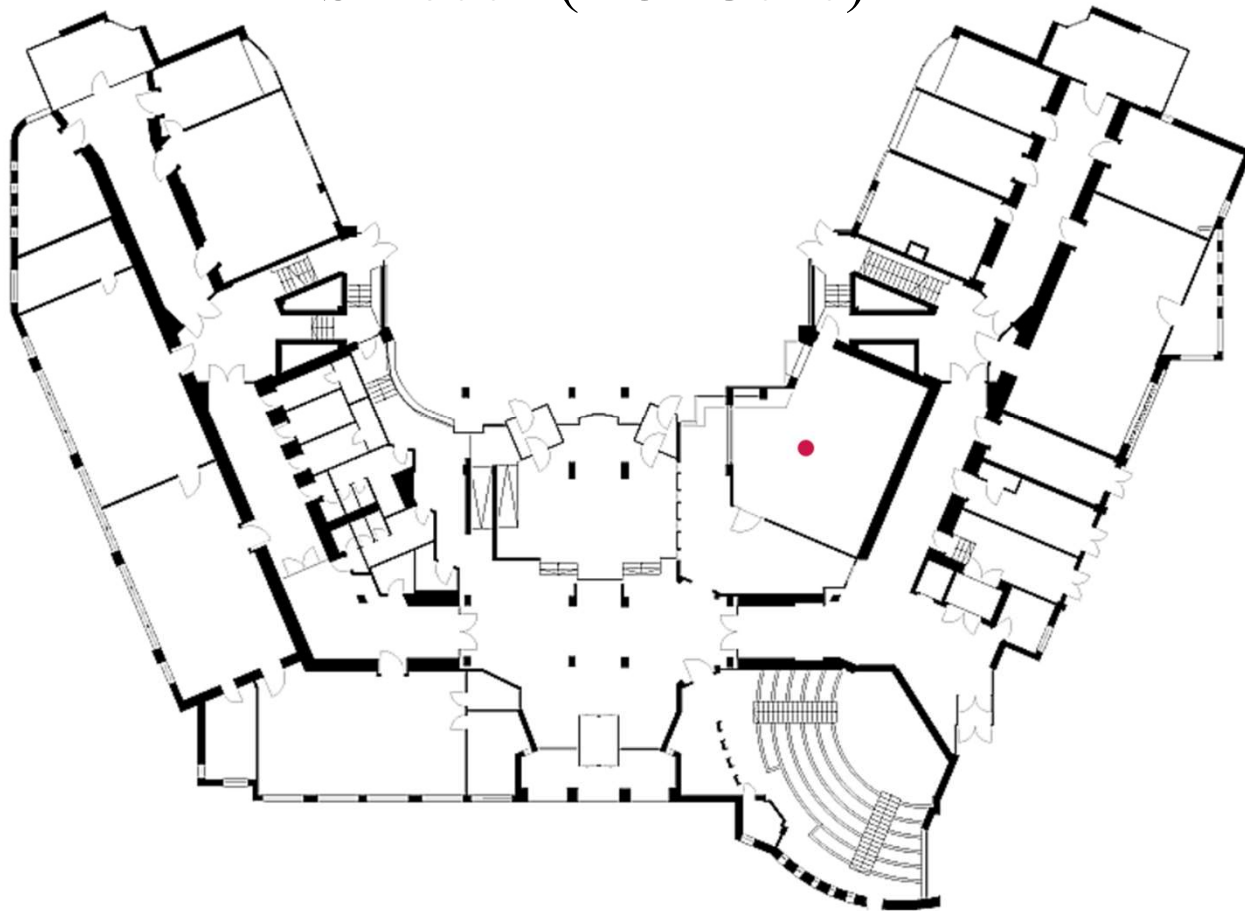


Diffraction

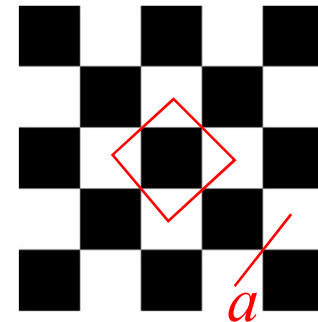
Tuesday 25, October

SR 6001 (BCEG010)



Determine the Fourier coefficients

$$f_{\vec{G}} = \frac{C}{a^2} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \exp(-i\vec{G} \cdot \vec{r}) dx dy$$



$$f_{\vec{G}} = \frac{C}{a^2} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \exp(-iG_x x) \exp(-iG_y y) dx dy$$

$$f_{\vec{G}} = \frac{C}{a^2} \frac{\left(\exp(-iG_x \sqrt{2}a/4) - \exp(iG_x \sqrt{2}a/4) \right) \left(\exp(-iG_y \sqrt{2}a/4) - \exp(iG_y \sqrt{2}a/4) \right)}{-G_x G_y}$$

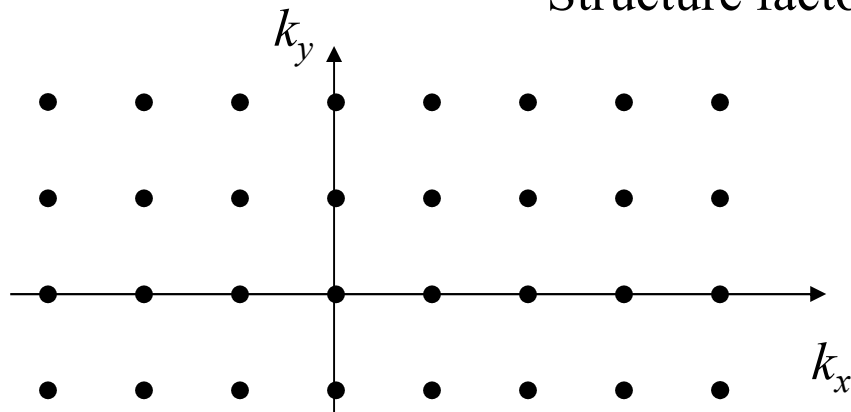
$$f_{\vec{G}} = \frac{4C}{a^2} \frac{\sin(G_x \sqrt{2}a/4) \sin(G_y \sqrt{2}a/4)}{G_x G_y}$$

Reciprocal lattice (Reziprokes Gitter)

Any periodic function can be written as a Fourier series

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$$

\uparrow Structure factor \nwarrow Reciprocal lattice vector G



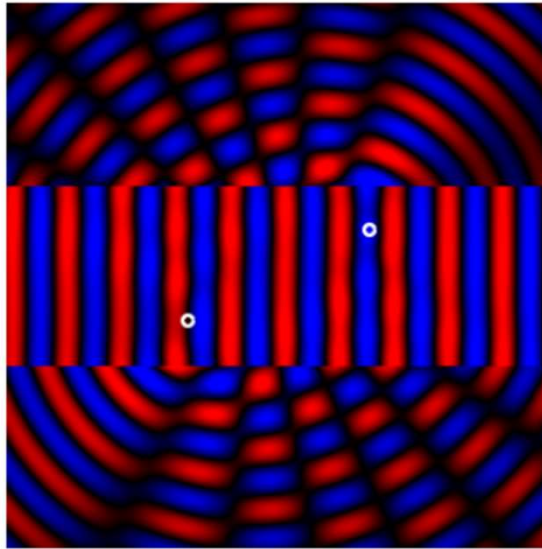
$$\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$$

v_i integers

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

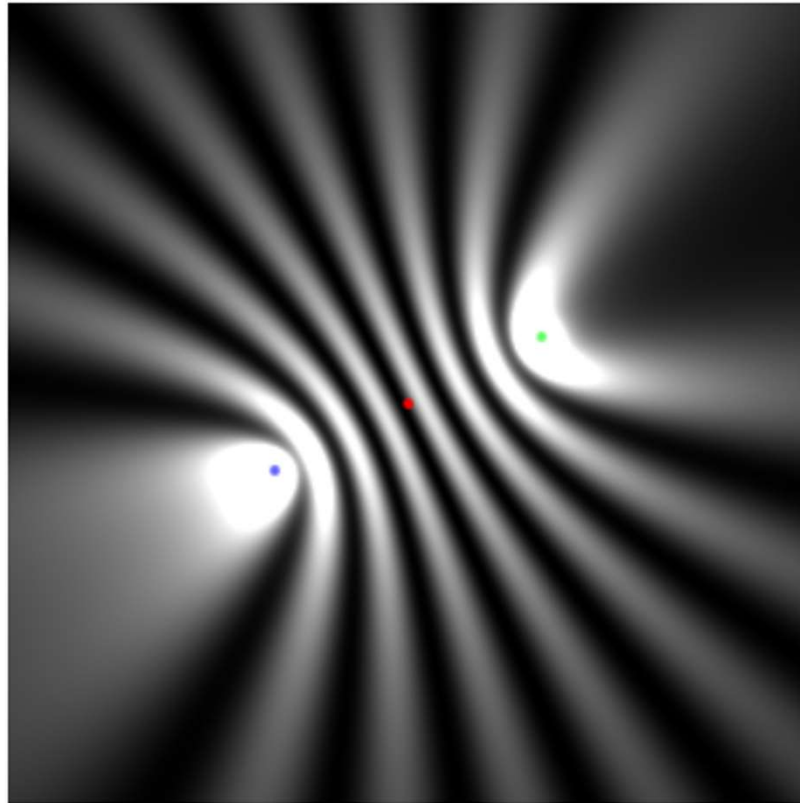
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Intensity of the scattered waves



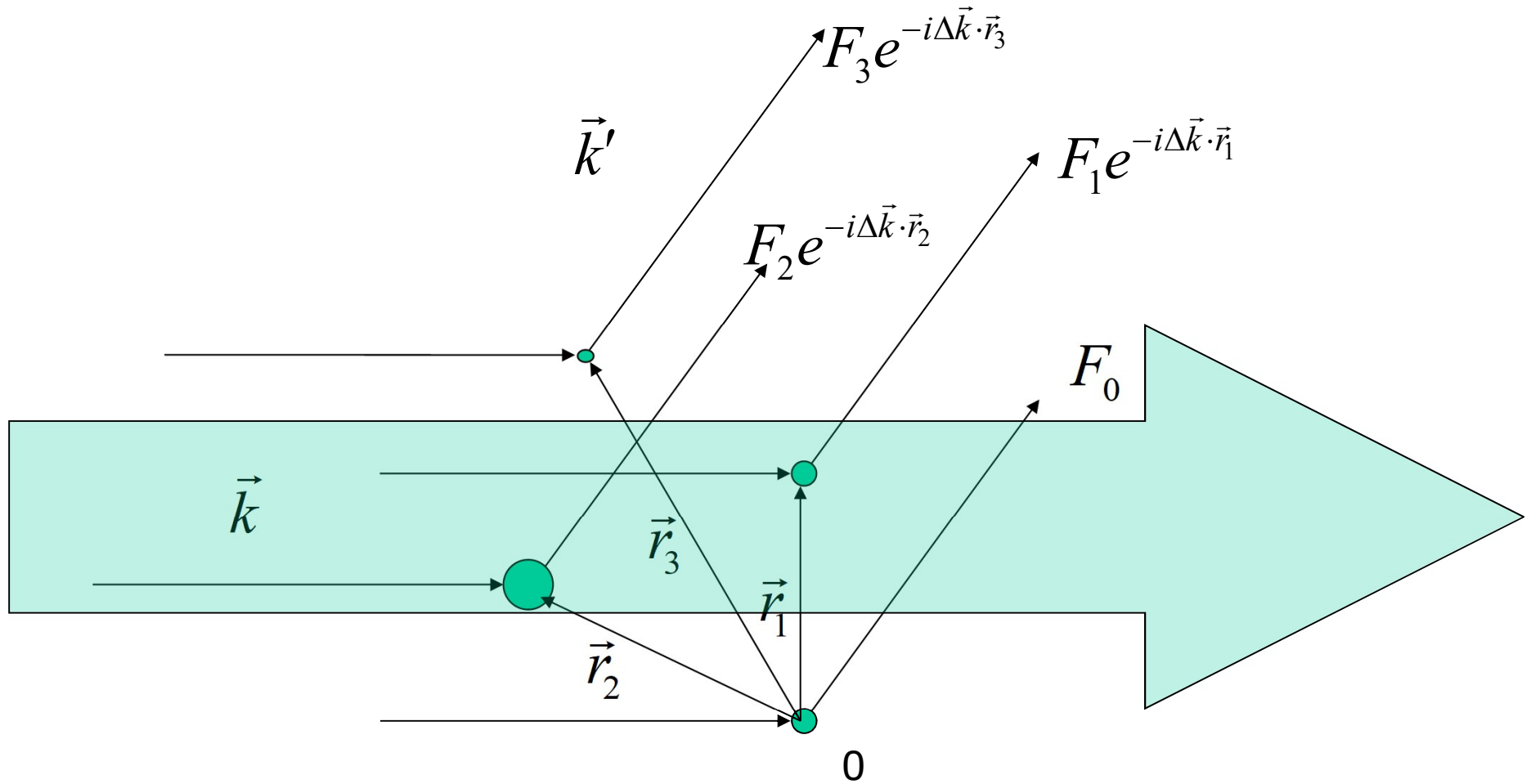
$$F_1 \frac{\cos(k|\vec{r} - \vec{r}_1| - \omega t + kx_1)}{\sqrt{|\vec{r} - \vec{r}_1|}} + F_2 \frac{\cos(k|\vec{r} - \vec{r}_2| - \omega t + kx_2)}{\sqrt{|\vec{r} - \vec{r}_2|}}.$$

Intensity of the scattered waves



$$\left(\frac{F_1}{\sqrt{|\vec{r} - \vec{r}_1|}} e^{i(k|\vec{r} - \vec{r}_1| + kx_1)} + \frac{F_2}{\sqrt{|\vec{r} - \vec{r}_2|}} e^{i(k|\vec{r} - \vec{r}_2| + kx_2)} \right) e^{-i\omega t}$$

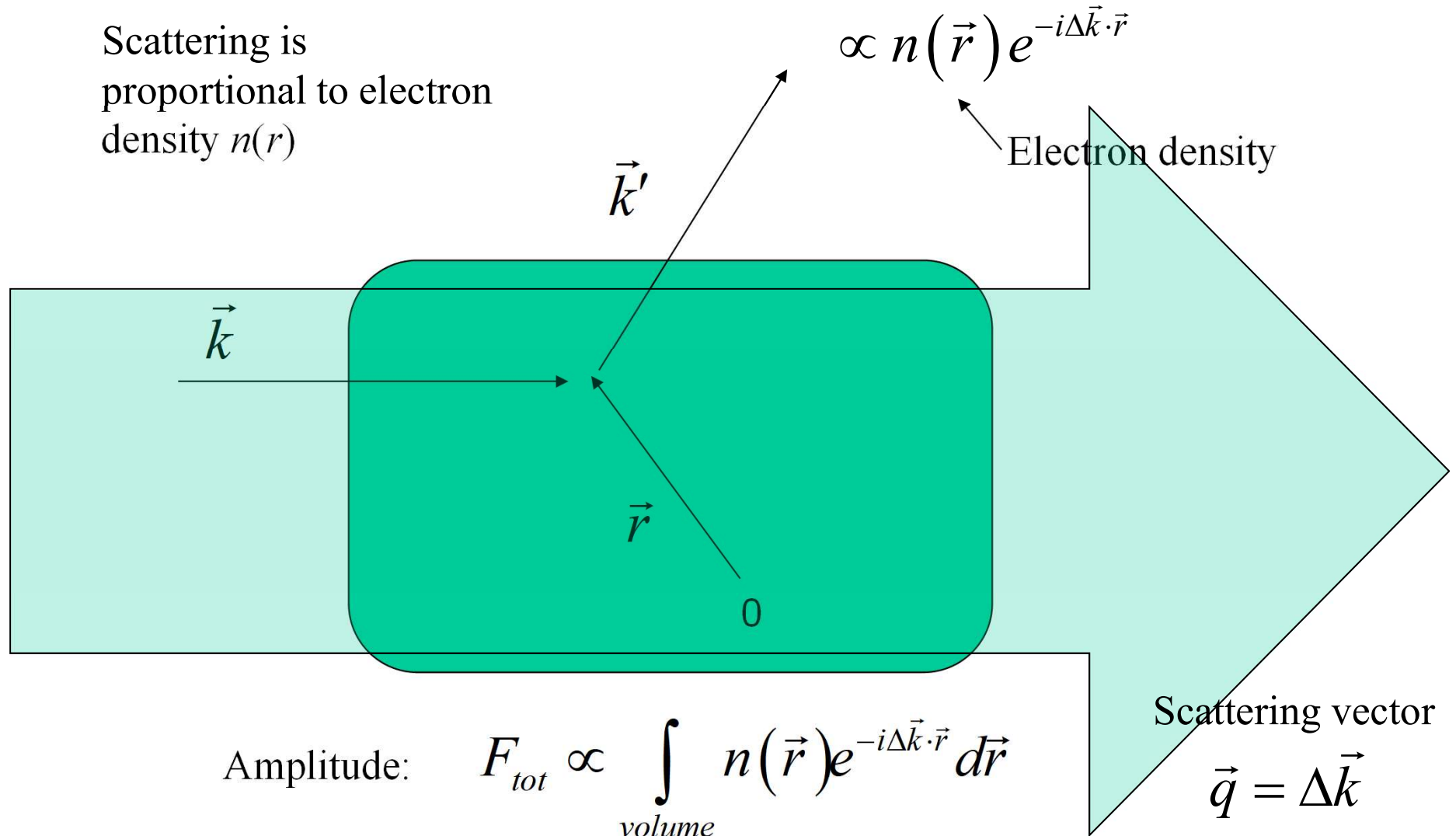
Interference



Amplitude:
$$F_{tot} = \sum_i F_i e^{-i\Delta \vec{k} \cdot \vec{r}_i}$$

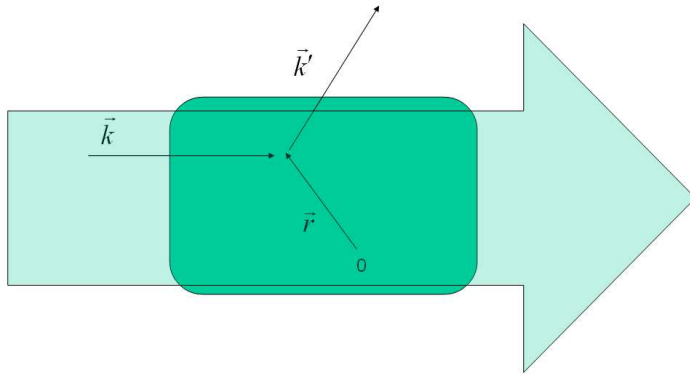
Interference

Scattering is
proportional to electron
density $n(r)$



The scattering amplitude is proportional to the Fourier transform of the electron density.

Scattering amplitude



$$F \propto \int n(\vec{r}) \exp(-i\Delta\vec{k} \cdot \vec{r}) dV$$

expand $n(r)$ in a Fourier series

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})$$

$$F \propto \sum_{\vec{G}} \int n_{\vec{G}} \exp(i(\vec{G} - \Delta\vec{k}) \cdot \vec{r}) dV$$

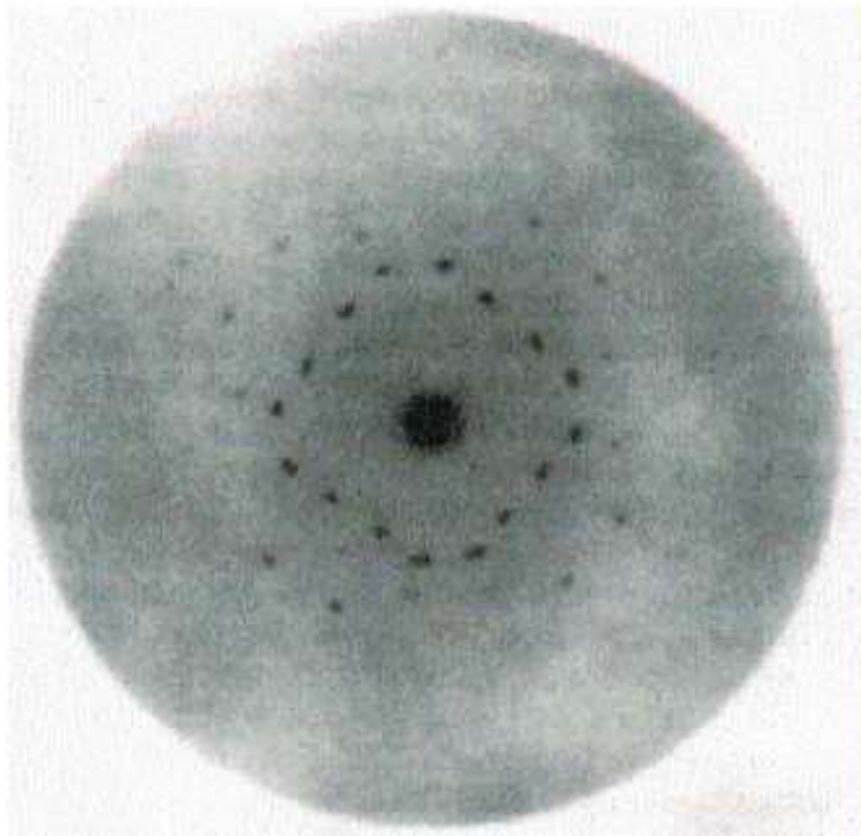
if $\vec{G} = \Delta\vec{k}$, all components add coherently

diffraction condition: $\boxed{\vec{G} = \Delta\vec{k}}$

The intensity of the peak at G is $|n_G|^2$

nobel prize 1914

first diffraction experiment of Max von Laue 1912
ZnS single crystal, exposure time 30'
the 5th diffraction pattern

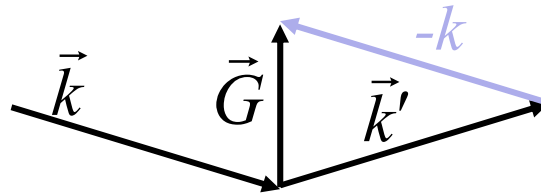


M. von Laue (1879-1960)

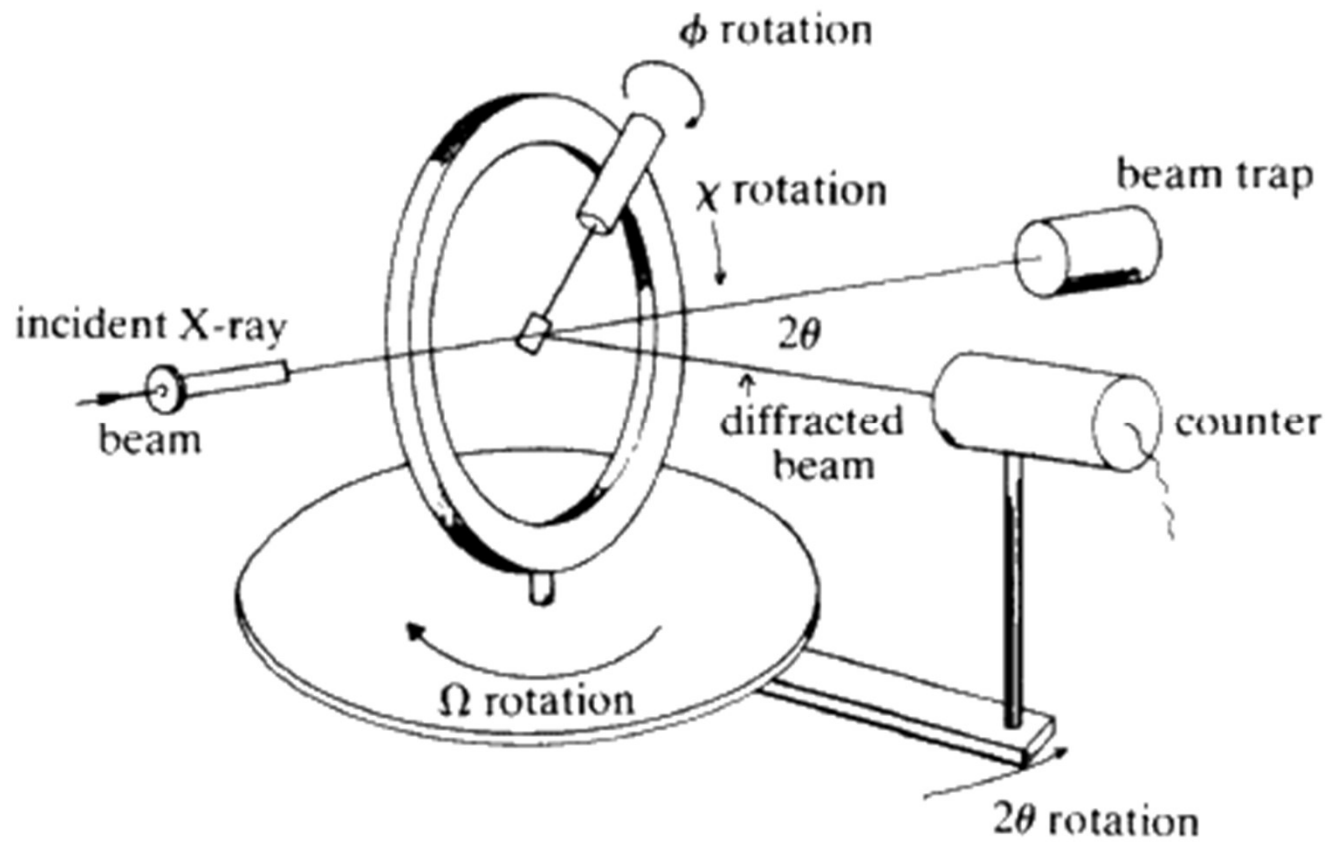
$$\vec{G} = \Delta \vec{k}$$

Diffraction condition (Laue condition)

$$\vec{k}' - \vec{k} = \Delta\vec{k} = \vec{G}$$

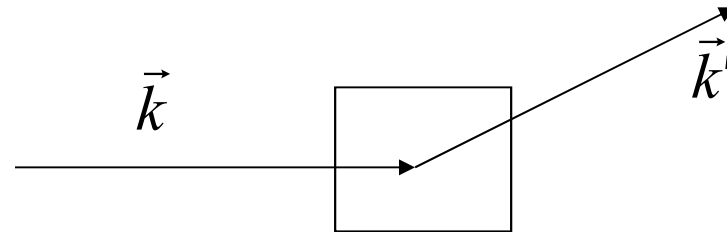


$$|\vec{k}| = |\vec{k}'| \text{ for elastic scattering}$$



θ sets the length of the scattering vector

Single crystal diffraction



$$\vec{G} = \Delta\vec{k} = \vec{q} \quad \leftarrow \text{Scattering wave vector}$$

Every time a diffraction peak is observed, record G . When many G vectors are known, determine the reciprocal lattice.

The sample and the detector must be turned to find all of the diffraction peaks.

| Gx | Gy | Gz | $ n_G ^2$ |
|--------|--------|--------|-----------|
| 2.4E10 | 2.4E10 | 0 | 10341 |
| 2.4E10 | 0 | 2.4E10 | 9989 |
| | | | |

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})$$

Determining real space primitive lattice vectors

$$\vec{a}_1 = 2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)}$$

$$\vec{a}_2 = 2\pi \frac{\vec{b}_3 \times \vec{b}_1}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)}$$

$$\vec{a}_3 = 2\pi \frac{\vec{b}_1 \times \vec{b}_2}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)}$$

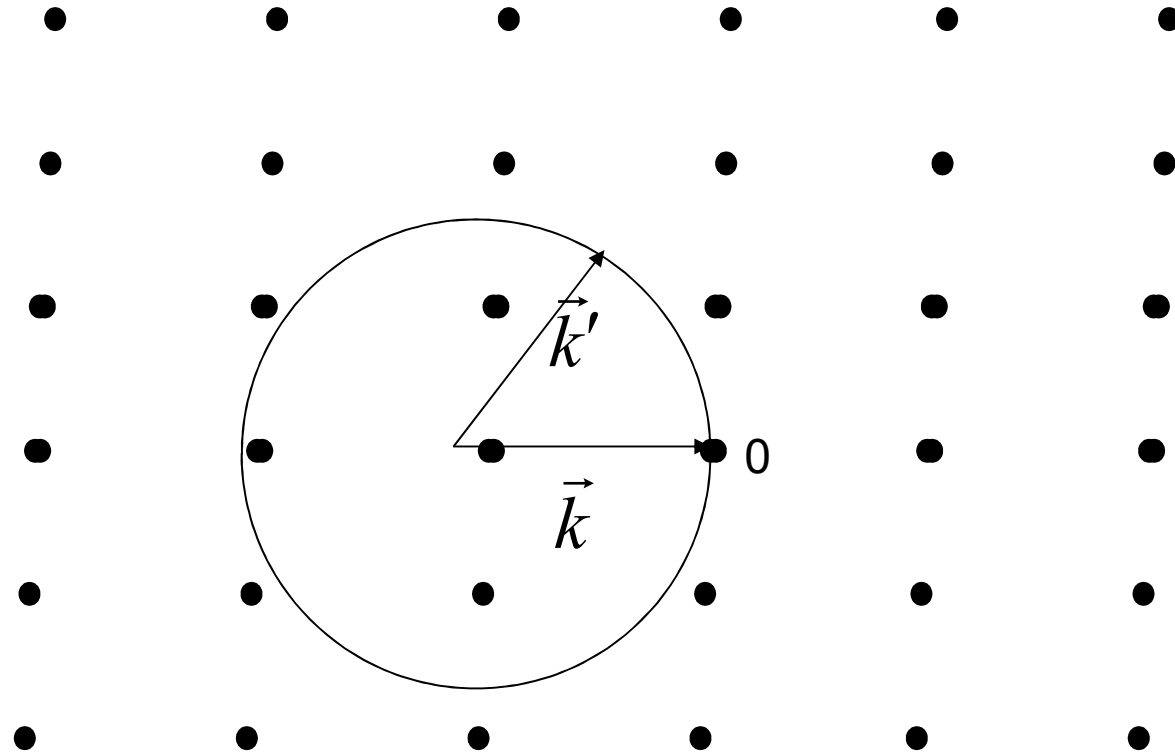
$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$$

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ determined
from diffraction experiment

Volume of the primitive unit cell $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

G vectors specify the Bravais lattice.

Ewald sphere $\Delta\vec{k} = \vec{G}$



Draw a vector representing the incoming radiation so that it ends at the origin. As the crystal is rotated around the origin, the condition for diffraction will be satisfied every time a reciprocal lattice point is on the sphere.

The number of diffraction peaks that will be observed in a diffraction experiment

Diffraction can occur whenever the diffraction condition, $\vec{k}' - \vec{k} = \vec{G}$, is satisfied. Here \vec{k} is the wave vector of the incoming waves, \vec{k}' is the wave vector of the scattered wave, and \vec{G} is a reciprocal lattice vector. For elastic scattering, $|\vec{k}| = |\vec{k}'|$ and diffraction can only occur for $2|\vec{k}| > |\vec{G}|$. Thus, there are only a finite number of diffraction peaks observable. The number of diffraction peaks can be estimated by dividing the volume of a sphere of radius $2|\vec{k}|$ by the volume of a primitive unit cell in reciprocal space. A more exact number can be obtained by testing if reciprocal lattice points lie inside the sphere. The form below calculates the primitive lattice vectors in reciprocal space from the primitive lattice vectors in real space and then determines the number of reciprocal lattice points that satisfy the diffraction condition.

Primitive lattice vectors:

$$\begin{aligned}\vec{a}_1 &= 4.12 \hat{x} + 0 \hat{y} + 0 \hat{z} \text{ [\AA]} \\ \vec{a}_2 &= 0 \hat{x} + 4.12 \hat{y} + 0 \hat{z} \text{ [\AA]} \\ \vec{a}_3 &= 0 \hat{x} + 0 \hat{y} + 4.12 \hat{z} \text{ [\AA]}\end{aligned}$$

$$\text{X-ray wavelength } \lambda = 1.540598 \text{ [\AA]}$$

$$\text{Cu K}\alpha = 1.540598 \text{ \AA}$$

$$\text{Cr K}\alpha = 2.28975 \text{ \AA}$$

$$\text{Mo K}\alpha = 0.7093165 \text{ \AA}$$

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Al (fcc) NaCl (fcc) CsCl (sc) SrTiO₃ (perovskite, sc)

GaAs (Zincblend, fcc) GaN (Wurtzite, hex)

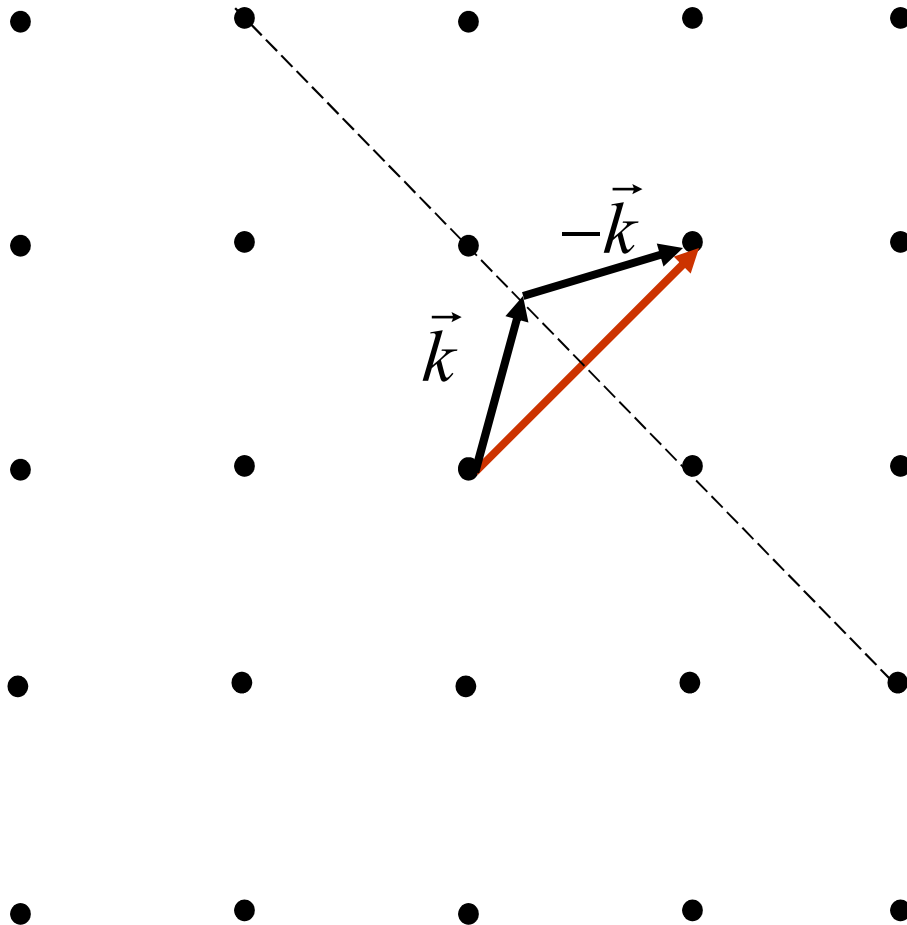
Primitive reciprocal lattice vectors

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 1.525 \hat{k}_x + 0.000 \hat{k}_y + 0.000 \hat{k}_z \text{ [\AA}^{-1}\text{]}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0.000 \hat{k}_x + 1.525 \hat{k}_y + 0.000 \hat{k}_z \text{ [\AA}^{-1}\text{]}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0.000 \hat{k}_x + 0.000 \hat{k}_y + 1.525 \hat{k}_z \text{ [\AA}^{-1}\text{]}$$

Diffraction condition



$$\vec{k}' - \vec{k} = \vec{G}$$

For every G there is a $-G$ so the diffraction condition can also be written as

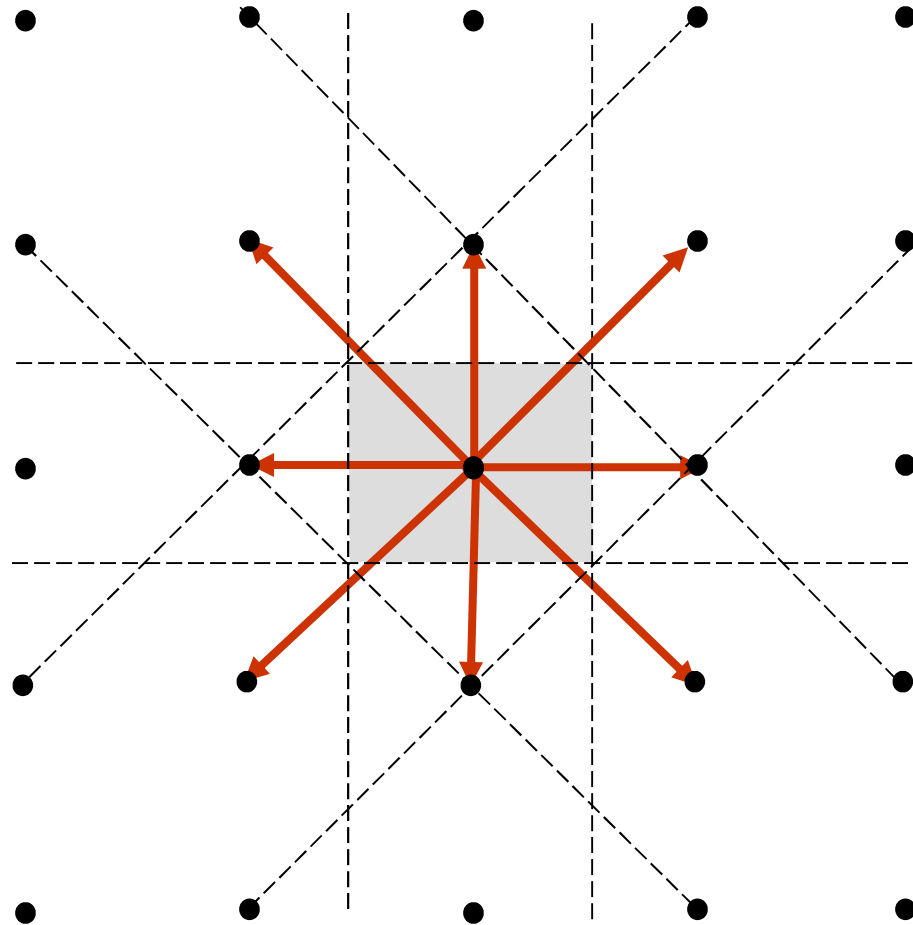
$$\vec{k} - \vec{k}' = \vec{G}$$

a wave will be diffracted if the wave vector ends on one of the planes

Brillouin zones

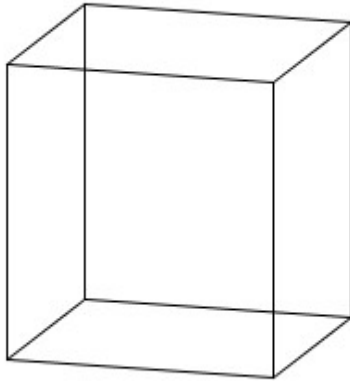


Leon Brillouin

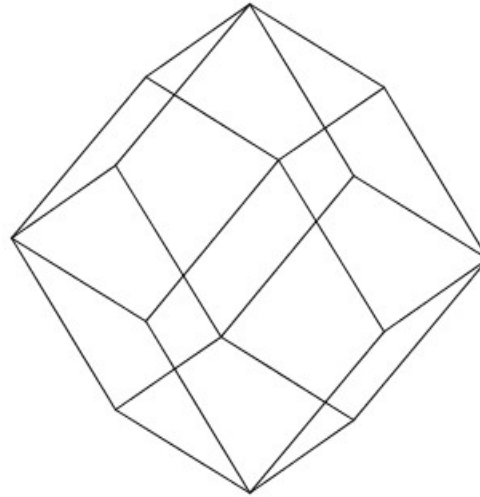


1st Brillouin zone consists of the k -states around the origin that can be reached without crossing a plane.

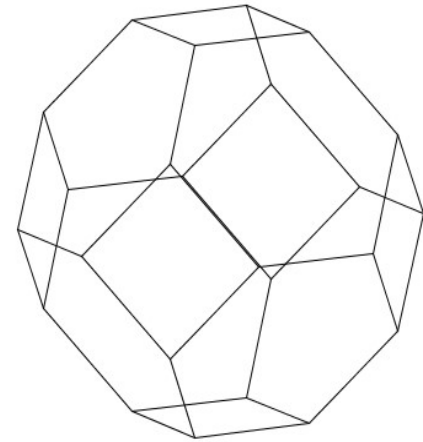
1st Brillouin zones



sc



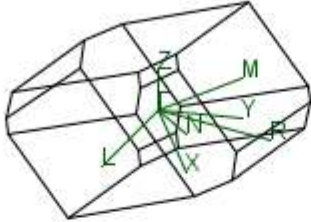
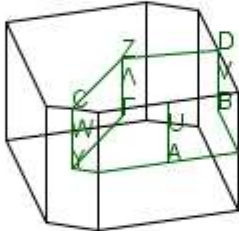
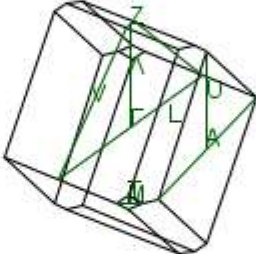
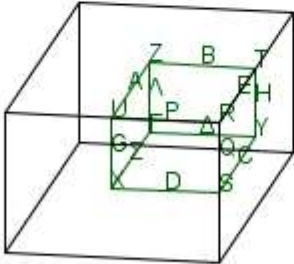
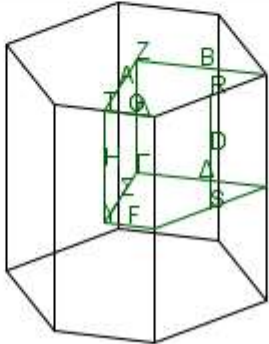

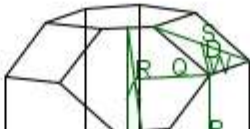
bcc



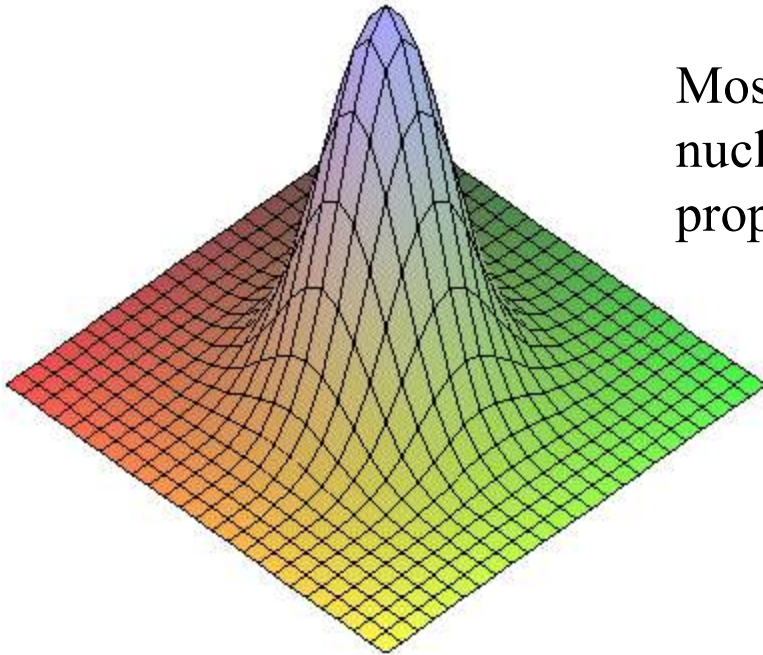
fcc

1st Brillouin is the Wigner-Seitz cell in reciprocal space.

Brillouin zones

| | | |
|---|---|---|
| <p>Triclinic</p> <p>$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$</p> |  <p>Triclinic</p> | |
| <p>Monoclinic</p> <p>$a \neq b \neq c$ $\alpha \neq 90^\circ$ $\beta = \gamma = 90^\circ$</p> |  <p>Monoclinic simple</p> |  <p>Monoclinic Base centered</p> |
| <p>Orthorhombic</p> <p>$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$</p> |  <p>Orthorhombic simple</p> |  <p>Base centered</p> |
| |  |  |

Electron density of an atom



Most of the electrons are concentrated around the nucleus. The integral over the electron density is proportional to the number of electrons.

$$n_j(\vec{r}) \propto \exp\left(-\frac{(\vec{r} - \vec{r}_j)^2}{r_0^2}\right)$$

Approximately a Gaussian centered at r_j

Electron density

Write the electron density as a Fourier series

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G} \cdot \vec{r}} = \sum_{\vec{T}} \sum_j n_j (\vec{r} - \vec{r}_j + \vec{T}),$$

position of atom j of the basis

Translation vector

Multiply by $e^{-i\vec{G}' \cdot \vec{r}}$ and integrate over a unit cell.

$$\sum_{\vec{G}} \int_{\text{u.c.}} n_{\vec{G}} e^{i\vec{G} \cdot \vec{r}} e^{-i\vec{G}' \cdot \vec{r}} d\vec{r} = \sum_j \int_{\text{u.c.}} n_j (\vec{r} - \vec{r}_j) e^{-i\vec{G}' \cdot \vec{r}} d\vec{r}.$$

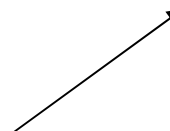
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Electron density

$$n_{\vec{G}} V = \sum_j \int n_j(\vec{r} - \vec{r}_j) e^{-i\vec{G} \cdot \vec{r}} d\vec{r}.$$

Make a substitution $\vec{r}' = \vec{r} - \vec{r}_j$.

$$n_{\vec{G}} = \frac{1}{V} \sum_j e^{-i\vec{G} \cdot \vec{r}_j} \underbrace{\int n_j(\vec{r}') e^{-i\vec{G} \cdot \vec{r}'} d\vec{r}'}.$$



Fourier transform of the electron density of atom j
= atomic form factor $f_j(G)$

Atomic form factor

$$f_j(\vec{G}) = \int n_j(\vec{r}) e^{-i\vec{G} \cdot \vec{r}} d\vec{r},$$

The atomic form factors can be looked up in a table.

The structure factors are given in terms of the atomic form factors.

$$n_{\vec{G}} = \frac{1}{V} \sum_j f_j(\vec{G}) e^{-i\vec{G} \cdot \vec{r}_j}$$

sum over the basis

position of atom j of the basis

Section 4.3.2. Parameterizations of electron atomic scattering factors

J. M. Cowley,^{b†} L. M. Peng,ⁱ G. Ren,^j S. L. Dudarev^c and M. J. Whelan^c

Table 4.3.2.2 | [pdf](#) |

Elastic atomic scattering factors of electrons for neutral atoms and s up to 2.0 \AA^{-1}

$$f(s) = \sum_i a_i \exp(-b_i s^2)$$

| Element | Z | a_1 | a_2 | a_3 | a_4 | a_5 | b_1 | b_2 | b_3 | b_4 | b_5 |
|---------|-----|--------|--------|--------|--------|--------|--------|--------|---------|---------|----------|
| H | 1 | 0.0349 | 0.1201 | 0.1970 | 0.0573 | 0.1195 | 0.5347 | 3.5867 | 12.3471 | 18.9525 | 38.6269 |
| He | 2 | 0.0317 | 0.0838 | 0.1526 | 0.1334 | 0.0164 | 0.2507 | 1.4751 | 4.4938 | 12.6646 | 31.1653 |
| Li | 3 | 0.0750 | 0.2249 | 0.5548 | 1.4954 | 0.9354 | 0.3864 | 2.9383 | 15.3829 | 53.5545 | 138.7337 |
| Be | 4 | 0.0780 | 0.2210 | 0.6740 | 1.3867 | 0.6925 | 0.3131 | 2.2381 | 10.1517 | 30.9061 | 78.3273 |
| B | 5 | 0.0909 | 0.2551 | 0.7738 | 1.2136 | 0.4606 | 0.2995 | 2.1155 | 8.3816 | 24.1292 | 63.1314 |
| C | 6 | 0.0893 | 0.2563 | 0.7570 | 1.0487 | 0.3575 | 0.2465 | 1.7100 | 6.4094 | 18.6113 | 50.2523 |
| N | 7 | 0.1022 | 0.3219 | 0.7982 | 0.8197 | 0.1715 | 0.2451 | 1.7481 | 6.1925 | 17.3894 | 48.1431 |
| O | 8 | 0.0974 | 0.2921 | 0.6910 | 0.6990 | 0.2039 | 0.2067 | 1.3815 | 4.6943 | 12.7105 | 32.4726 |
| F | 9 | 0.1083 | 0.3175 | 0.6487 | 0.5846 | 0.1421 | 0.2057 | 1.3439 | 4.2788 | 11.3932 | 28.7881 |
| Ne | 10 | 0.1269 | 0.3535 | 0.5582 | 0.4674 | 0.1460 | 0.2200 | 1.3779 | 4.0203 | 9.4934 | 23.1278 |
| Na | 11 | 0.2142 | 0.6853 | 0.7692 | 1.6589 | 1.4482 | 0.3334 | 2.3446 | 10.0830 | 48.3037 | 138.2700 |
| Mg | 12 | 0.2314 | 0.6866 | 0.9677 | 2.1882 | 1.1339 | 0.3278 | 2.2720 | 10.9241 | 39.2898 | 101.9748 |
| Al | 13 | 0.2390 | 0.6573 | 1.2011 | 2.5586 | 1.2312 | 0.3138 | 2.1063 | 10.4163 | 34.4552 | 98.5344 |



513.001 Molecular and Solid State Physics

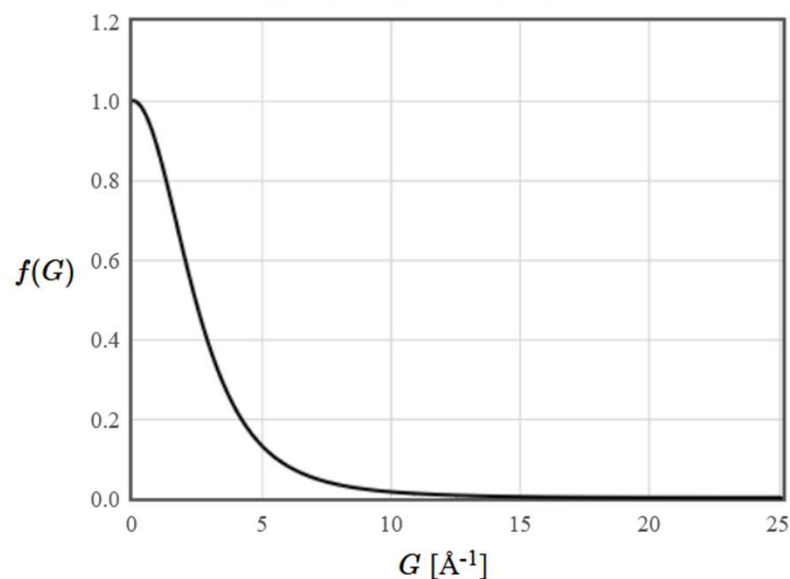
Atomic form factors

In the range of scattering vectors between $0 < q < 25 \text{ \AA}^{-1}$, the atomic form factor is well approximated by the expression, [1]

$$f(q) = \sum_{i=1}^4 a_i \exp \left(-b_i \left(\frac{q}{4\pi} \right)^2 \right) + c,$$

where the values of a_i , b_i , and c are tabulated below. The different atomic form factors for the elements can be plotted using the form below.

Atomic form factor for H



H ▼

$|\vec{G}| = 10 \text{ \AA}^{-1}$ $f(G) = 0.0156257014$

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| Element | a_1 | b_1 | a_2 | b_2 | a_3 | b_3 | a_4 | b_4 | c |
|-----------------|----------|---------|----------|---------|----------|---------|----------|---------|----------|
| H | 0.489918 | 20.6593 | 0.262003 | 7.74039 | 0.196767 | 49.5519 | 0.049879 | 2.20159 | 0.001305 |
| H ¹⁻ | 0.897661 | 53.1368 | 0.565616 | 15.187 | 0.415815 | 186.576 | 0.116973 | 3.56709 | 0.002389 |
| He | 0.8734 | 9.1037 | 0.6309 | 3.3568 | 0.3112 | 22.9276 | 0.178 | 0.9821 | 0.0064 |

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Primitive lattice vectors:

$$\begin{aligned}\vec{a}_1 &= 4.12\text{E-10} \hat{x} + 0 \hat{y} + 0 \hat{z} \text{ [m]} \\ \vec{a}_2 &= 0 \hat{x} + 4.12\text{E-10} \hat{y} + 0 \hat{z} \text{ [m]} \\ \vec{a}_3 &= 0 \hat{x} + 0 \hat{y} + 4.12\text{E-10} \hat{z} \text{ [m]}\end{aligned}$$

Basis:

The positions of the atoms are given in fractional coordinates between -1 and 1.

| | | | | | | |
|------|-----|---------------|-----|---------------|-----|-------------|
| Cs1+ | 0 | $\vec{a}_1 +$ | 0 | $\vec{a}_2 +$ | 0 | \vec{a}_3 |
| Cl1- | 0.5 | $\vec{a}_1 +$ | 0.5 | $\vec{a}_2 +$ | 0.5 | \vec{a}_3 |
| | | $\vec{a}_1 +$ | | $\vec{a}_2 +$ | | \vec{a}_3 |
| | | $\vec{a}_1 +$ | | $\vec{a}_2 +$ | | \vec{a}_3 |
| | | $\vec{a}_1 +$ | | $\vec{a}_2 +$ | | \vec{a}_3 |

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Al (fcc)

NaCl (fcc)

CsCl (sc)

SrTiO3 (sc)

GaAs (Zincblend, fcc)

GaN (Wurtzite, hex)

Primitive reciprocal lattice vectors

$$\begin{aligned}\vec{b}_1 &= 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 1.525\text{e+10} \hat{k}_x + 0.000 \hat{k}_y + 0.000 \hat{k}_z \text{ [m}^{-1}\text{]} \\ \vec{b}_2 &= 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0.000 \hat{k}_x + 1.525\text{e+10} \hat{k}_y + 0.000 \hat{k}_z \text{ [m}^{-1}\text{]} \\ \vec{b}_3 &= 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0.000 \hat{k}_x + 0.000 \hat{k}_y + 1.525\text{e+10} \hat{k}_z \text{ [m}^{-1}\text{]}\end{aligned}$$

Structure factors

The value of $|n_{\vec{G}}|$ for the 000 diffraction peak is the total number of electrons in the primitive unit cell. The intensities of the peaks in an x-ray diffraction experiment

| hkl | $ \vec{G} \text{ \AA}^{-1}$ | $ n_{\vec{G}} $ | $ n_{\vec{G}} ^2$ | $\text{Re}\{n_{\vec{G}}\}$ | $\text{Im}\{n_{\vec{G}}\}$ |
|-------|------------------------------|-----------------|-------------------|----------------------------|----------------------------|
| 000 | 0.000 | 72.00 | 5184 | 72.00 | 0.000 |
| -100 | 1.525 | 34.43 | 1185 | 34.43 | 5.333e-8 |
| 0-10 | 1.525 | 34.43 | 1185 | 34.43 | 5.333e-8 |
| 00-1 | 1.525 | 34.43 | 1185 | 34.43 | 5.333e-8 |
| 001 | 1.525 | 34.43 | 1185 | 34.43 | -5.333e-8 |

Structure factor

$$n_{\vec{G}} = \frac{1}{V} \sum_j f_j(G) e^{-i\vec{G} \cdot \vec{r}_j}$$

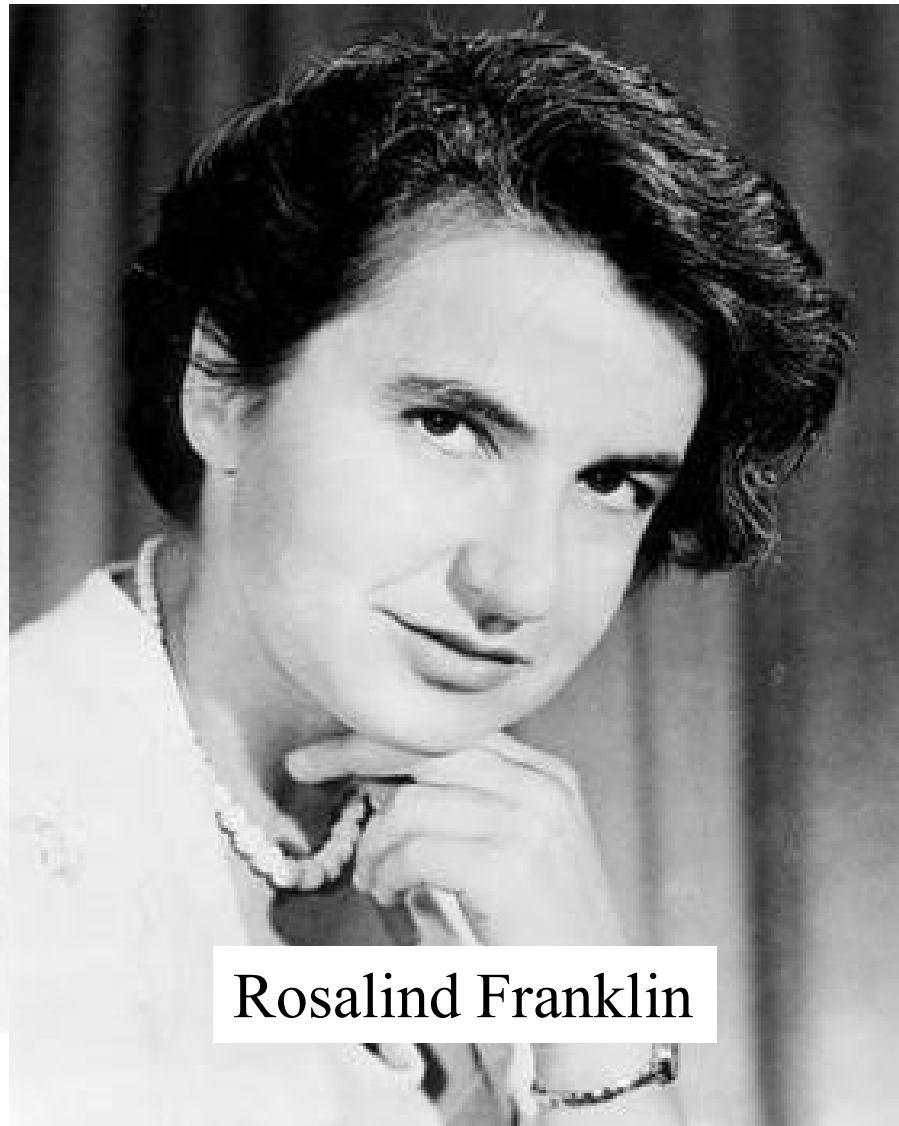
A structure factor is the Fourier transform of the electron density of the basis of a crystal evaluated at a reciprocal lattice vector. Since the electron density of the basis can be approximated as a sum over the electron densities of the atoms in the basis, the Fourier transform of the electron density of the basis is a sum of the Fourier transforms of the electron densities of the atoms in the basis.

An x-ray experiment measures the scattered intensity $|F_G|^2$. The phase information is lost. This is proportional to $|n_G|^2$.

crystal structure solution

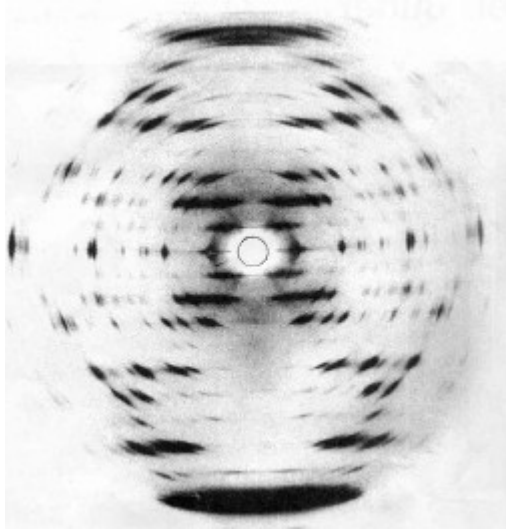
structural solution of the DNA

F.Crick, J.Watson, M.Wilkins
nobel laureate 1962 for medicine



Rosalind Franklin

crystal structure solution



"Guess" the crystal structure

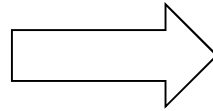
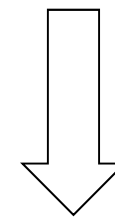
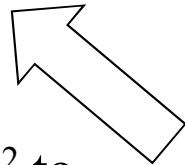


Table 4.3.2.2 | pdf |
Elastic atomic scattering factors of electrons for neutral atoms and s up to 2.0 Å⁻¹

| Element | Z | a ₁ | a ₂ | a ₃ | a ₄ | a ₅ | b ₁ | b ₂ | b ₃ |
|---------|----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| H | 1 | 0.0349 | 0.1201 | 0.1970 | 0.0573 | 0.1195 | 0.5347 | 3.5867 | 12.3471 |
| He | 2 | 0.0317 | 0.0838 | 0.1526 | 0.1334 | 0.0164 | 0.2507 | 1.4751 | 4.4938 |
| Li | 3 | 0.0750 | 0.2249 | 0.5548 | 1.4954 | 0.9354 | 0.3864 | 2.9383 | 15.3829 |
| Be | 4 | 0.0780 | 0.2210 | 0.6740 | 1.3867 | 0.6925 | 0.3131 | 2.2381 | 10.1517 |
| B | 5 | 0.0909 | 0.2551 | 0.7738 | 1.2136 | 0.4606 | 0.2995 | 2.1155 | 8.3816 |
| C | 6 | 0.0893 | 0.2563 | 0.7570 | 1.0487 | 0.3575 | 0.2465 | 1.7100 | 6.4094 |
| N | 7 | 0.1022 | 0.3219 | 0.7982 | 0.8197 | 0.1715 | 0.2451 | 1.7481 | 6.1925 |
| O | 8 | 0.0974 | 0.2921 | 0.6910 | 0.6990 | 0.2039 | 0.2067 | 1.3815 | 4.6943 |
| F | 9 | 0.1083 | 0.3175 | 0.6487 | 0.5846 | 0.1421 | 0.2057 | 1.3439 | 4.2788 |
| Ne | 10 | 0.1269 | 0.3535 | 0.5582 | 0.4674 | 0.1460 | 0.2200 | 1.3779 | 4.0203 |
| Na | 11 | 0.2142 | 0.6853 | 0.7692 | 1.6589 | 1.4482 | 0.3334 | 2.3446 | 10.0830 |
| Mg | 12 | 0.2314 | 0.6866 | 0.9677 | 2.1882 | 1.1339 | 0.3278 | 2.2720 | 10.9241 |
| Al | 13 | 0.2390 | 0.6573 | 1.2011 | 2.5586 | 1.2312 | 0.3138 | 2.1063 | 10.4163 |
| Si | 14 | 0.2519 | 0.6372 | 1.3795 | 2.5082 | 1.0500 | 0.3075 | 2.0174 | 9.6746 |
| P | 15 | 0.2548 | 0.6106 | 1.4541 | 2.3204 | 0.8477 | 0.2908 | 1.8740 | 8.5176 |
| S | 16 | 0.2497 | 0.5628 | 1.3899 | 2.1865 | 0.7715 | 0.2681 | 1.6711 | 7.0267 |
| Cl | 17 | 0.2443 | 0.5397 | 1.3919 | 2.0197 | 0.6621 | 0.2468 | 1.5242 | 6.1537 |
| Ar | 18 | 0.2385 | 0.5017 | 1.3428 | 1.8899 | 0.6079 | 0.2289 | 1.3694 | 5.2561 |

Compare $|n_G|^2$ to
the
measurements



From the atomic form
factors, calculate the
structure factors n_G .

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})$$

x-ray diffraction

The shape and the dimensions of the unit cell can be deduced from the positions of the Bragg reflections; the content of the unit cell, on the other hand, must be determined from the intensities of the reflections.

Solid State Physics, Ibach and Lüth

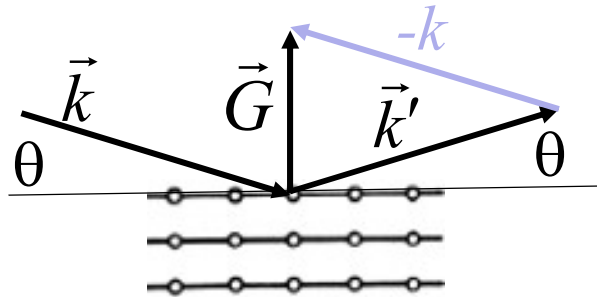
Diffraction condition: $\Delta\vec{k} = \vec{G}$

The intensity of the peaks is proportional to the squared Fourier coefficients of the electron density.

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})$$

x-ray diffraction

$$\vec{G}_{hkl} \perp (hkl)$$



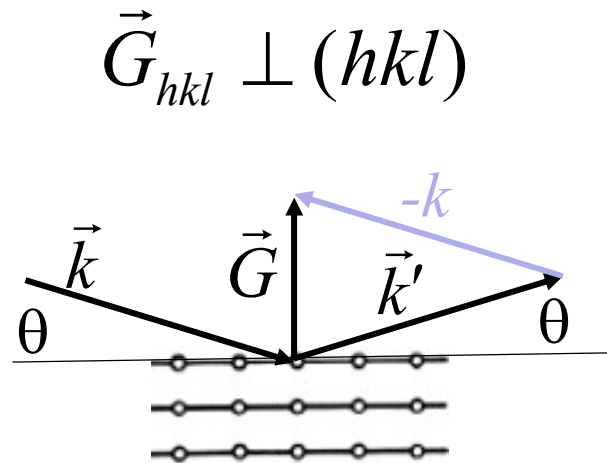
for $\theta = \pi/2$, $2|k| = |G|$ and

constructive interference takes place when $2d_{hkl} = \lambda$.

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

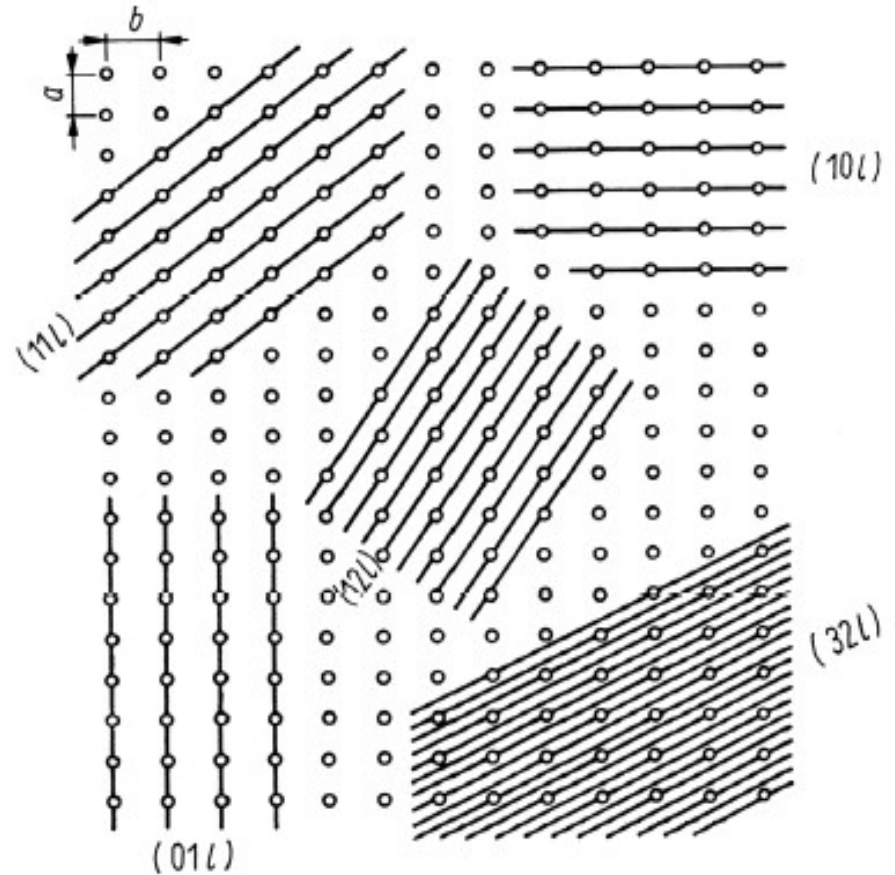
$$|\vec{G}_{hkl}| = \frac{2\pi}{d_{hkl}}$$

x-ray diffraction

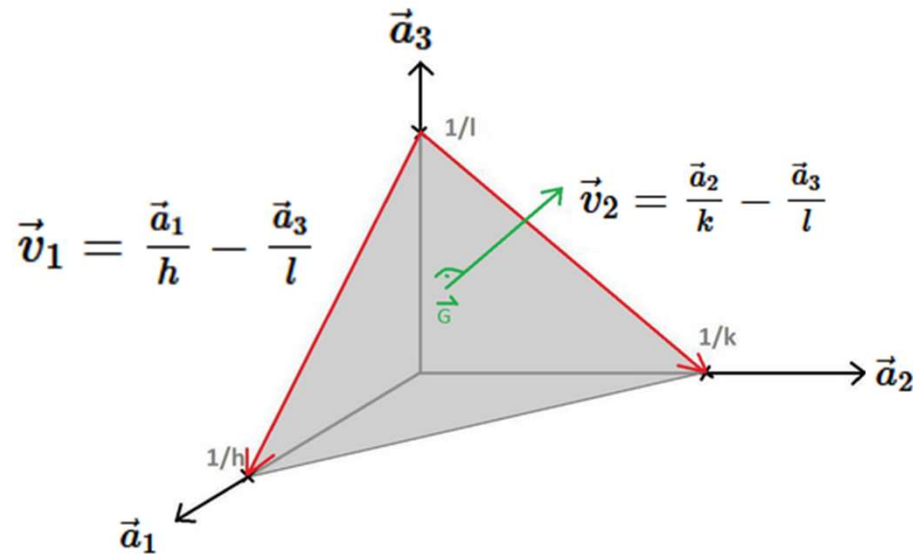


$$|\vec{G}_{hkl}| = \frac{2\pi}{d_{hkl}}$$

distance between the net planes



The reciprocal lattice vector \vec{G}_{hkl} is orthogonal to the (hkl) plane



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

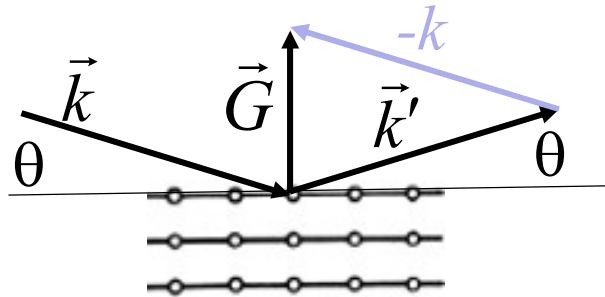
$$\vec{v}_1 \cdot \vec{G}_{hkl} = \left(\frac{1}{h} h\vec{b}_1 \cdot \vec{a}_1 - \frac{1}{l} l\vec{a}_3 \cdot \vec{b}_3 \right) = 2\pi - 2\pi = 0$$

$$\vec{v}_2 \cdot \vec{G}_{hkl} = \left(\frac{1}{k} k\vec{a}_2 \cdot \vec{b}_2 - \frac{1}{l} l\vec{b}_3 \cdot \vec{a}_3 \right) = 2\pi - 2\pi = 0$$

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

x-ray diffraction

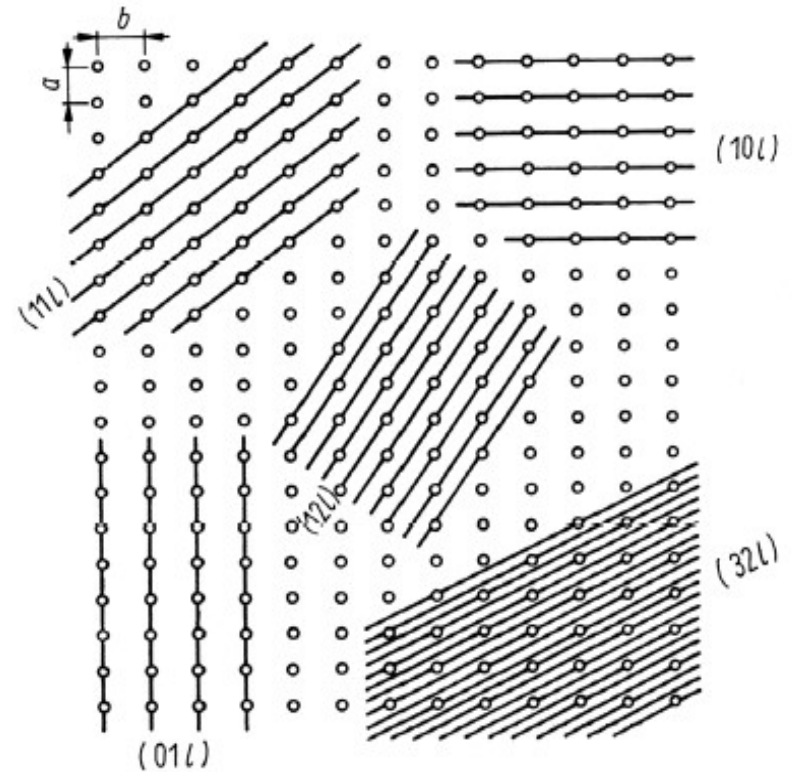
$$\vec{G}_{hkl} \perp (hkl)$$



$$|\vec{G}_{hkl}| = |\Delta\vec{k}| = 2|\vec{k}|\sin\theta = \frac{2\pi}{d_{hkl}}$$

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

$$|\vec{k}| = \frac{2\pi}{\lambda}$$



distance between the net planes

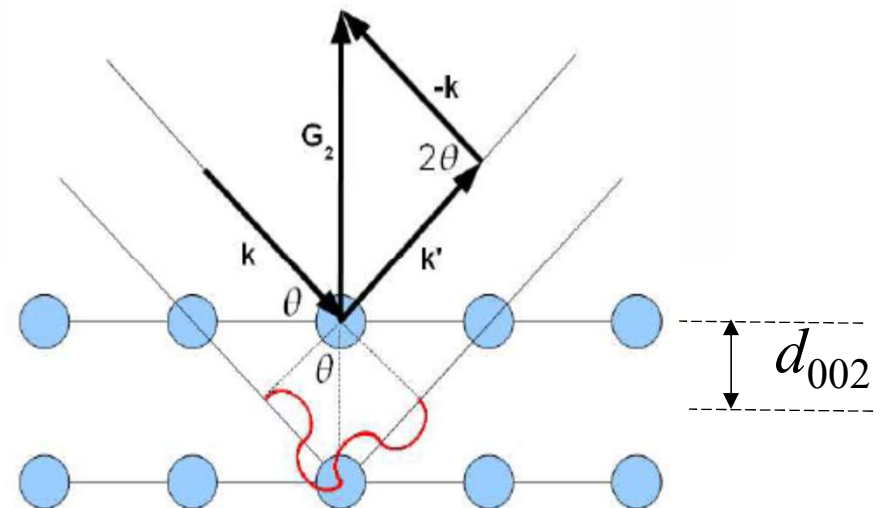
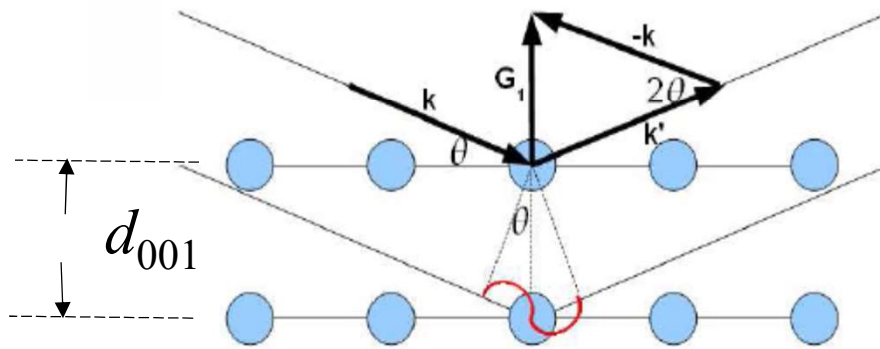
$$2d_{hkl} \sin\theta = \lambda \quad \leftarrow \text{another formulation of the diffraction condition}$$

Bragg and Laue conditions

Bragg condition: $2d \sin \theta = n\lambda$

Laue condition: $\Delta \vec{k} = \vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

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

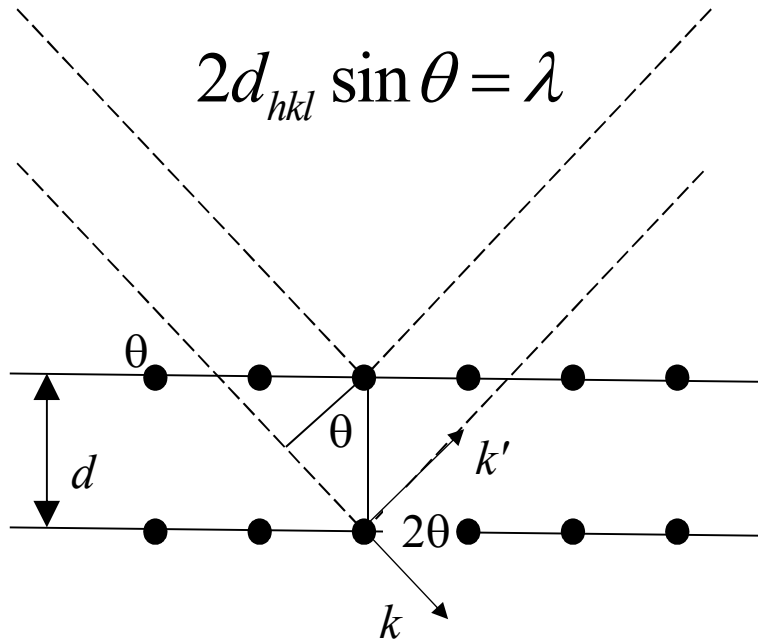


$$n = 1 \Leftrightarrow 001$$

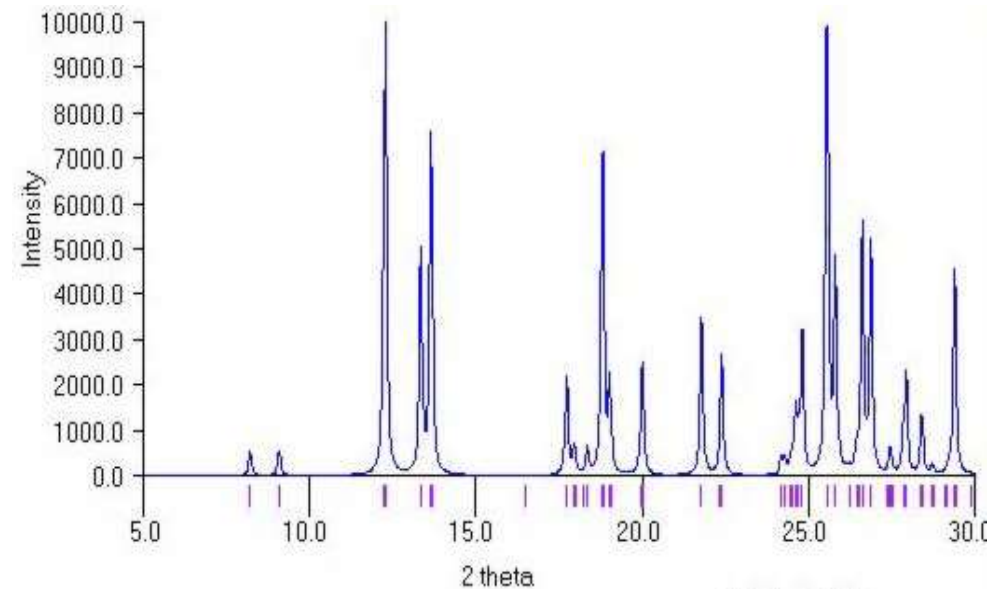
$$n = 2 \Leftrightarrow 002$$

Powder diffraction

Powder diffraction is performed on a powder of many small crystals. Ideally, every possible crystalline orientation is represented equally in a powdered sample. The relative intensities of the diffraction peaks indicate which crystal structures are present.

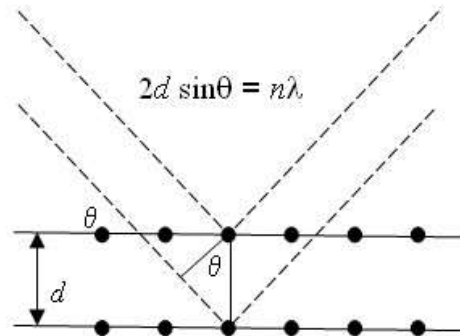


X-rays: Bragg diffraction

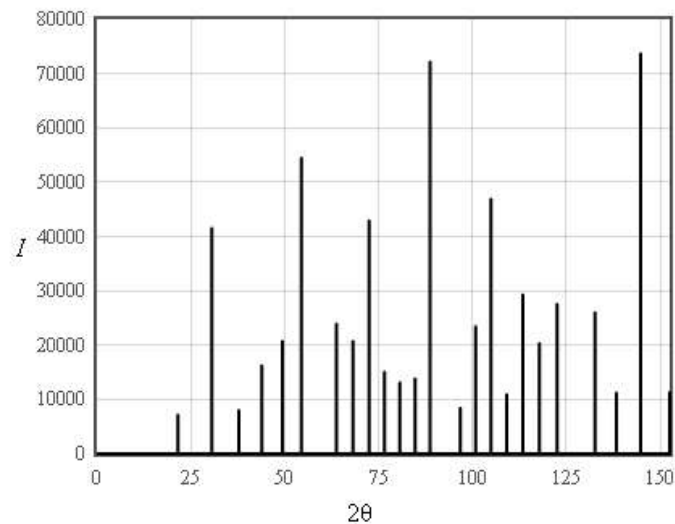


Powder diffraction

For powder diffraction, a crystal is ground into a fine powder so that there are many small crystals with random orientations. X-rays strike the surface of the sample at an angle θ and an x-ray detector is placed at an angle θ to the surface. Only planes parallel to the surface will diffract x-rays to the detector.



Since there are many small crystals with random orientations in the sample, all possible crystal planes that can diffract the x-rays will contribute to the measured signal when θ satisfies the Bragg condition. The form below can calculate the powder diffraction pattern for any crystal with up to five atoms per primitive unit cell. Some buttons are provided that load the form with the data for certain crystals.



Primitive lattice vectors:

$\vec{a}_1 =$ $\hat{x} +$ $\hat{y} +$ \hat{z} [m]
 $\vec{a}_2 =$ $\hat{x} +$ $\hat{y} +$ \hat{z} [m]
 $\vec{a}_3 =$ $\hat{x} +$ $\hat{y} +$ \hat{z} [m]

Basis:

The positions of the atoms are given in fractional coordinates between -1 and 1.

| | | | | | | |
|-------------------------------|----------------------------------|----------------|----------------------------------|----------------|----------------------------------|-------------|
| Cs1+ | <input type="text" value="0"/> | $\vec{a}_1 + $ | <input type="text" value="0"/> | $\vec{a}_2 + $ | <input type="text" value="0"/> | \vec{a}_3 |
| Cl1- | <input type="text" value="0.5"/> | $\vec{a}_1 + $ | <input type="text" value="0.5"/> | $\vec{a}_2 + $ | <input type="text" value="0.5"/> | \vec{a}_3 |
| <input type="text" value=""/> | <input type="text" value=""/> | $\vec{a}_1 + $ | <input type="text" value=""/> | $\vec{a}_2 + $ | <input type="text" value=""/> | \vec{a}_3 |
| <input type="text" value=""/> | <input type="text" value=""/> | $\vec{a}_1 + $ | <input type="text" value=""/> | $\vec{a}_2 + $ | <input type="text" value=""/> | \vec{a}_3 |
| <input type="text" value=""/> | <input type="text" value=""/> | $\vec{a}_1 + $ | <input type="text" value=""/> | $\vec{a}_2 + $ | <input type="text" value=""/> | \vec{a}_3 |

X-ray wavelength λ [Å] =

http://rruff.geo.arizona.edu/AMS/all_minerals.php

American Mineralogist Crystal Structure Database

| | | | | |
|--|-------------------------------|---------------------------------|-----------------------------------|-----------------------------|
| Abellaite | Abelsonite | Abenakiite-(Ce) | Abernathyite | Abhurite |
| Abswurbachite | Acanthite | Acetamide | Acetylene-hydrate | Achavalite |
| Actinium | Actinolite | Acuminite | Adachiite | Adamantane |
| Adamantane-methane-hydrate | Adamite | Adamsite-(Y) | Adelite | Admontite |
| Adolfpateraite | Adranosite | Adranosite-(Fe) | Aegirine | Aenigmatite |
| Aerinite | Aerugite | Aeschynite-(La) | Aeschynite-(Y) | Africanite |
| Afrinite | Afwillite | | | |
| Agardite-(Y) | Agrellite | | | |
| Ahlfeldite | Ahrensrite | | | |
| Ajoite | Akaganeite | | | |
| Akhtenskite | Akimotoite | | | |
| Aktashite | Alabandite | | | |
| Albertiniite | Albite | | | |
| Alcaparrosaite | Alflarsenite | | | |
| Algodonite | Alinite | | | |
| Allanite-(Ce) | Allanite-(La) | | | |
| Allantoin | Allargentum | | | |
| Allorite | Alluaivite | | | |
| Almeidaite | Alnaperboei | | | |
| Altaite | Althausite | | | |
| Alum-(Na) | Aluminite | | | |
| Aluminoceledonite | Aluminoceri | | | |
| Aluminotaramite | Aluminum | | | |
| Alumotantite | Alunite | | | |
| Amarantite | Amarillite | | | |
| Americium | Amesite | | | |

American Mineralogist Crystal Structure Database

4 matching records for this search.

☐ **Aluminium**

 Wyckoff R W G

Crystal Structures 1 (1963) 7-83

Second edition. Interscience Publishers, New York, New York

Cubic closest packed, ccp, structure

_database_code_amcsd 0011137

4.04958 4.04958 4.04958 90 90 90

atom x y z

Al 0 0 0

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View JMOl 3-D Structure \(p. link\)](#)

Aluminium

Wyckoff R W G

Crystal Structures 1 (1963) 7-83

Second edition. Interscience Publishers, New York, New York

Cubic closest packed, ccp, structure

_database_code_amcsd 0011137

CELL PARAMETERS: 4.0496 4.0496 4.0496 90.000 90.000 90.000

SPACE GROUP: Fm3m

X-RAY WAVELENGTH: 1.541838

Cell Volume: 66.409

Density (g/cm3): 2.698

MAX. ABS. INTENSITY / VOLUME**2: 34.61439413

RIR: 4.177

RIR based on corundum from Acta Crystallographica A38 (1982) 733-739

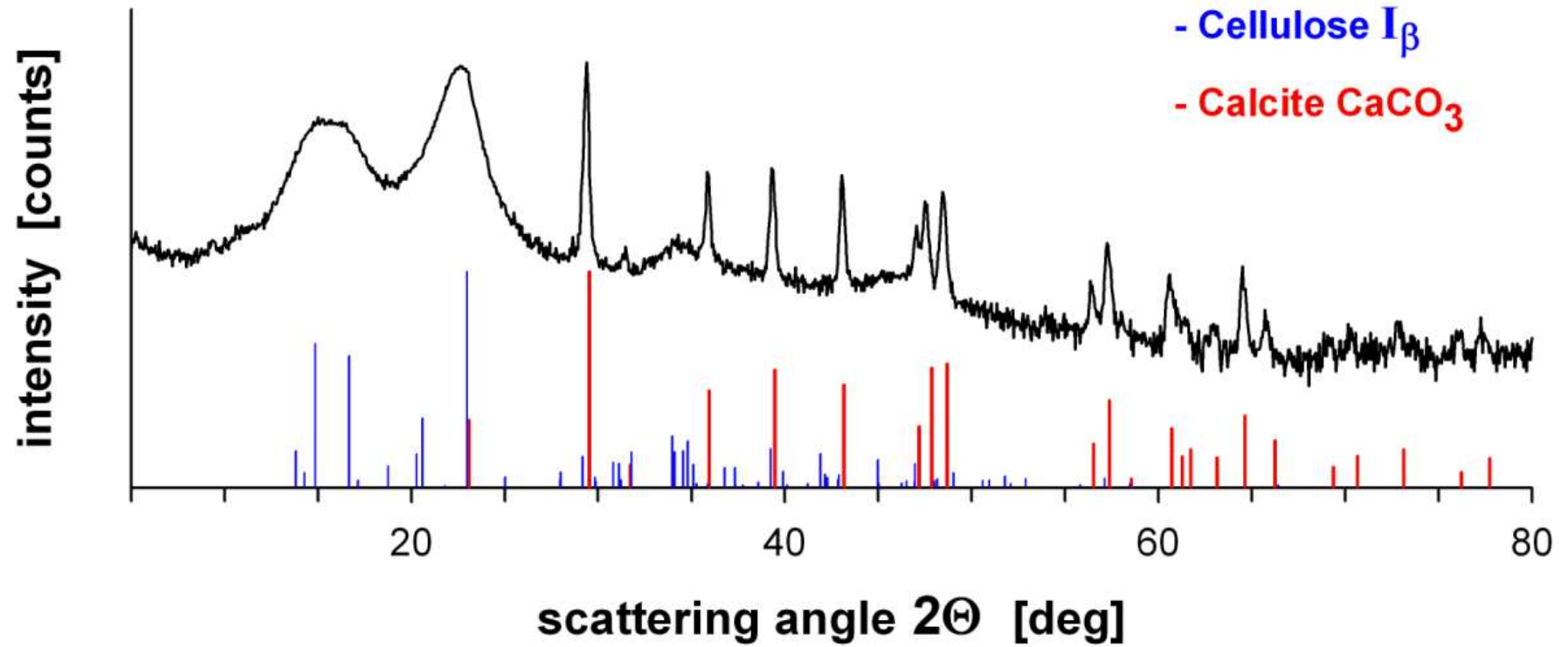
| 2-THETA | INTENSITY | D-SPACING | H | K | L | Multiplicity |
|---------|-----------|-----------|---|---|---|--------------|
| 38.50 | 100.00 | 2.3380 | 1 | 1 | 1 | 8 |
| 44.76 | 47.49 | 2.0248 | 2 | 0 | 0 | 6 |
| 65.16 | 28.01 | 1.4317 | 2 | 2 | 0 | 12 |
| 78.30 | 30.71 | 1.2210 | 3 | 1 | 1 | 24 |
| 82.52 | 8.74 | 1.1690 | 2 | 2 | 2 | 8 |

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reference, see Downs et al. (1993) American Mineralogist 78, 1104-1107.

copy paper

- Cellulose I_β

- Calcite CaCO₃



Powder diffraction

Phase identification

Every crystal has a specific "fingerprint" given by the positions and intensities of the diffraction peaks. The composition of a multi-phase specimen can be determined by fitting its diffraction pattern to the diffraction patterns of pure crystals which can be looked up in a database.

International Centre for Diffraction Data www.icdd.com

550,000 reference materials

Phase transitions, thermal expansion, piezoelectricity, piezomagnetism, bulk modulus, compliance tensor can be measured.