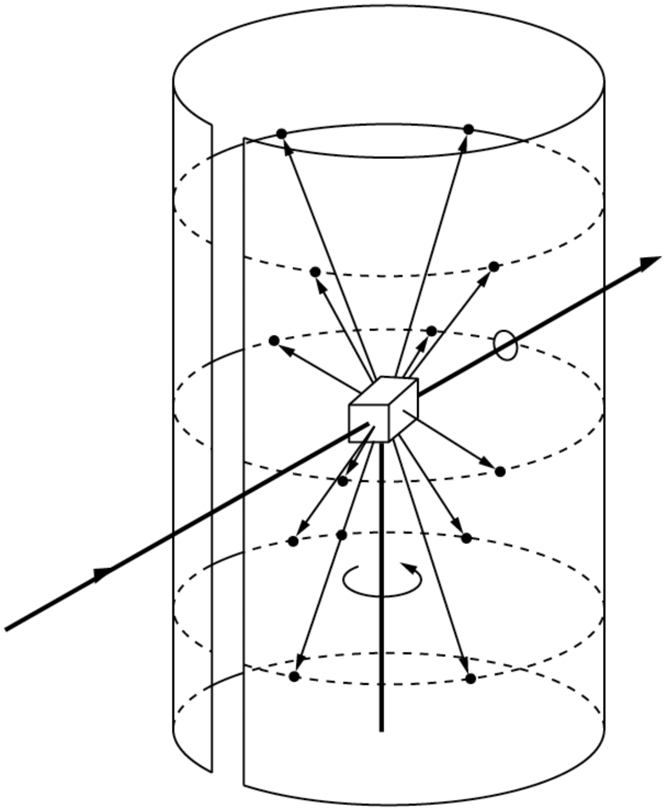
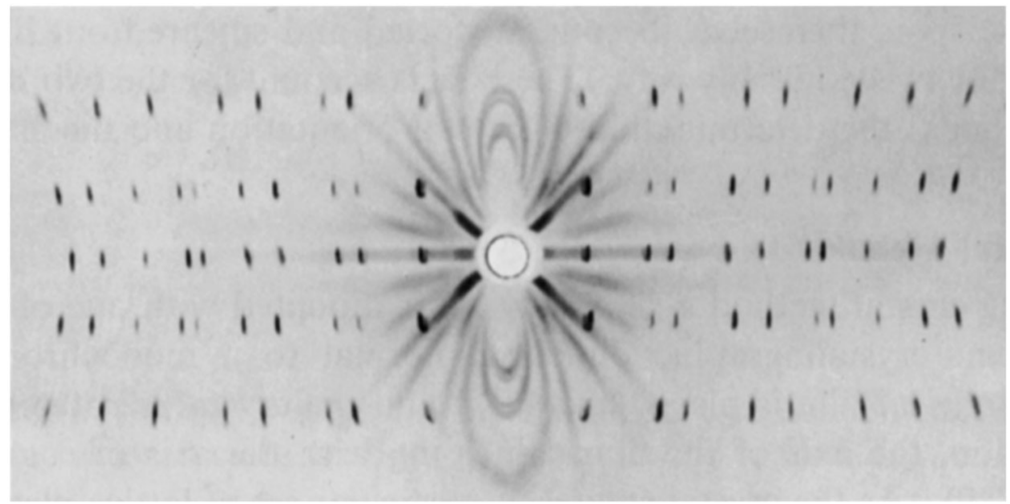


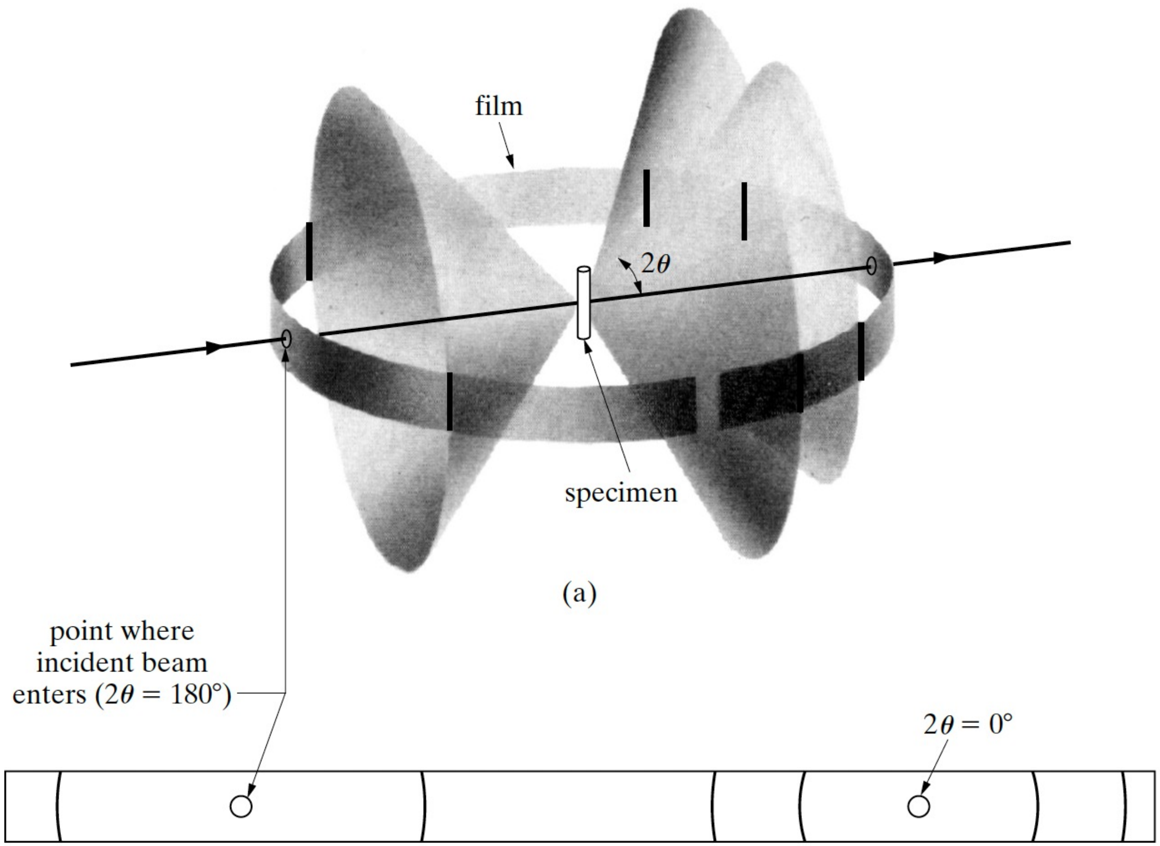


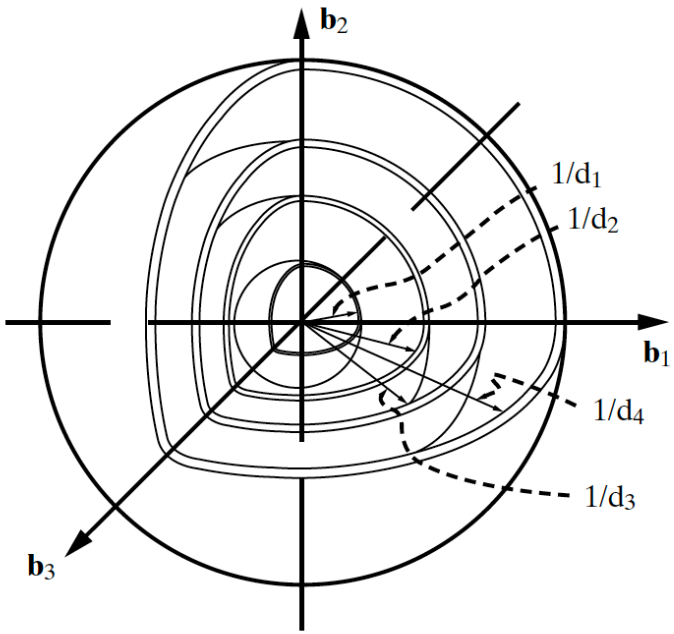
Rotating-crystal pattern of a quartz crystal (hexagonal) rotated about its c axis. Filtered copper radiation. (The streaks are due to the white radiation not removed by the filter.)

B.D. Cullity & S.R. Strock "Elements of X-ray Diffraction" (2014)

Powder method

- Monochromatic X-ray beam, $k = 2\pi/\lambda$
- Powder or polycrystalline sample

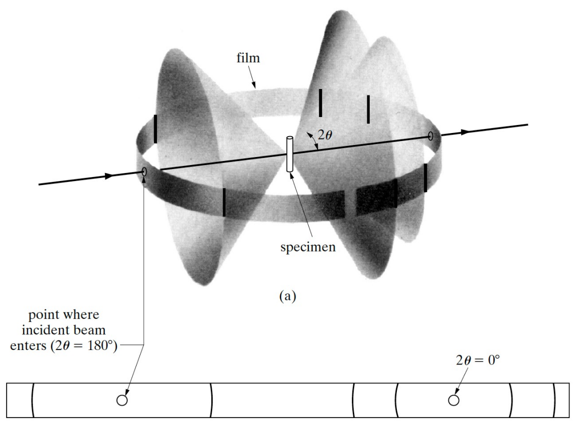


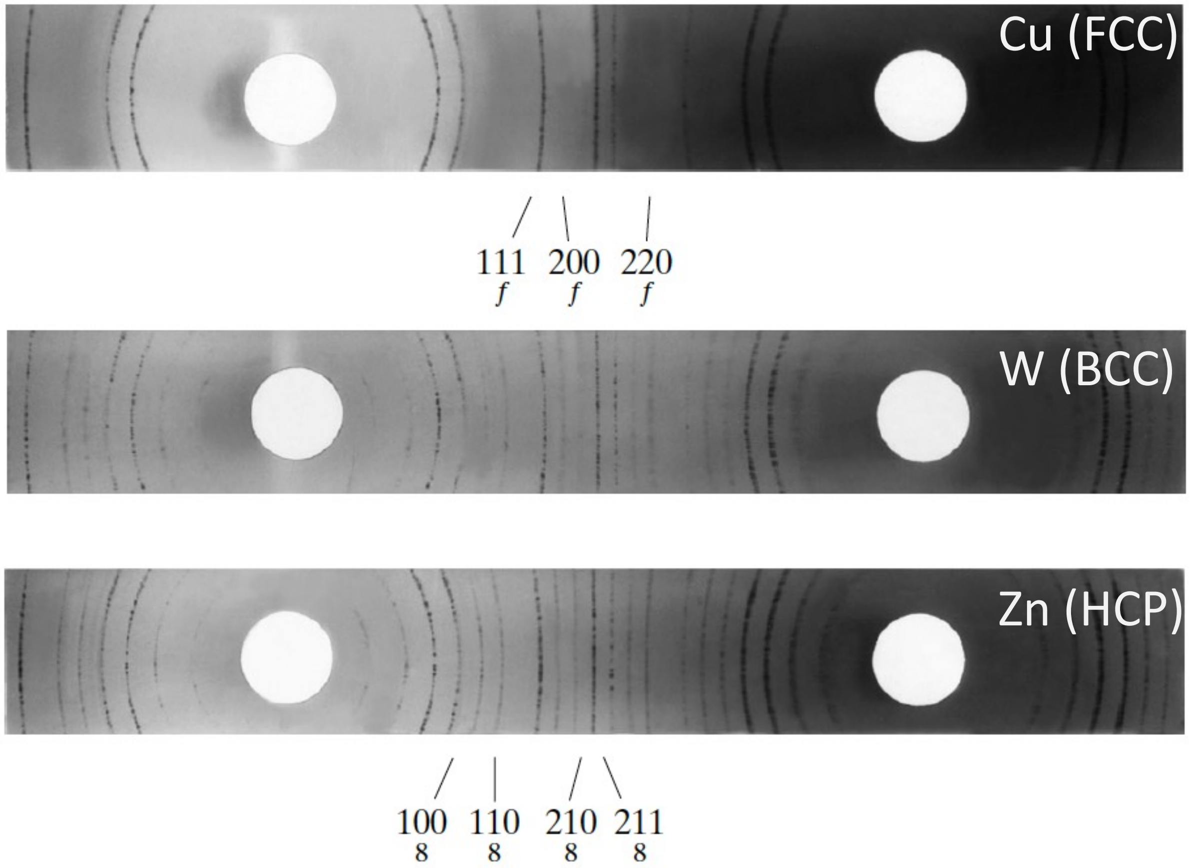


B.D. Cullity & S.R. Strock "Elements of X-ray Diffraction" (2014)

Powder method

- Monochromatic X-ray beam, $k = 2\pi/\lambda$
- Powder or polycrystalline sample

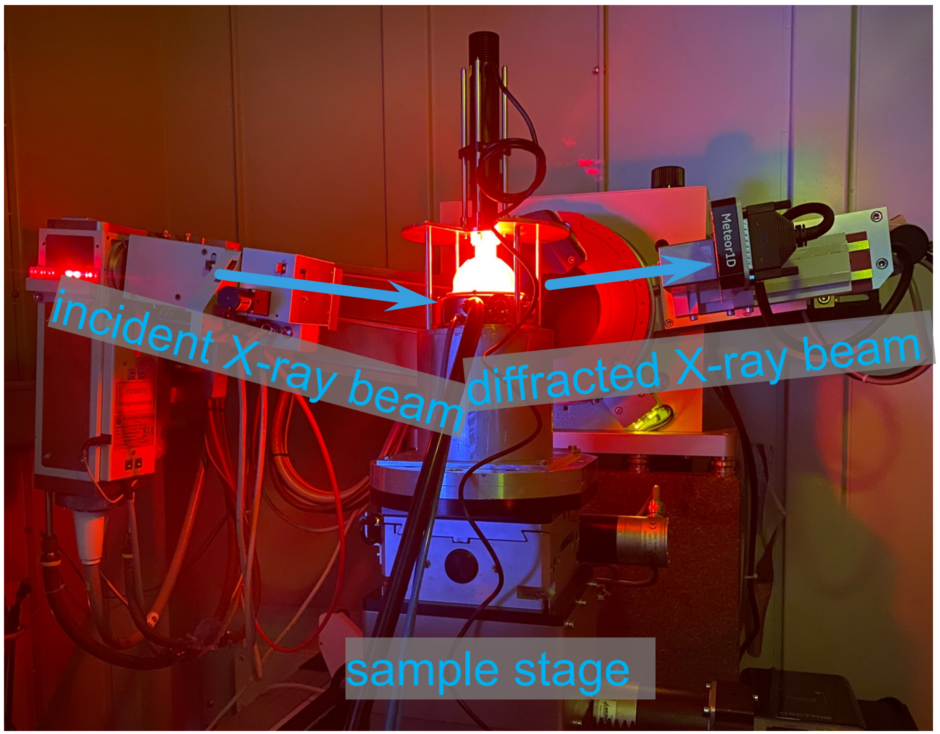




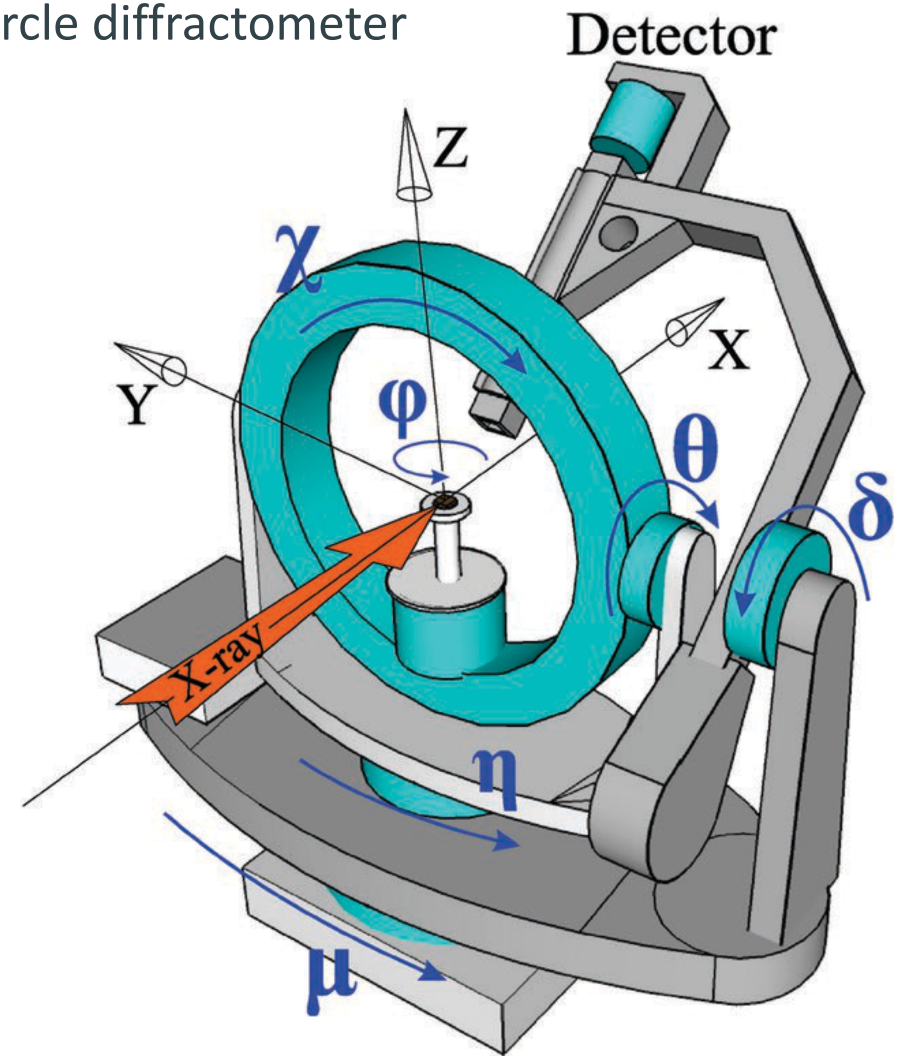
B.D. Cullity & S.R. Strock "Elements of X-ray Diffraction" (2014)

Scans in reciprocal space

Two-circle diffractometer



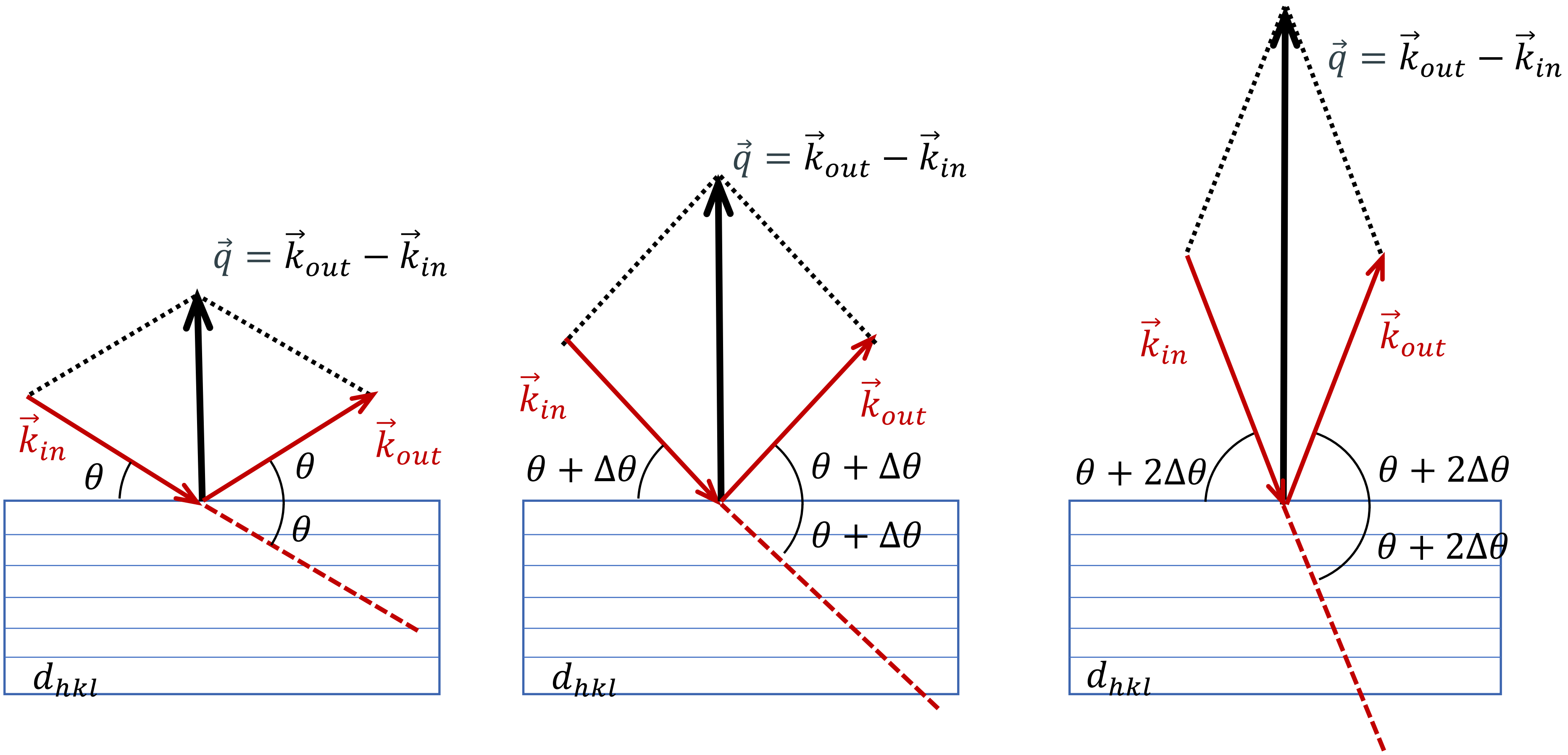
Six-circle diffractometer



D. Grigoriev et al., J. Appl. Cryst. ***49*** *961-967 (2016)*

Q-scan ($\theta - 2\theta$ scan)

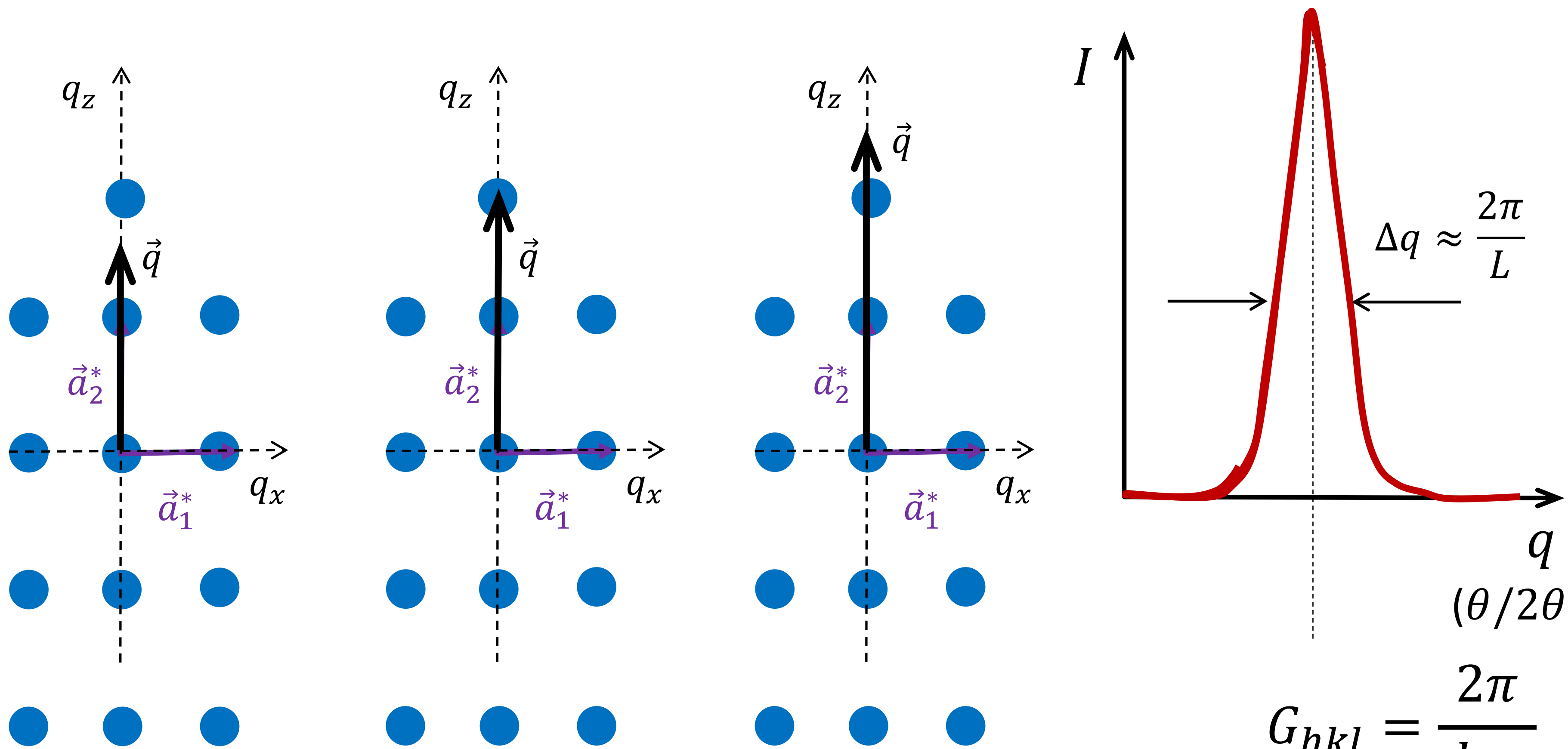
real space



Q-scan ($\theta - 2\theta$ scan)

reciprocal space

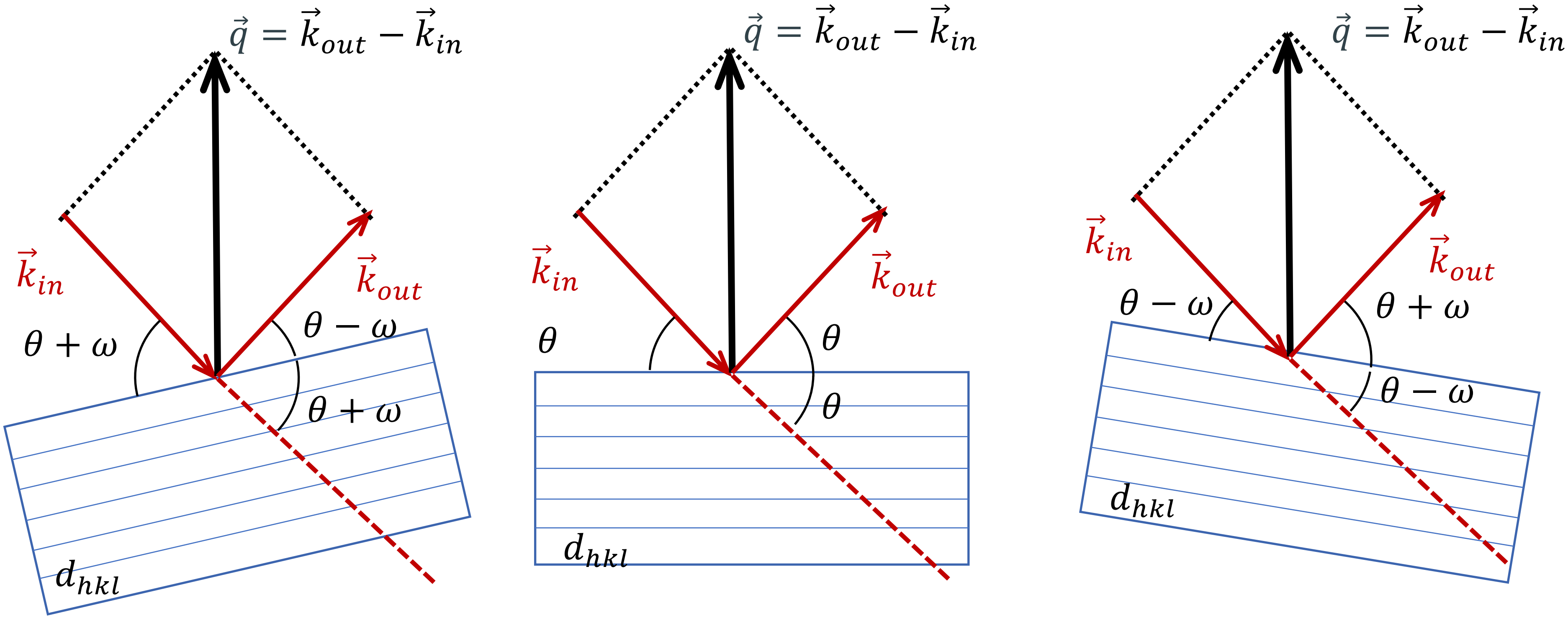
- Separation between planes
- Size of a single crystal domains



$$G_{hkl} = \frac{2\pi}{d_{hkl}}$$

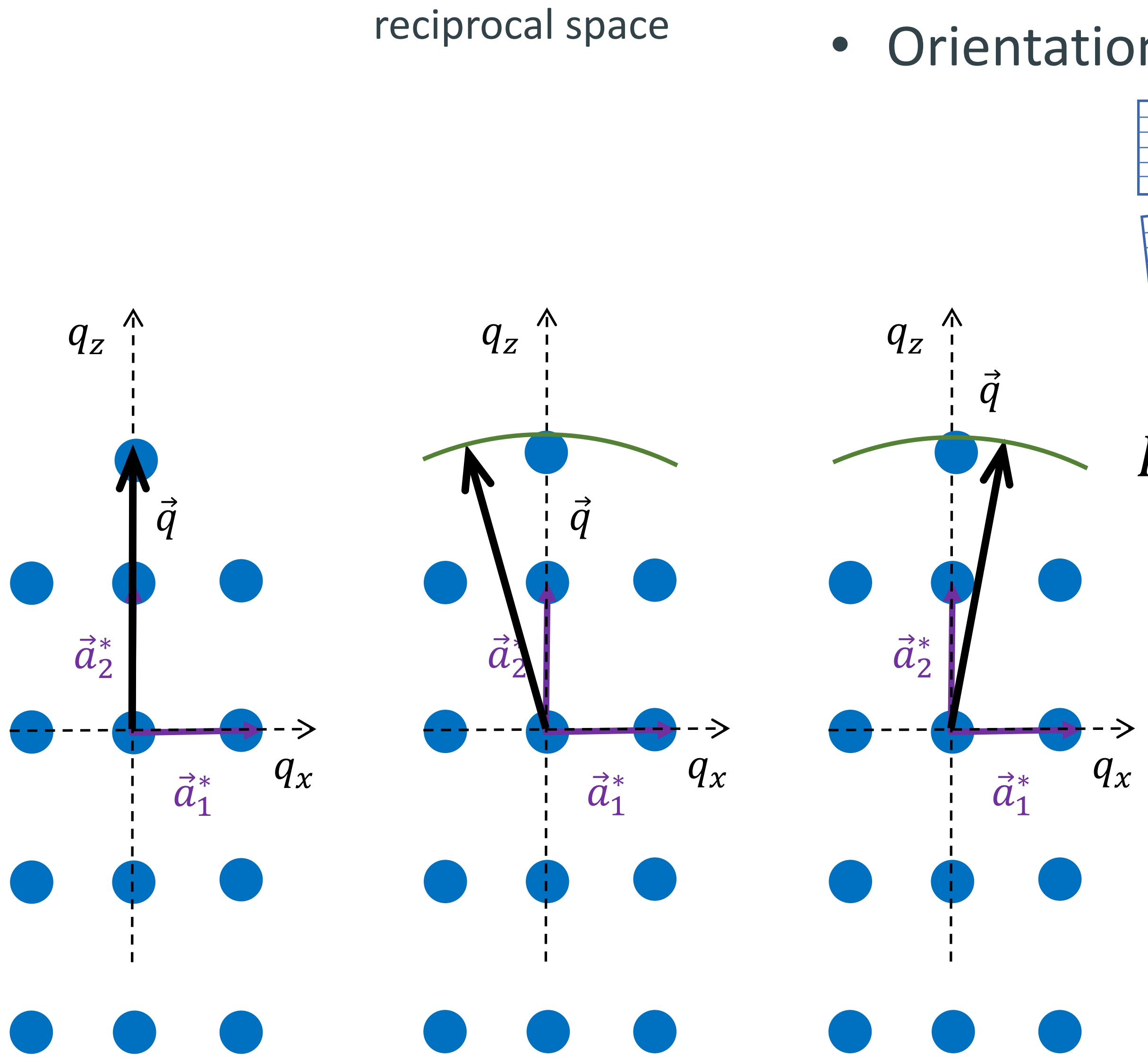
Rocking scan (θ scan, ω scan)

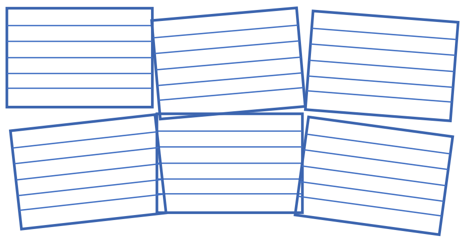
real space

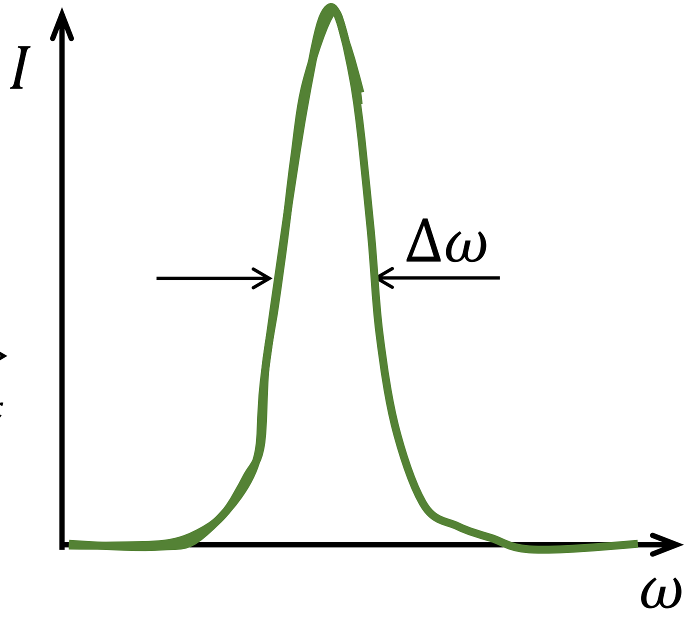


Rocking scan (θ scan, ω scan)

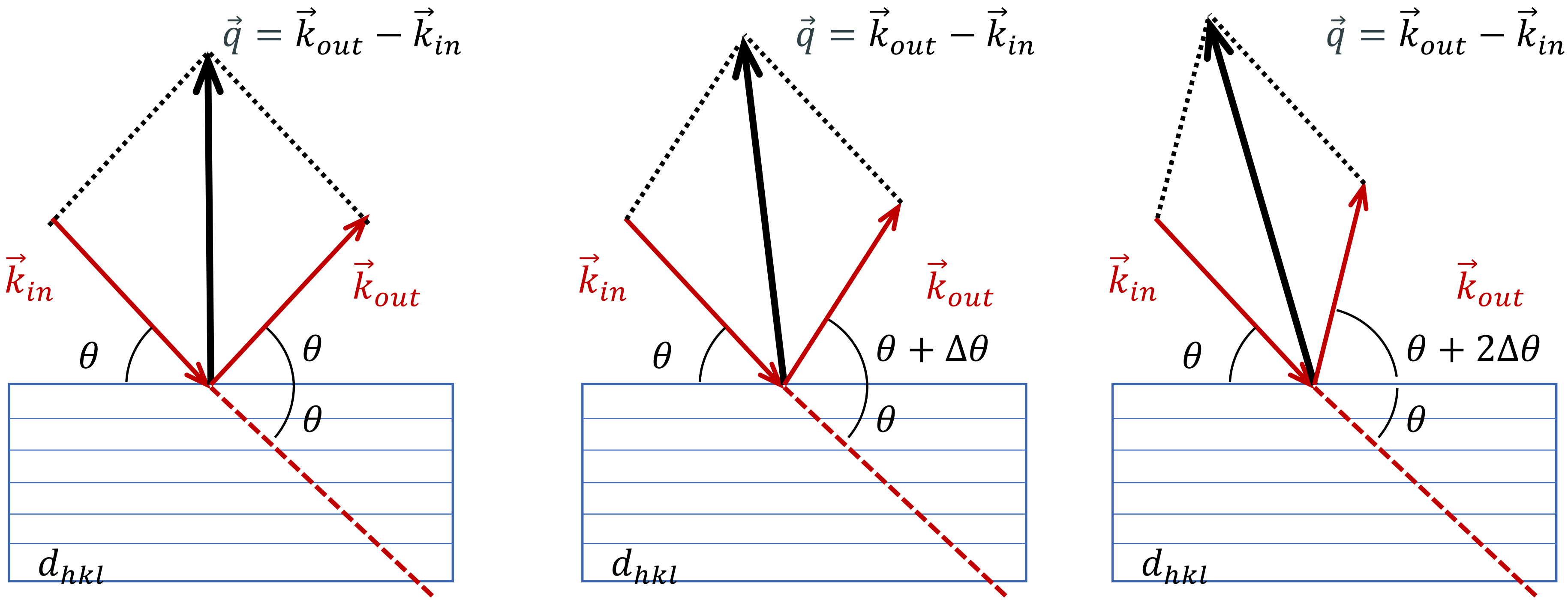
- Orientation of domains (mozaicity)







real space

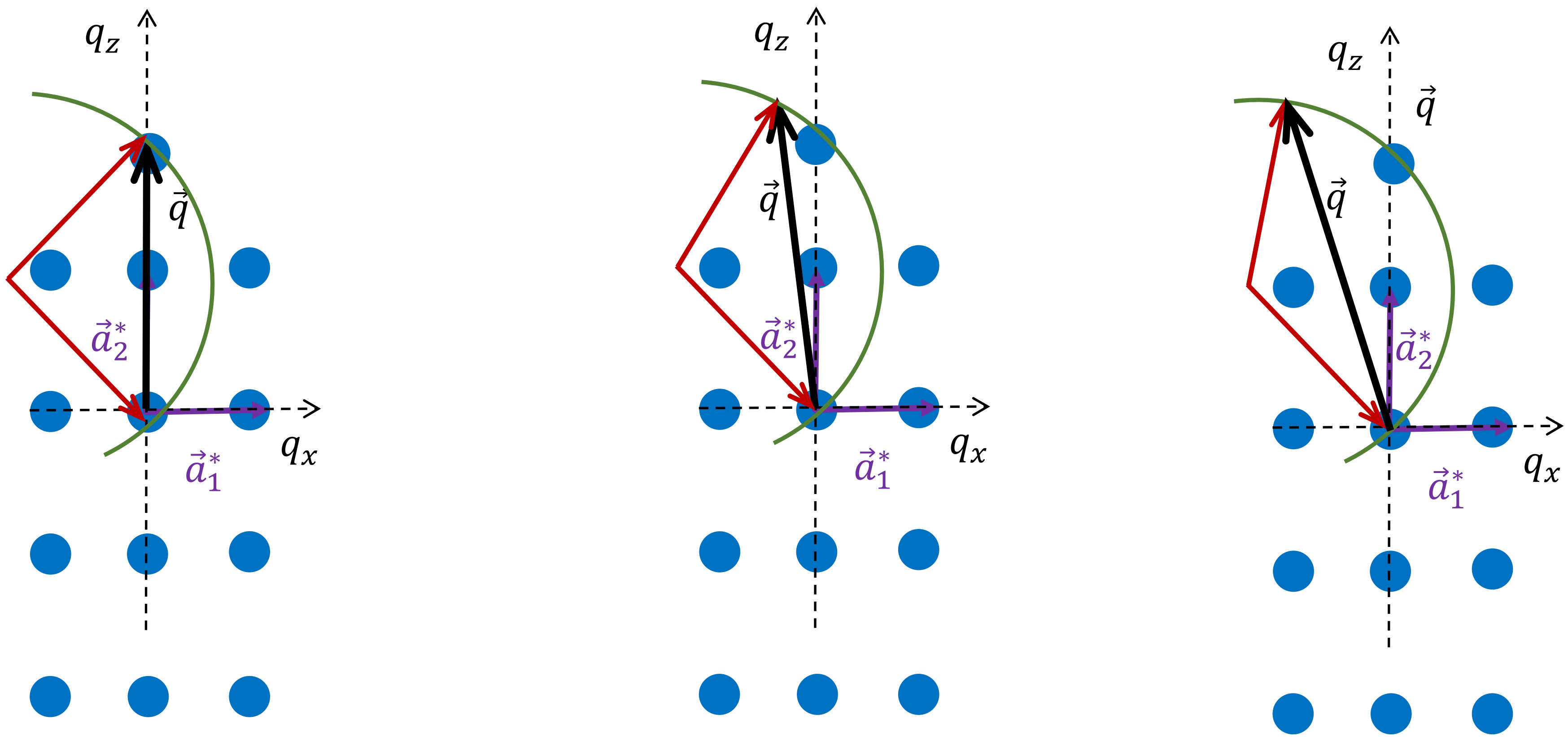


$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$
$\vec{k}_{in}$
$\vec{k}_{out}$
θ
θ
θ
d_{hkl}
$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$
$\vec{k}_{in}$
$\vec{k}_{out}$
θ
$\theta + \Delta\theta$
θ
d_{hkl}
$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$
$\vec{k}_{in}$
$\vec{k}_{out}$
θ
$\theta + 2\Delta\theta$
θ
d_{hkl}

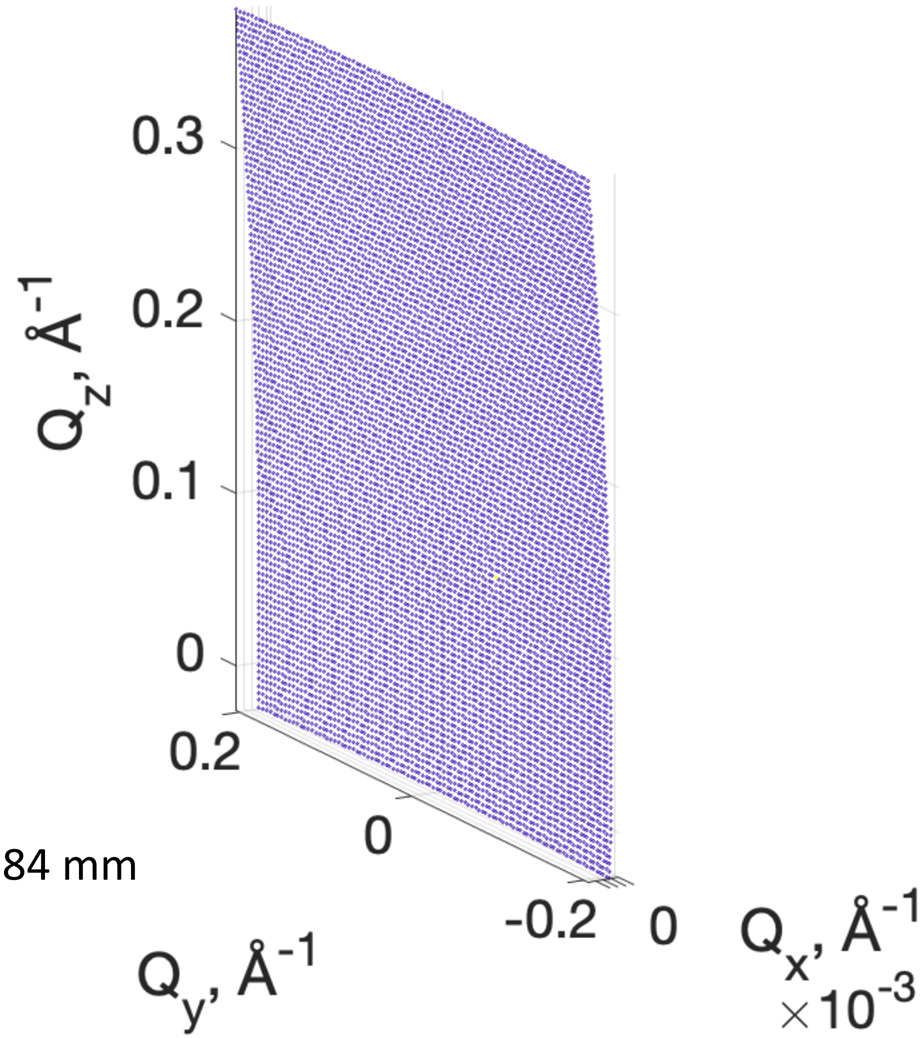
Rocking scan (θ scan, ω scan)

- Cross section of reciprocal space with Ewald sphere

reciprocal space

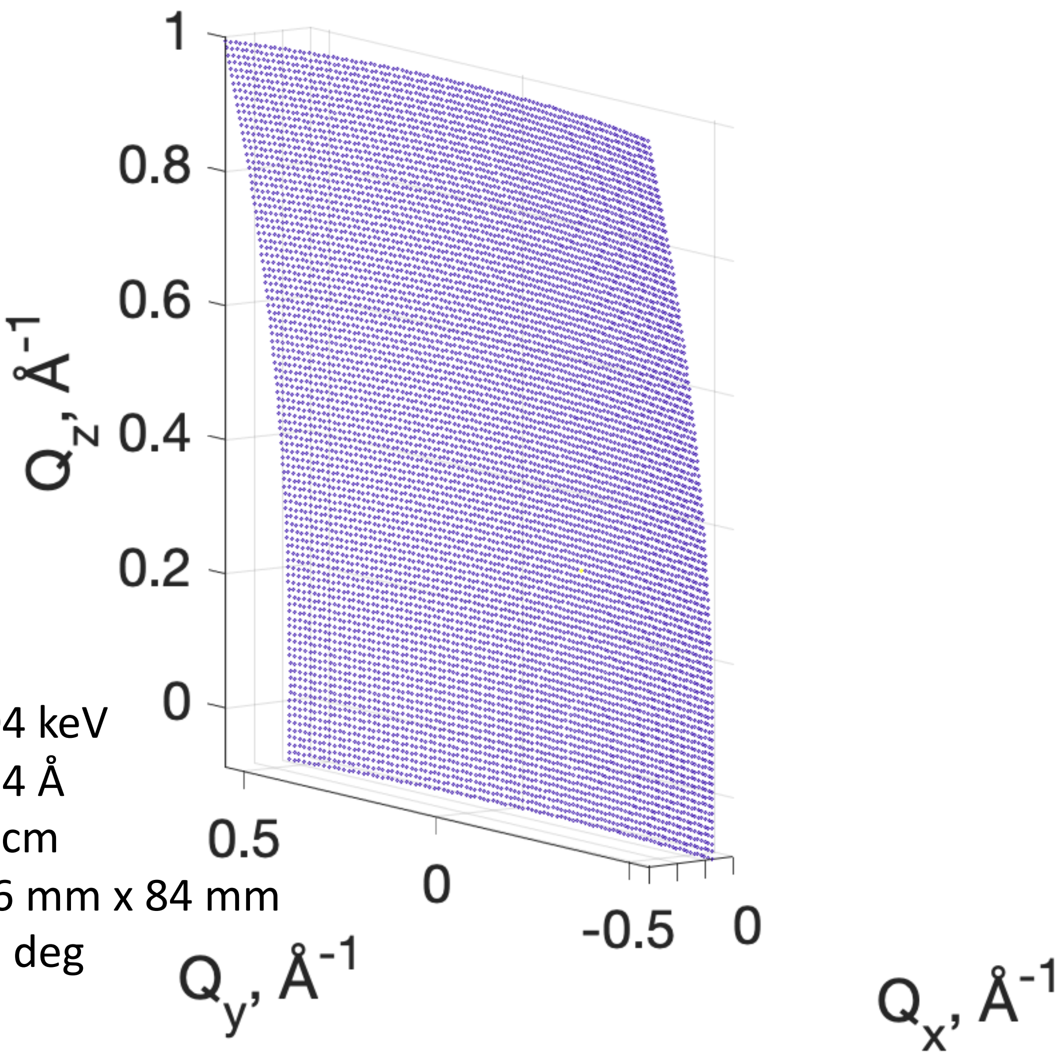


Our GIWAXS setup



- Energy (E): 8.04 keV
- Wavelength (λ): 1.54 Å
- Sample-detector distance (L): 100 cm
- Size of Pilatus 300K detector: 106 mm x 84 mm
- Incident angle (α_i): 0.5 deg

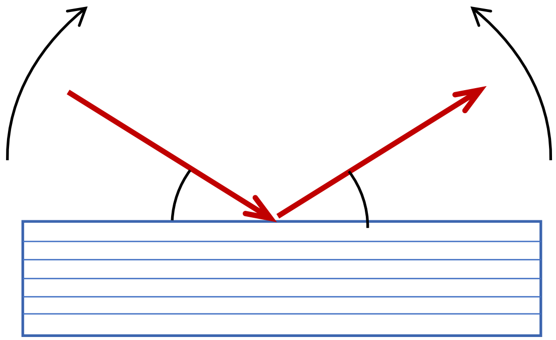
Our GIWAXS setup



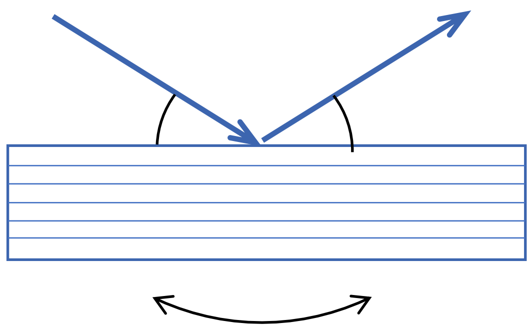
- Energy (E): 8.04 keV
- Wavelength (λ): 1.54 Å
- Sample-detector distance (L): 37 cm
- Size of Pilatus 300K detector: 106 mm x 84 mm
- Incident angle (α_i): 0.5 deg

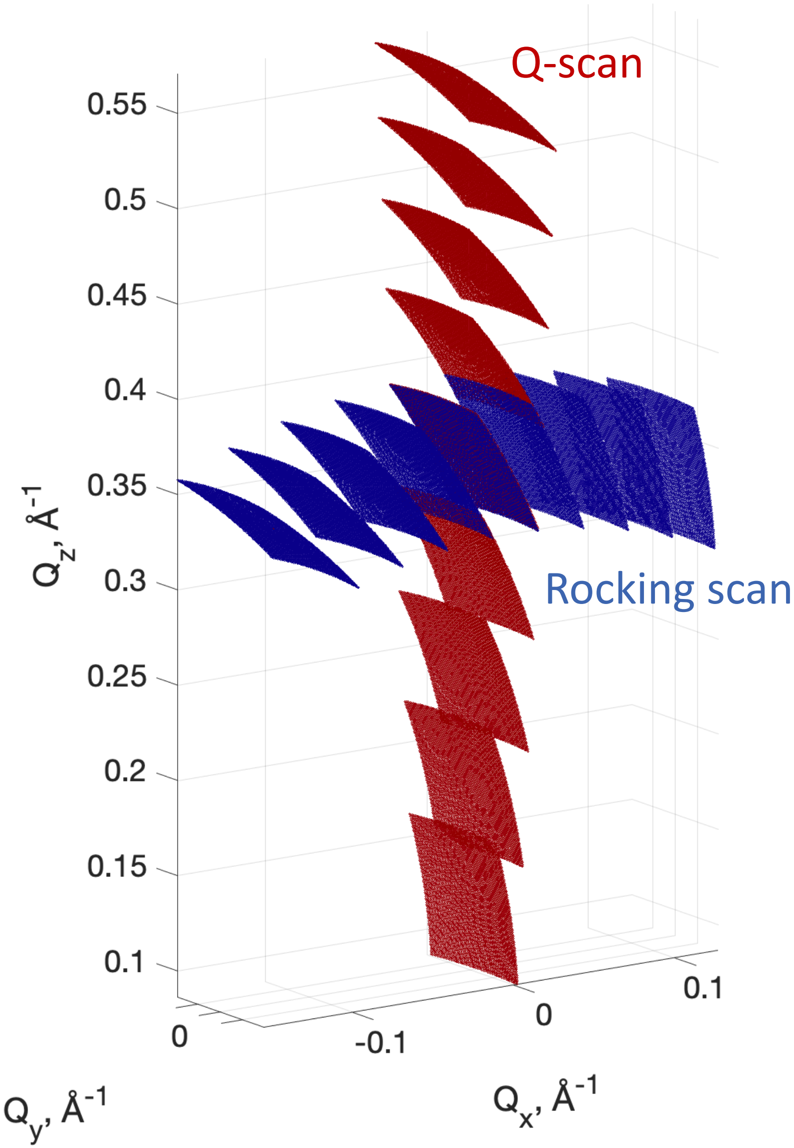
Different scans with a 2D detector

Q-scan



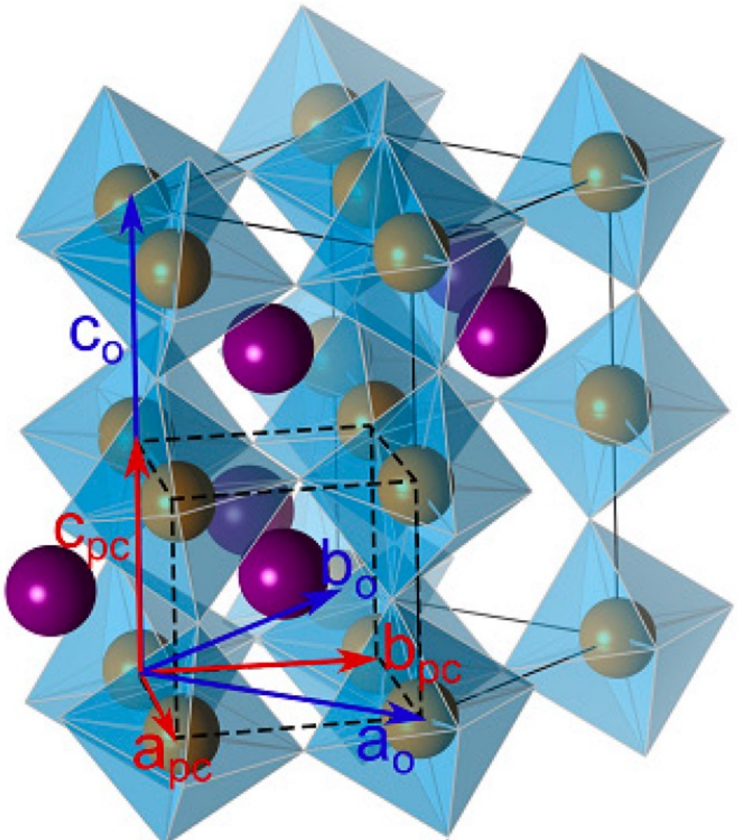
Rocking scan





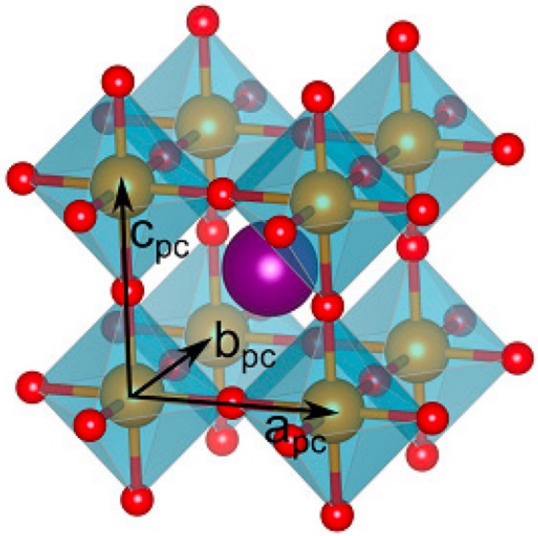
Pseudocubic lattice

Orthorhombic unit cell of $SmNiO_3$



$$a_o = 5.3283\ \text{Å}$$
$$b_o = 5.4374\ \text{Å}$$
$$c_o = 7.5675\ \text{Å}$$
$$\alpha = \beta = \gamma = 90°$$

Pseudocubic unit cell

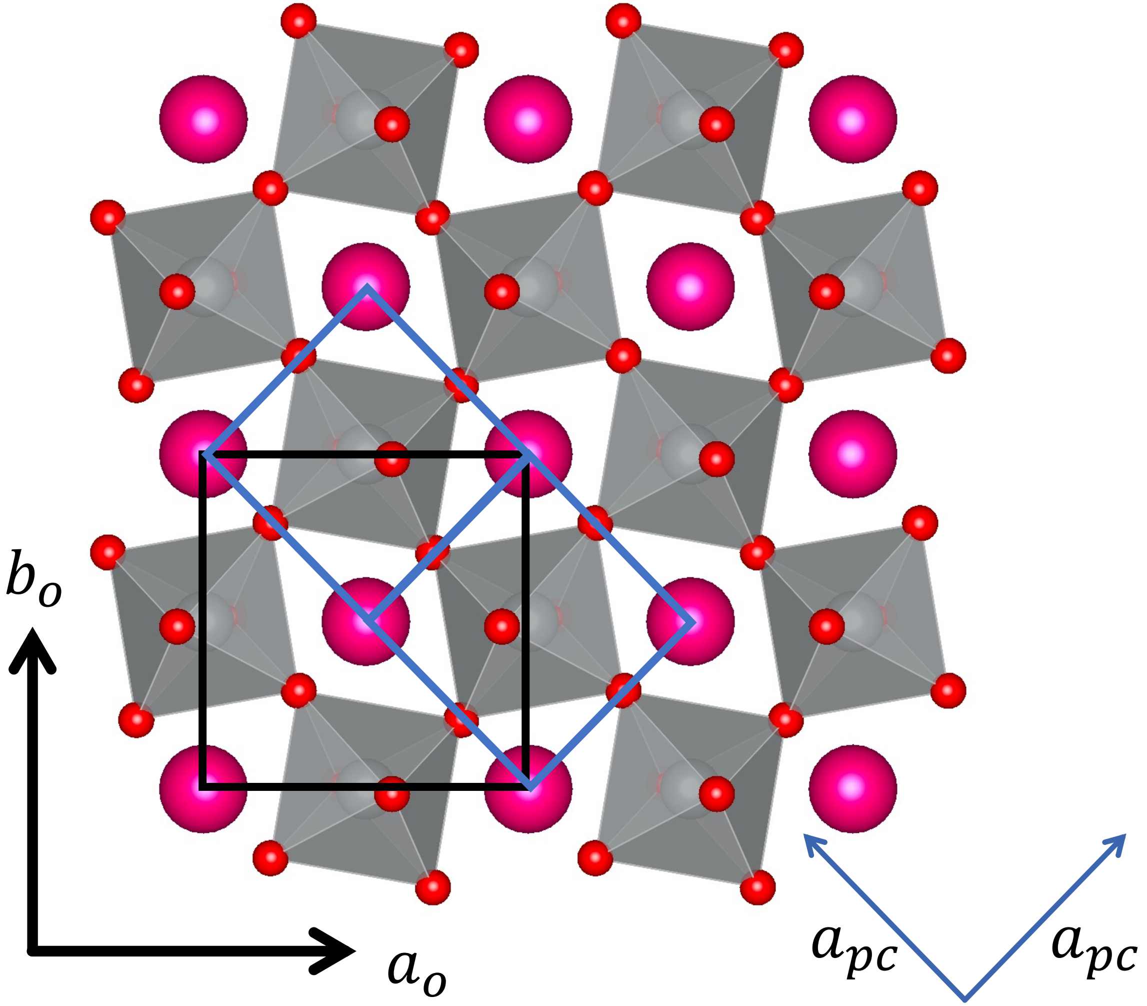


$$a_{pc} = b_{pc} = 3.806\ \text{Å}$$
$$c_{pc} = 3.784\ \text{Å}$$
$$\alpha = \beta = 90°$$
$$\gamma = 88.84° \approx 90°$$

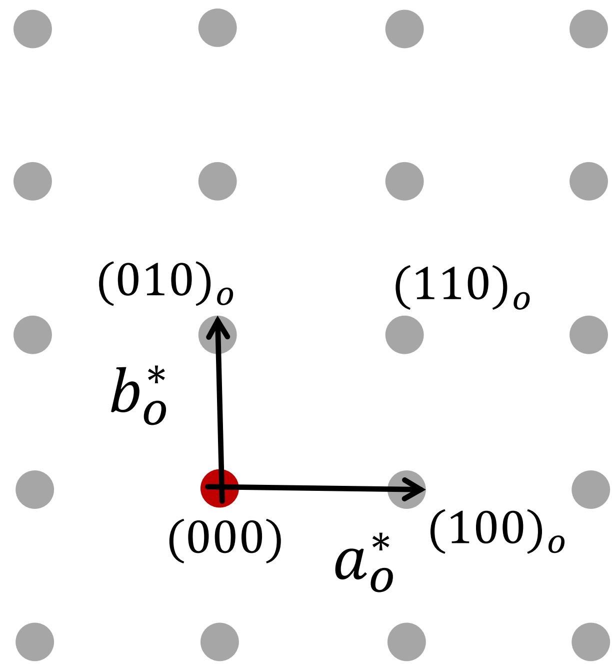
S. Catalano et al., Rep. Prog. Phys., ***81*** *046501 (2018)*

Pseudocubic lattice

Real space

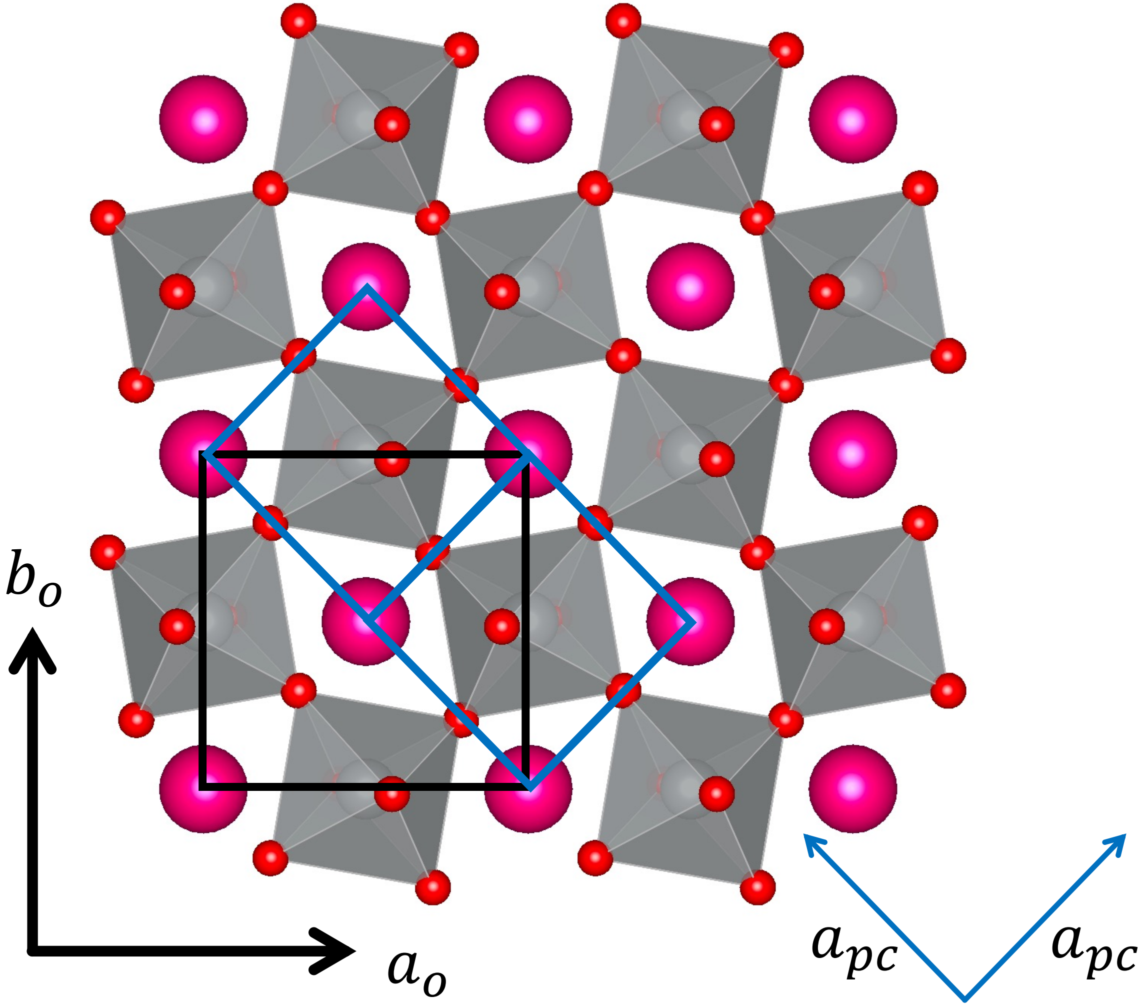


Reciprocal space

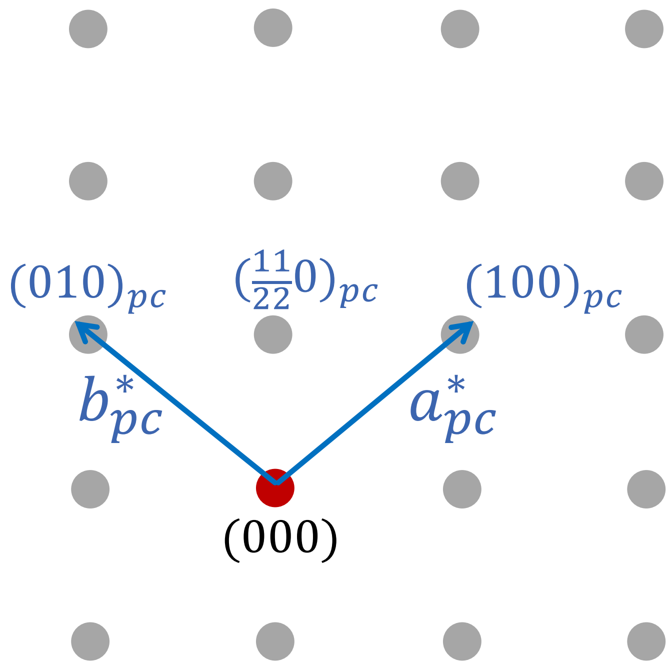


Pseudocubic lattice

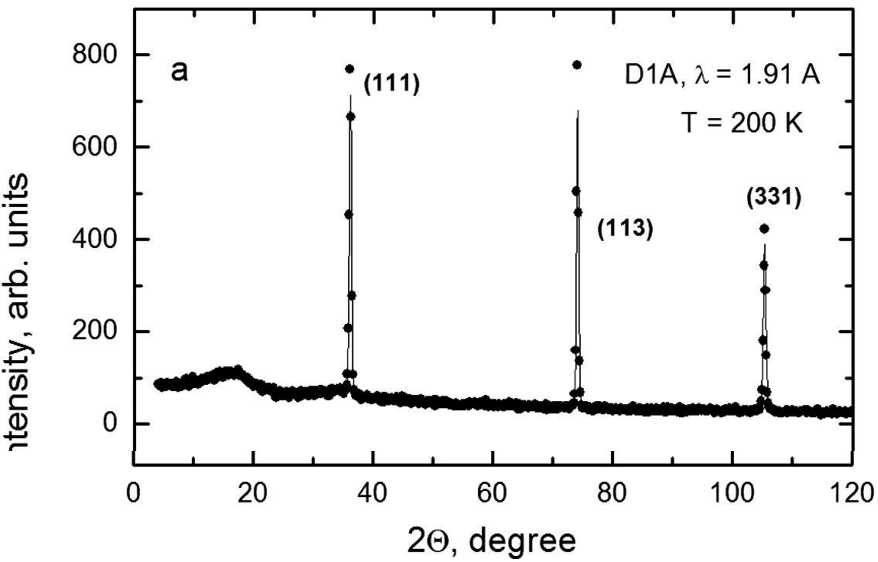
Real space

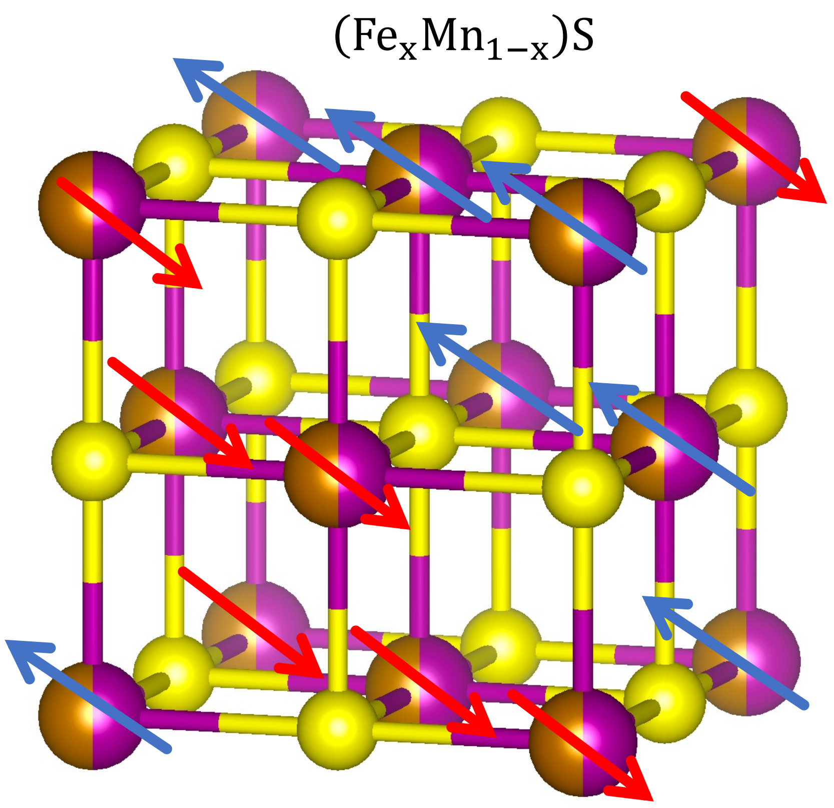


Reciprocal space



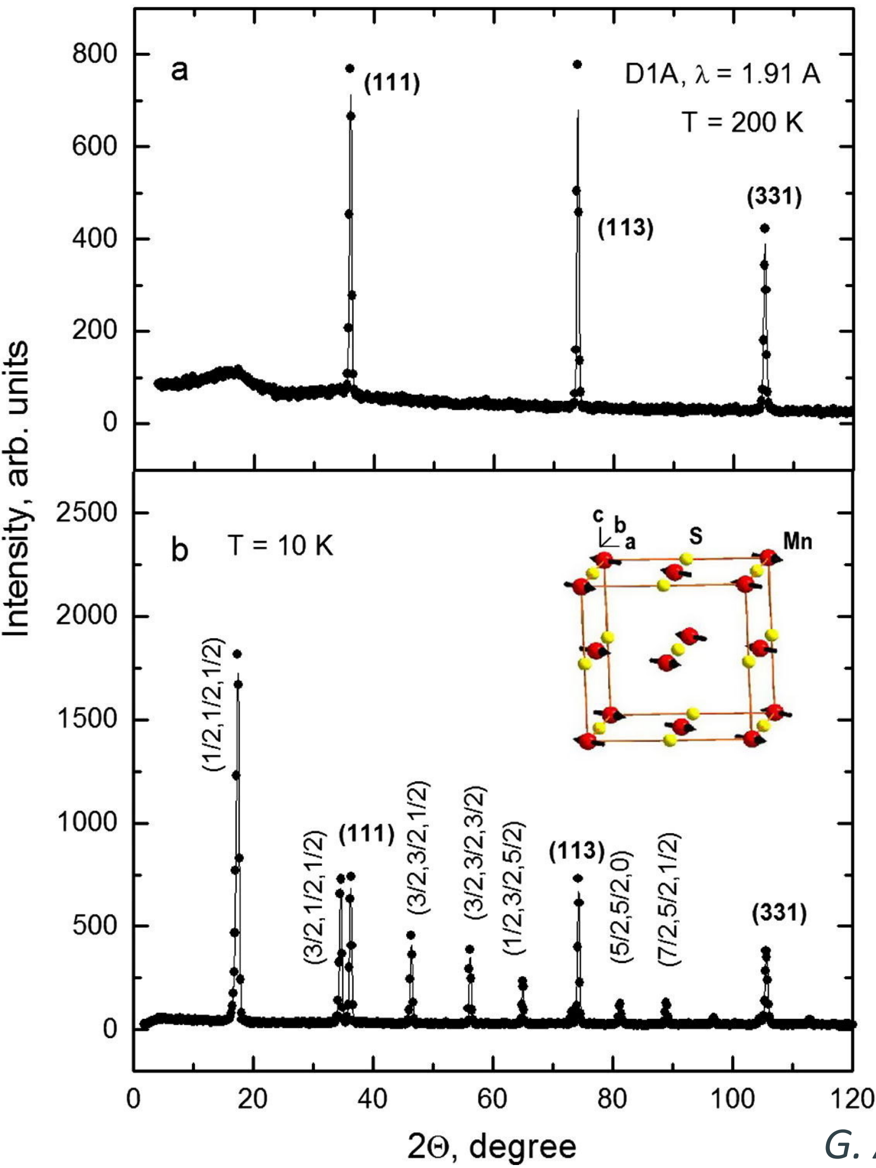
Doubling of the unit cell



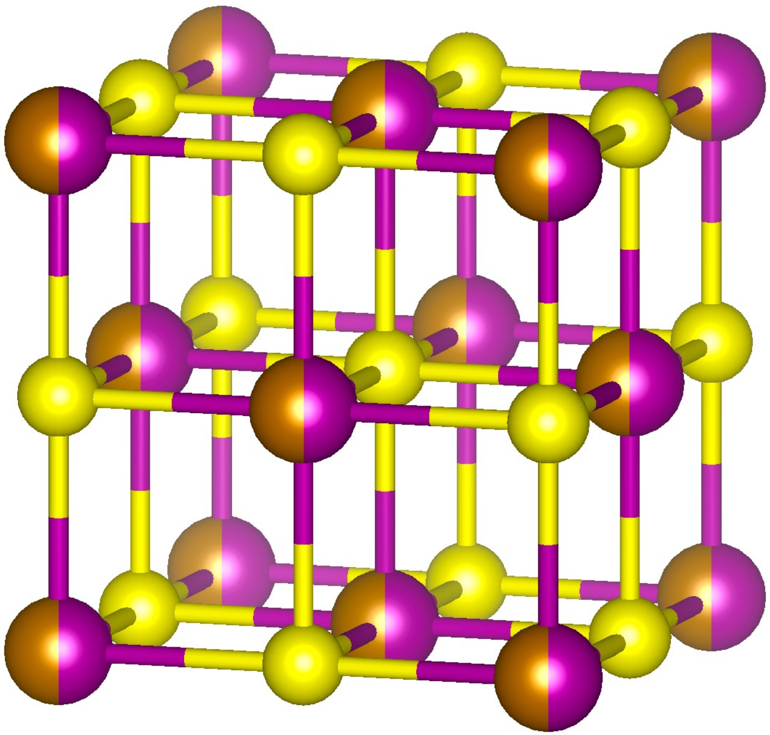


G. Abramova et al. / J. Alloys Compd. 632 563–567 (2015)

Doubling of the unit cell



$(Fe_x Mn_{1-x})S$

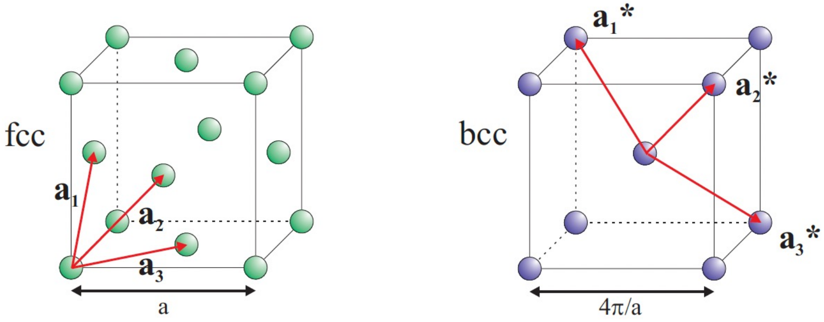


Neutrons are sensitive to magnetic moment

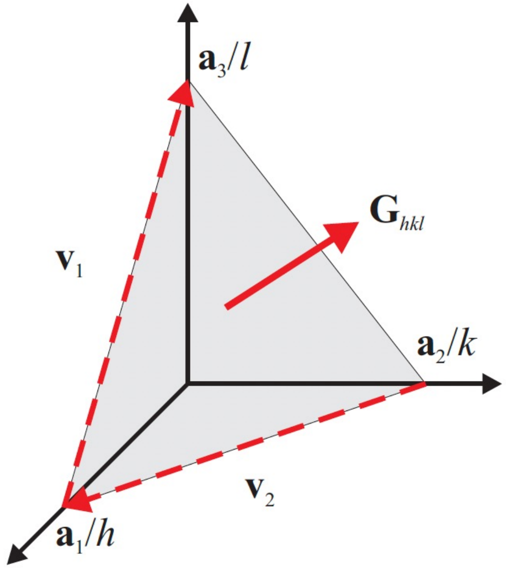
G. Abramova et al. / J. Alloys Compd. 632 563–567 (2015)

What to remember

- Reciprocal lattice and real lattice are related by Fourier transform



- The set of parallel crystal planes (hkl) uniquely determine the reciprocal lattice vector $\vec{G}_{hkl}$



- Bragg peaks correspond to constructive interference of the scattered waves