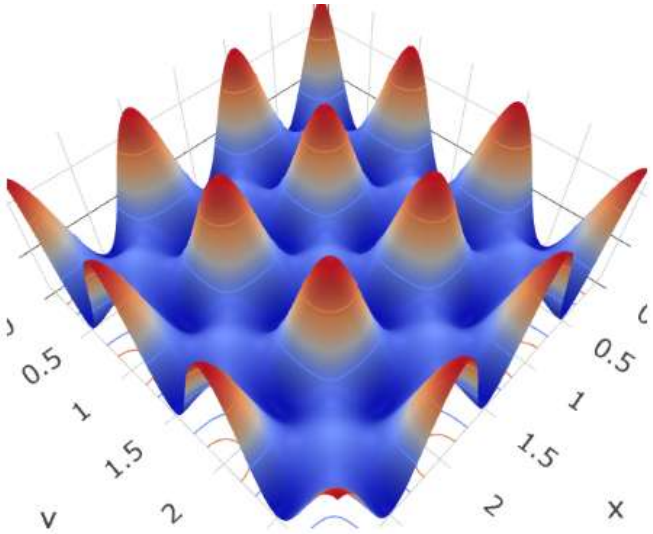
Powder diffraction
Electron diffraction
Neutron diffraction

Periodic functions



$$f(\vec{r}) = \sum_{hkl} f_{\vec{G}_{hkl}} \exp\left(i\vec{G}_{hkl} \cdot \vec{r}\right)$$

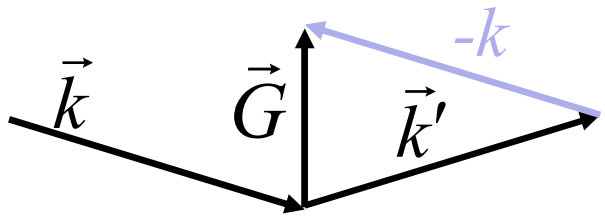
$$\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$\exp\left(i\vec{G} \cdot \vec{a}_1\right) = 1, \qquad \vec{G} \cdot \vec{a}_1 = 2\pi h$$

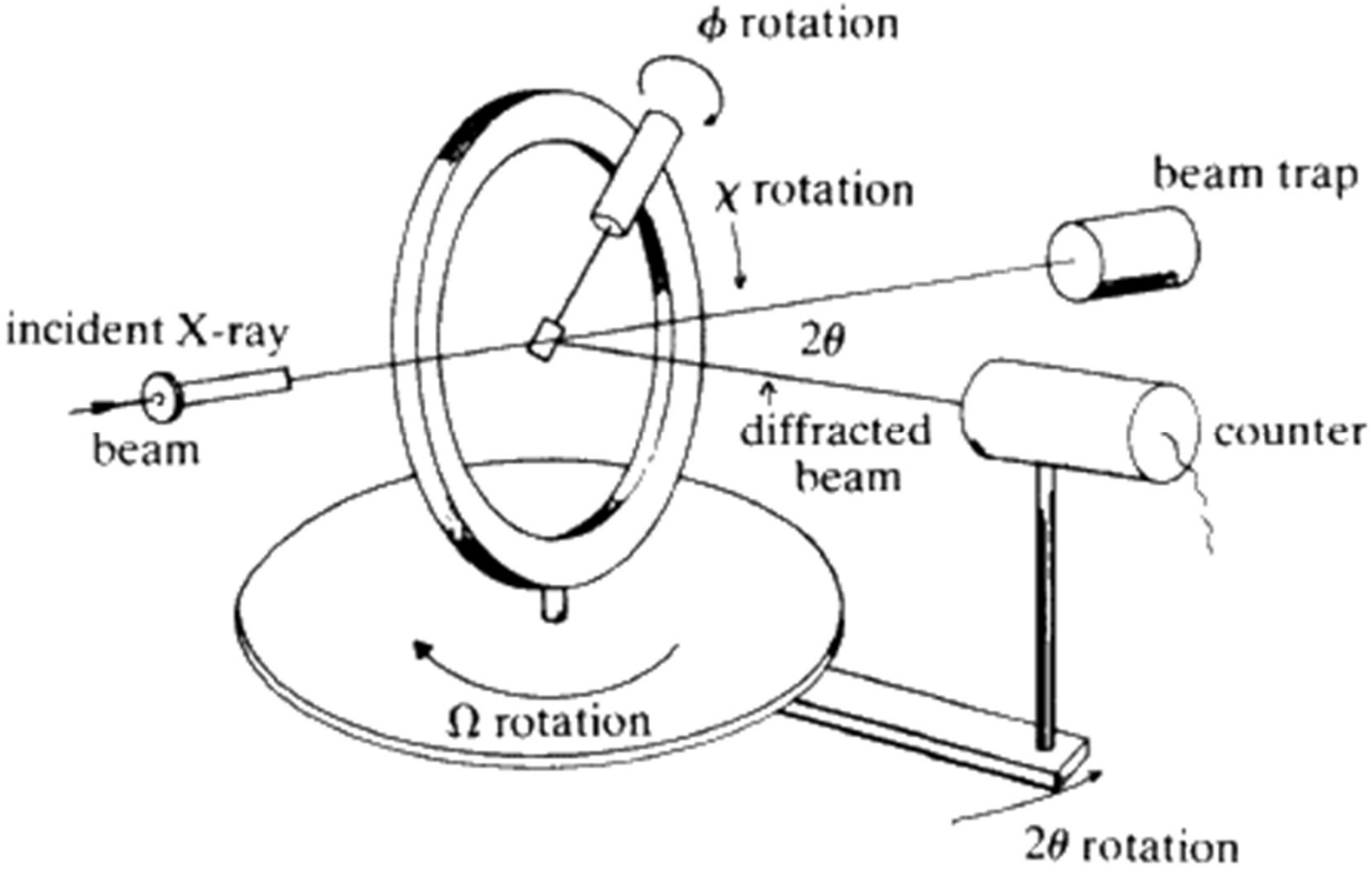
$$\exp\left(i\vec{G} \cdot \vec{a}_2\right) = 1, \qquad \vec{G} \cdot \vec{a}_2 = 2\pi k$$

$$\exp\left(i\vec{G} \cdot \vec{a}_3\right) = 1, \qquad \vec{G} \cdot \vec{a}_3 = 2\pi l,$$

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



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

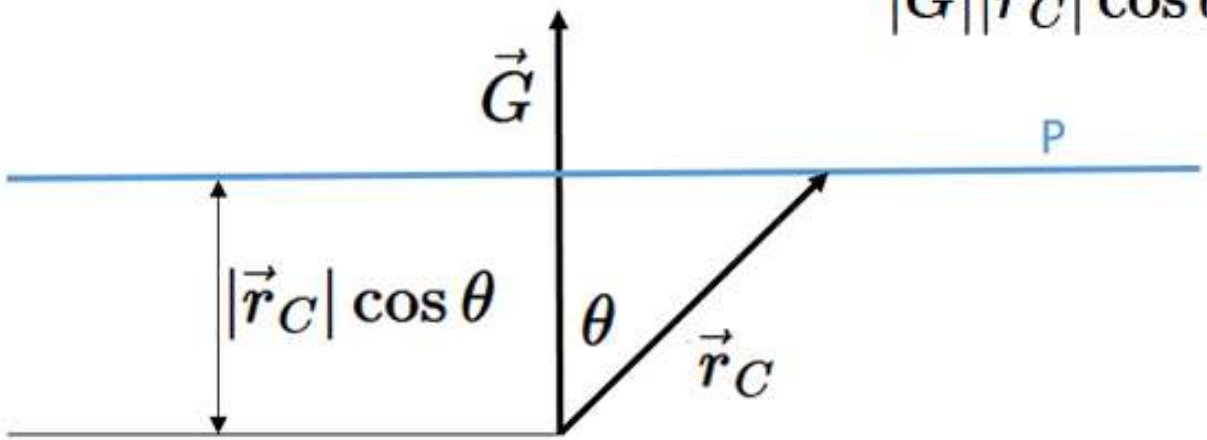


http://serc.carleton.edu/research_education/geochemsheets/techniques/SXD.html

Netplanes

$$\vec{G} \cdot \vec{r}_C = C$$

$$|\vec{G}||\vec{r}_C| \cos\theta = C$$



$$\vec{G} \cdot \vec{r}_n = 2\pi n, \qquad n = \cdots -2, -1, 0, 1, 2, \cdots$$

Bravais lattice points: $\vec{T} = u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3$

$$\vec{G} \cdot \vec{T} = \left(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3\right) \cdot (u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3) = 2\pi(hu + kv + wl)$$

The Bravais lattice points lie on the netplanes.

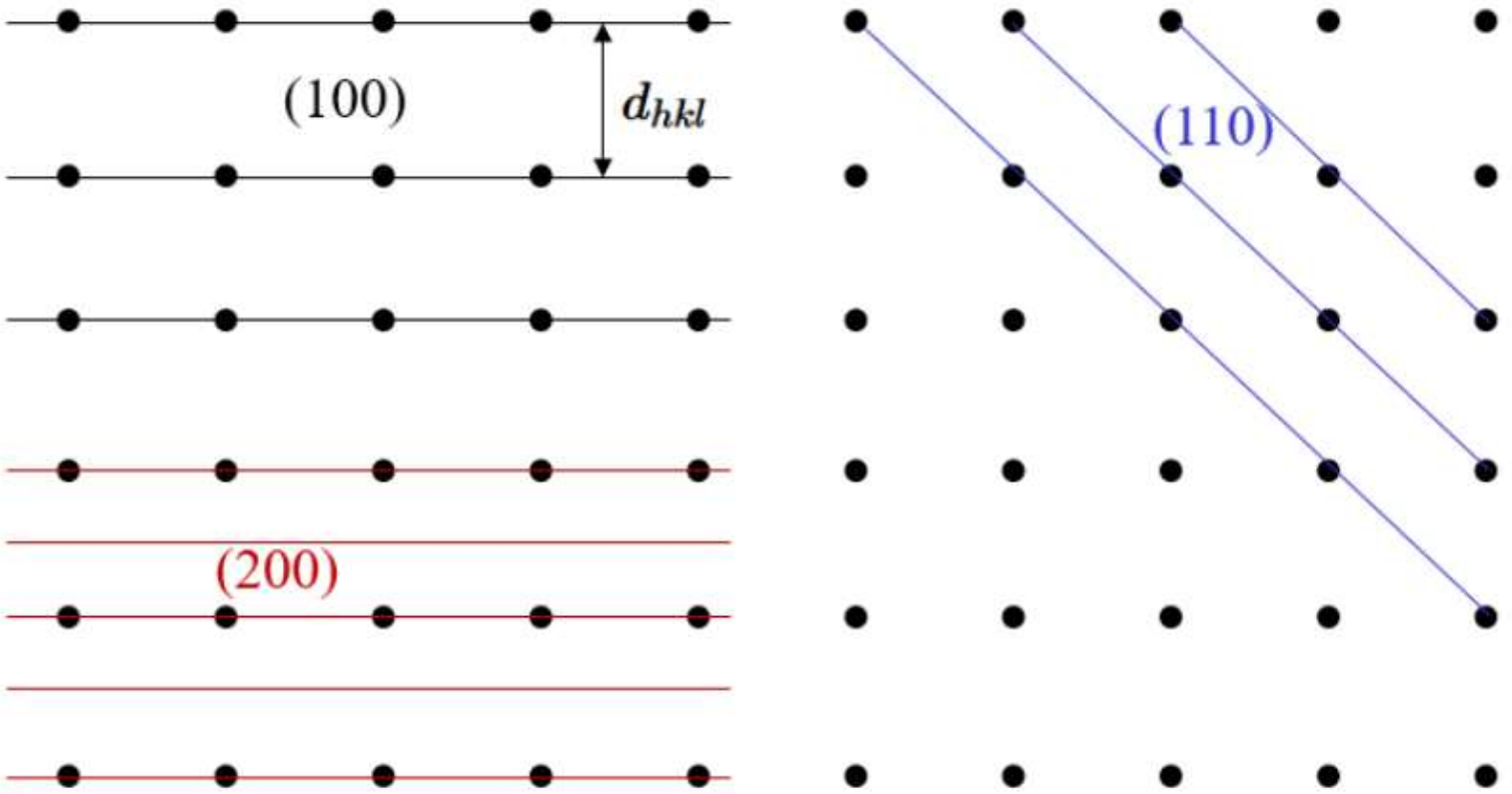
Netplanes and Lattice Planes

$$|\vec{G}_{hkl}|\vec{r}|\cos\theta = 2\pi n$$

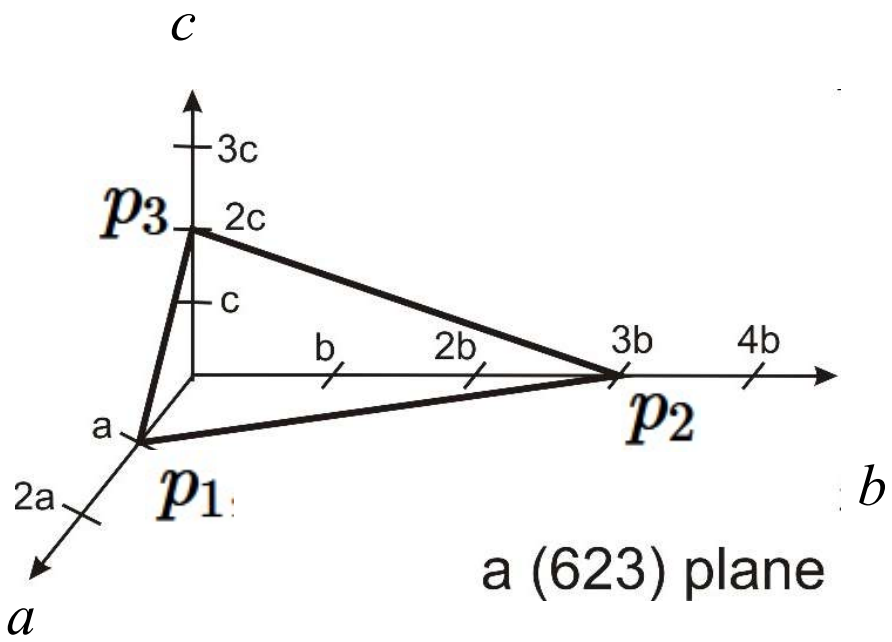
$n = 1$ and $\theta = 0$

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

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



Miller indices: Crystal planes



a (623) plane

A plane with the intercepts $1/h, 1/k, 1/l$ is the (h,k,l) plane.

$$\vec{G} \cdot p_1 \vec{a}_1 = C = 2\pi h p_1,$$
$$\vec{G} \cdot p_2 \vec{a}_2 = C = 2\pi k p_2,$$
$$\vec{G} \cdot p_3 \vec{a}_3 = C = 2\pi l p_3.$$

$$h = \frac{C}{2\pi p_1},$$
$$k = \frac{C}{2\pi p_2},$$
$$l = \frac{C}{2\pi p_3}.$$

$\vec{G}_{hkl}$ is normal to the (hkl) plane

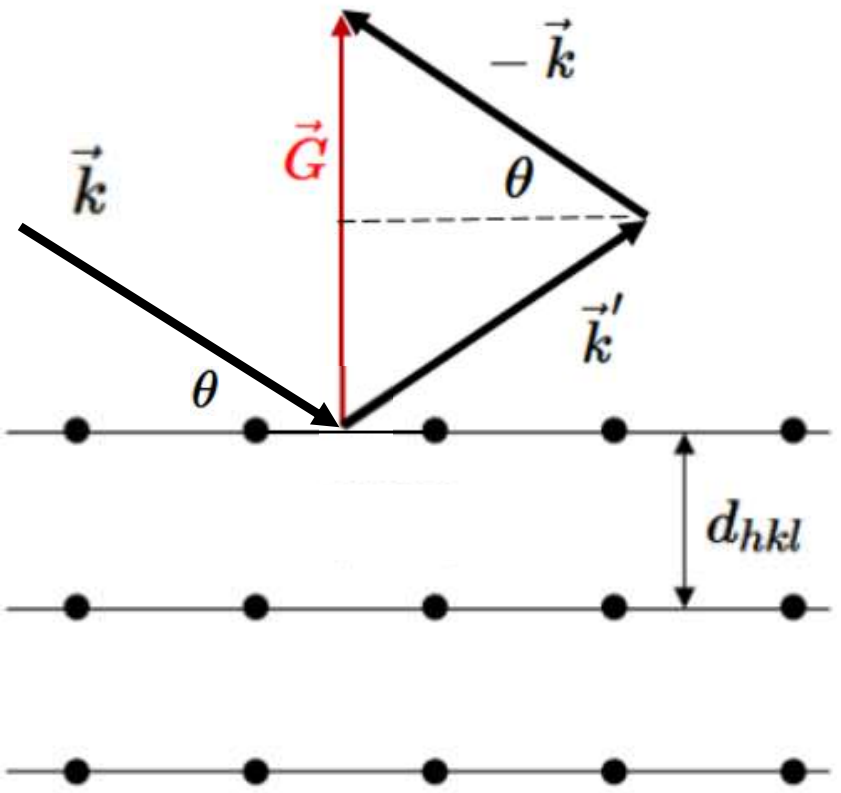
Weiss zone law

$$\vec{G}_{hkl} \cdot \vec{T}_{uvw} = 0 = \left(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3\right) \cdot (u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3) = 2\pi(hu + kv + wl)$$

$\vec{T}_{uvw}$ is in the (hkl) plane if $(hu + kv + wl) = 0$

Bragg diffraction

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



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

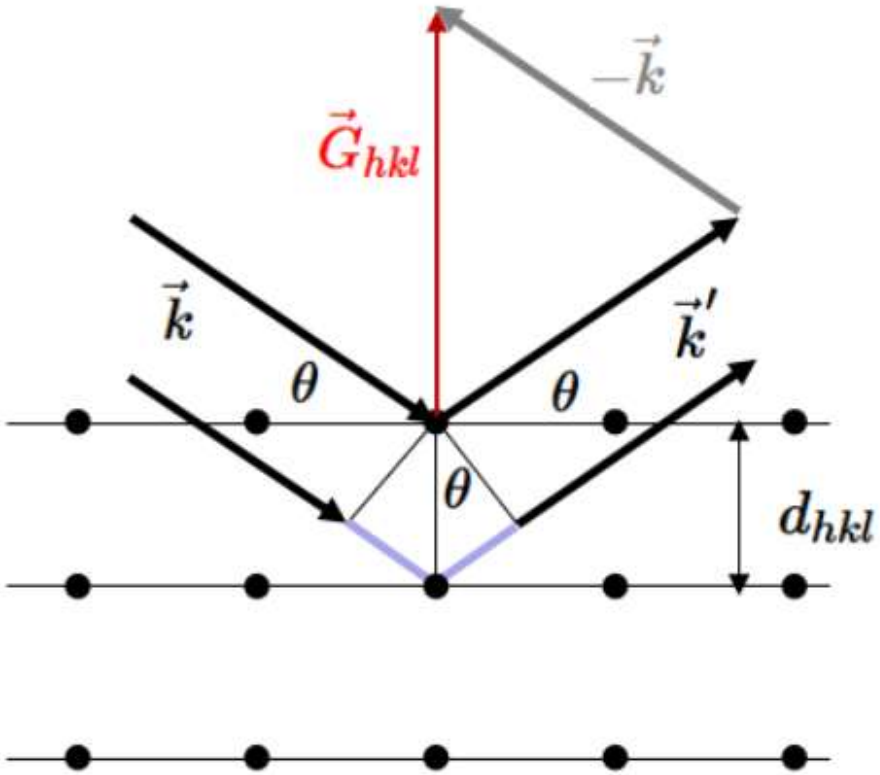
$$d_{hkl} = \frac{2\pi}{|\vec{G}_{hkl}|} \text{ and } \lambda = \frac{2\pi}{|\vec{k}|}$$

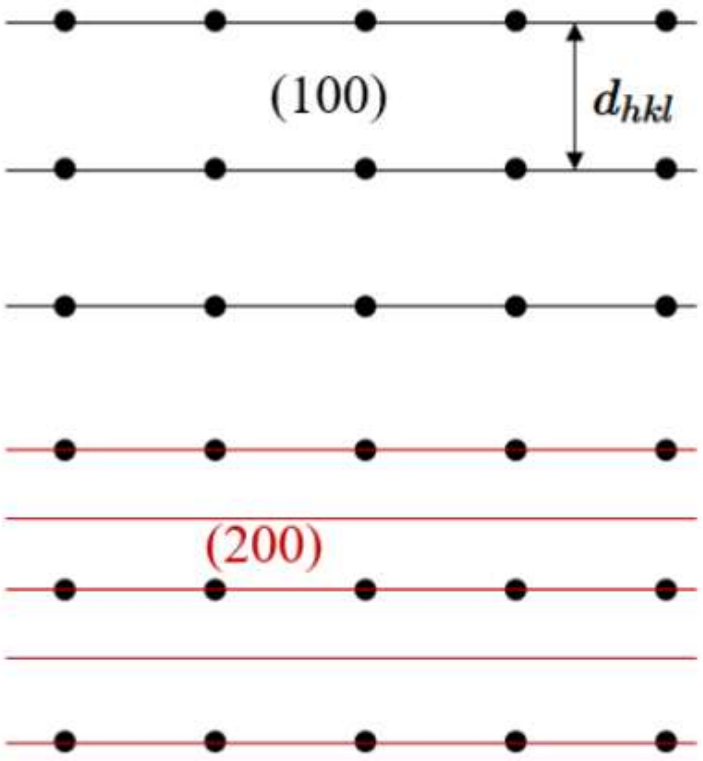
$$\lambda = 2d_{hkl} \sin\theta.$$

θ is the angle between $\vec{k}$ and the *hkl* netplane.

Bragg diffraction

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



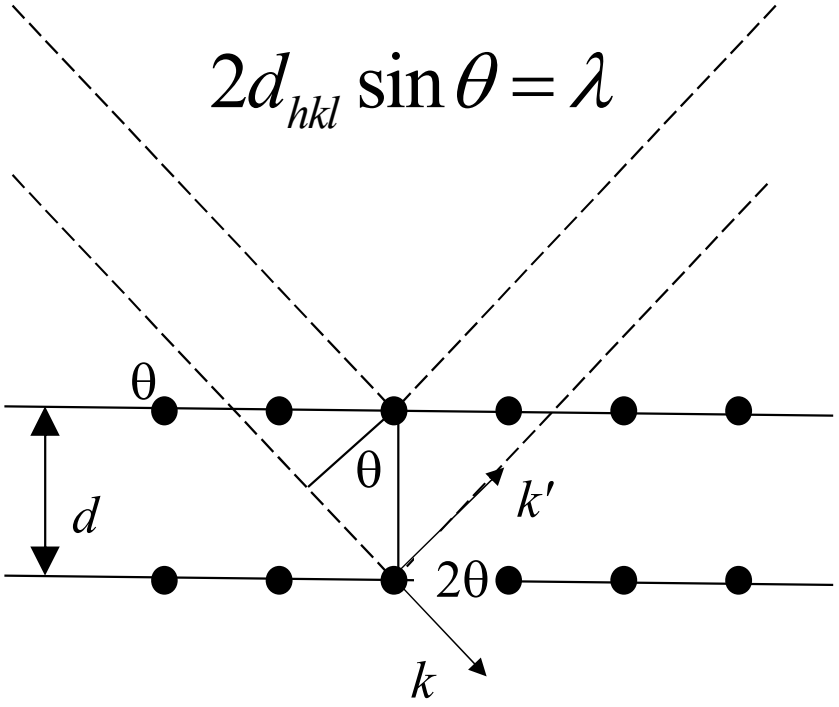


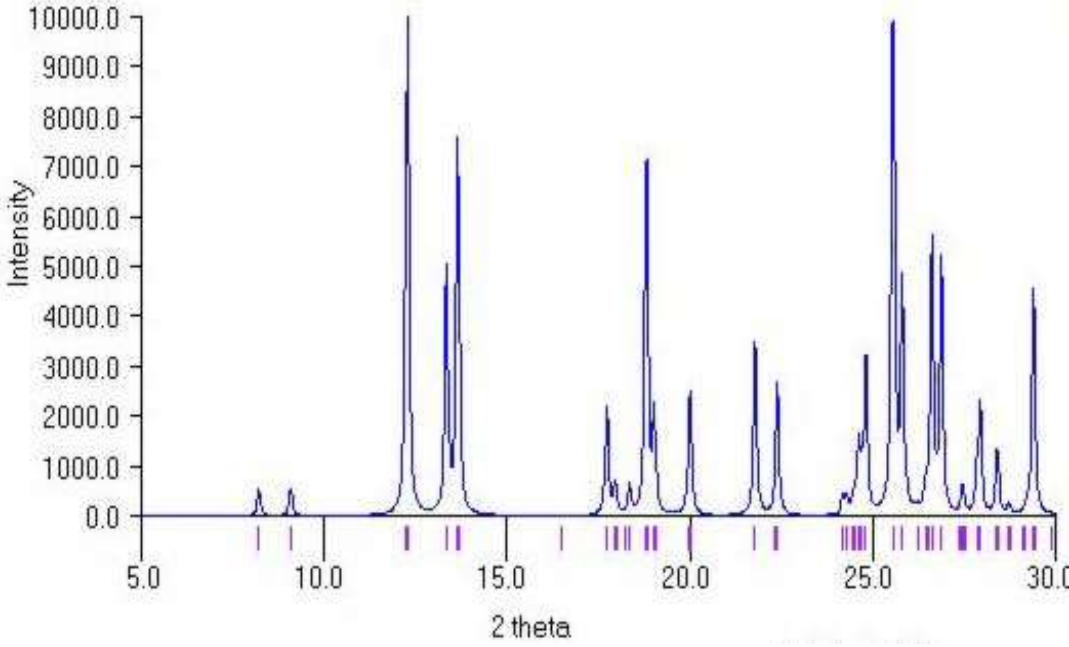
$$n\lambda = 2d_{hkl} \sin\theta.$$

↖ coprime

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.

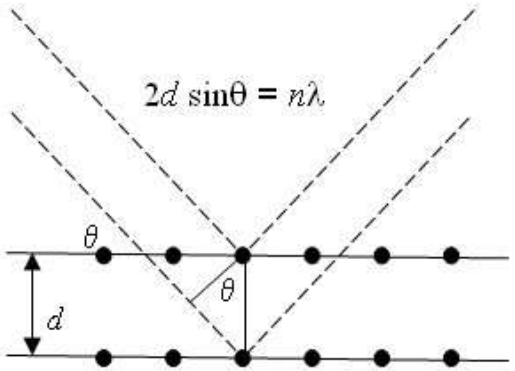




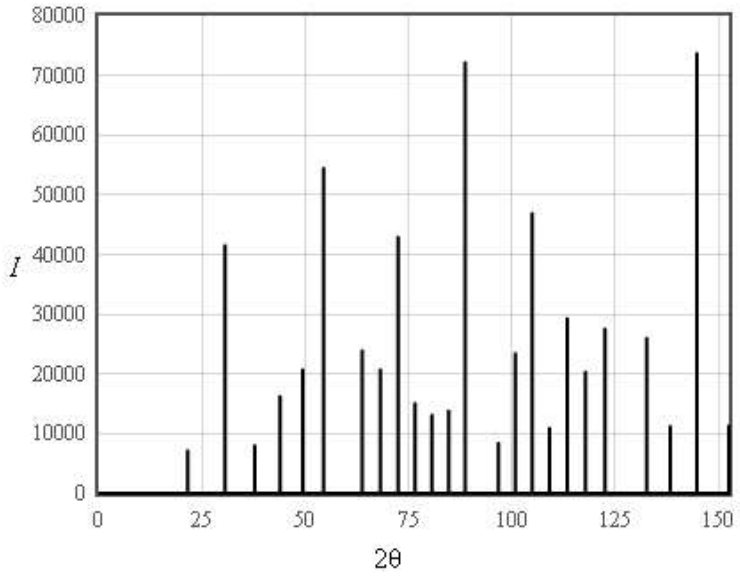
X-rays: Bragg diffraction

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 satisifies 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:

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

Basis:

The positions of the atoms are given in fractional coodinates 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	$\vec{a}_3$
		$\vec{a}_1 +$		$\vec{a}_2 +$		$\vec{a}_3$
		$\vec{a}_1 +$		$\vec{a}_2 +$		$\vec{a}_3$
		$\vec{a}_1 +$		$\vec{a}_2 +$		$\vec{a}_3$

X-ray wavelength λ [Å] = 1.540598 Cu Kα

submit

Al (fcc) | NaCl (fcc) | CsCl (sc) | SrTiO3 (perovskite, sc) | GaAs (Zincblend, fcc) | GaN (Wurtzite, hex)

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

American Mineralogist Crystal Structure Database

Abellaite	Abelsonite	Abenakiite-(Ce)	Abernathyite	Abhurite
Abswurmbachite	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)	Afghanite
Afmite	Afwillite			
Agardite-(Y)	Agrellite			
Ahlfeldite	Ahrensite			
Ajoite	Akaganeite			
Akhtenskite	Akimotoite			
Aktashite	Alabandite			
Albertiniite	Albite			
Alcaparrosaite	Alflarsenite			
Algodonite	Alinite			
Allanite-(Ce)	Allanite-(La)			
Allantoin	Allargentum			
Alloriite	Alluaivite			
Almeidaite	Alnaperboe			
Altaite	Althausite			
Alum-(Na)	Aluminite			
Aluminoceladonite	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 P
Cubic closest packed, ccp, str
_database_code_amcsd 0011137
4.04958 4.04958 4.04958 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 malink)

```
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
================================================================================
 XPOW Copyright 1993 Bob Downs, Ranjini Swaminathan and Kurt Bartelmehs
reference, see Downs et al. (1993) American Mineralogist 78, 1104-1107.
```

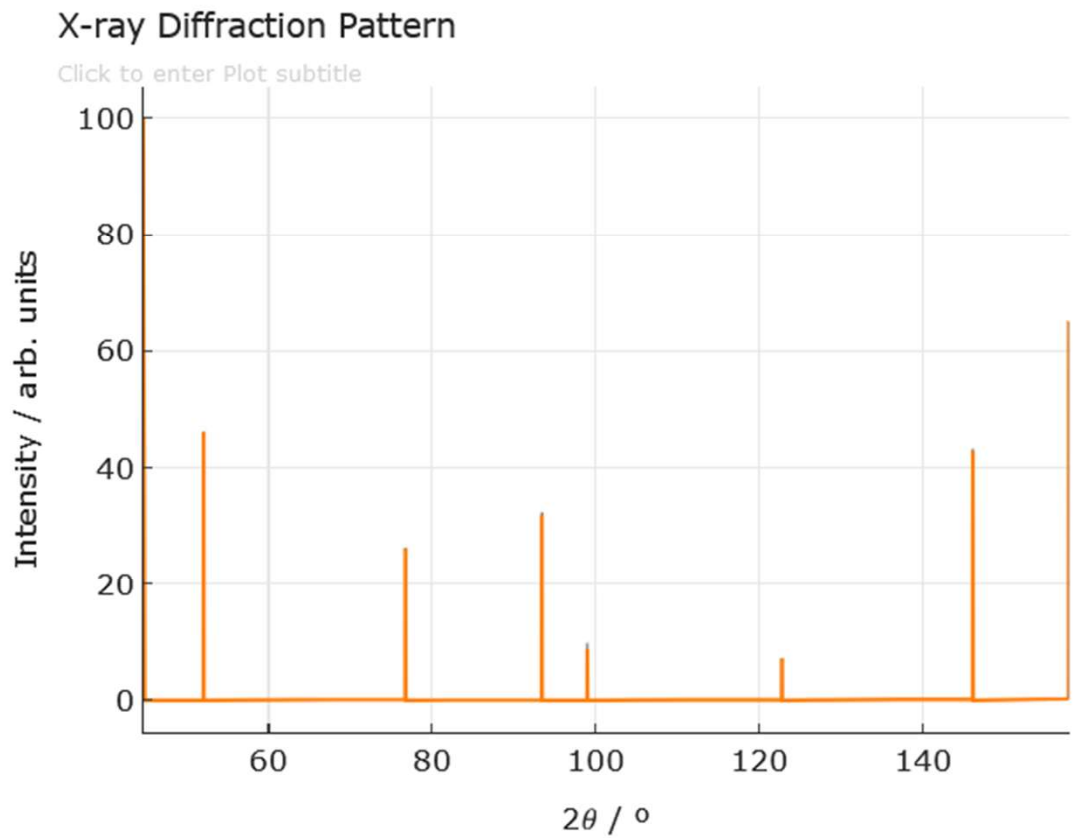
Materials Explorer

Diffraction Patterns

Data Methods API

Mode

X-ray Diffraction (Powder)



Radiation source

CuKα (1.542 Å)

Shape Factor

0.94

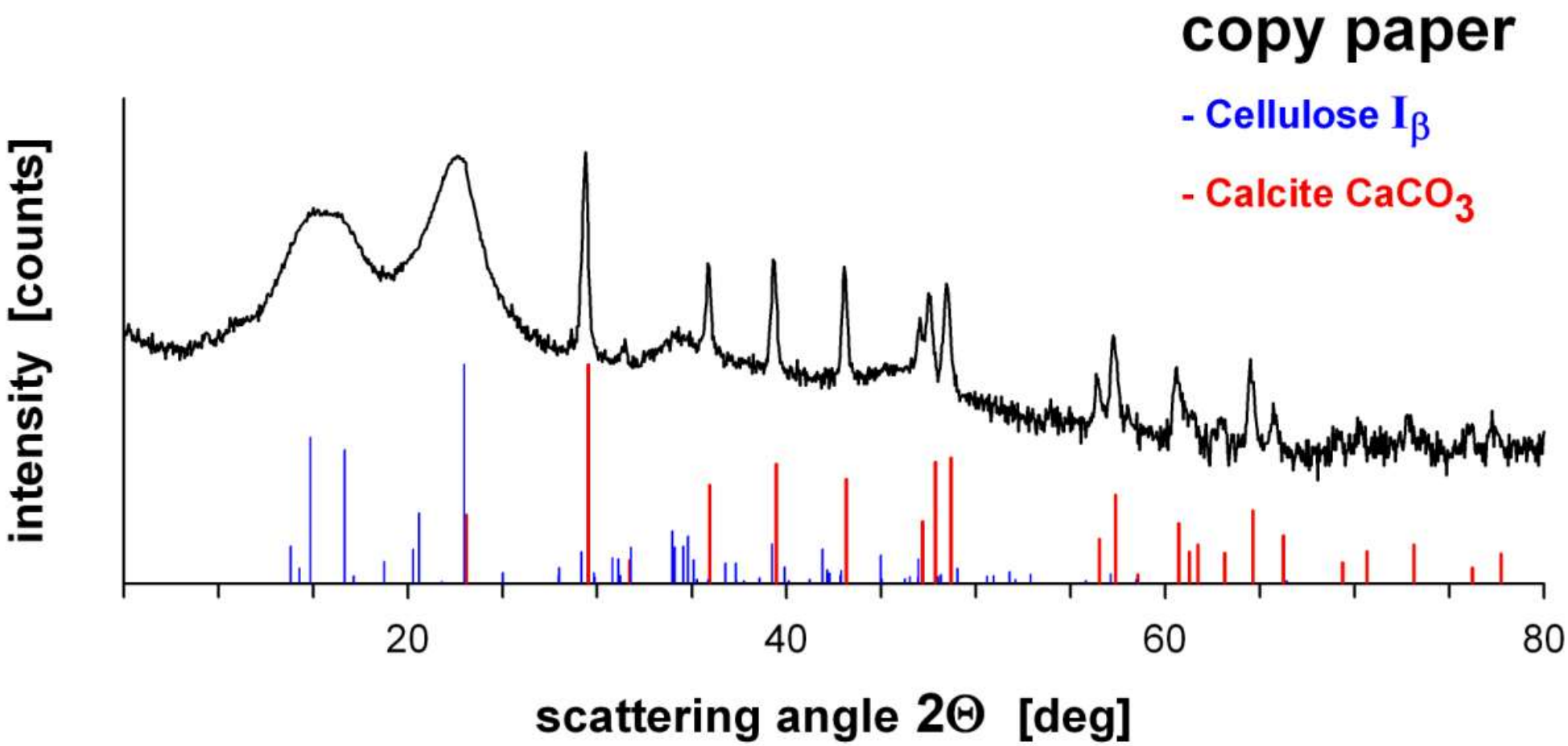
Peak Profile

Gaussian

Scherrer crystallite size / nm

10

0.1 1 10 100


copy paper
- Cellulose I_β
- Calcite $CaCO_3$
intensity [counts]
20
40
60
80
scattering angle 2Θ [deg]

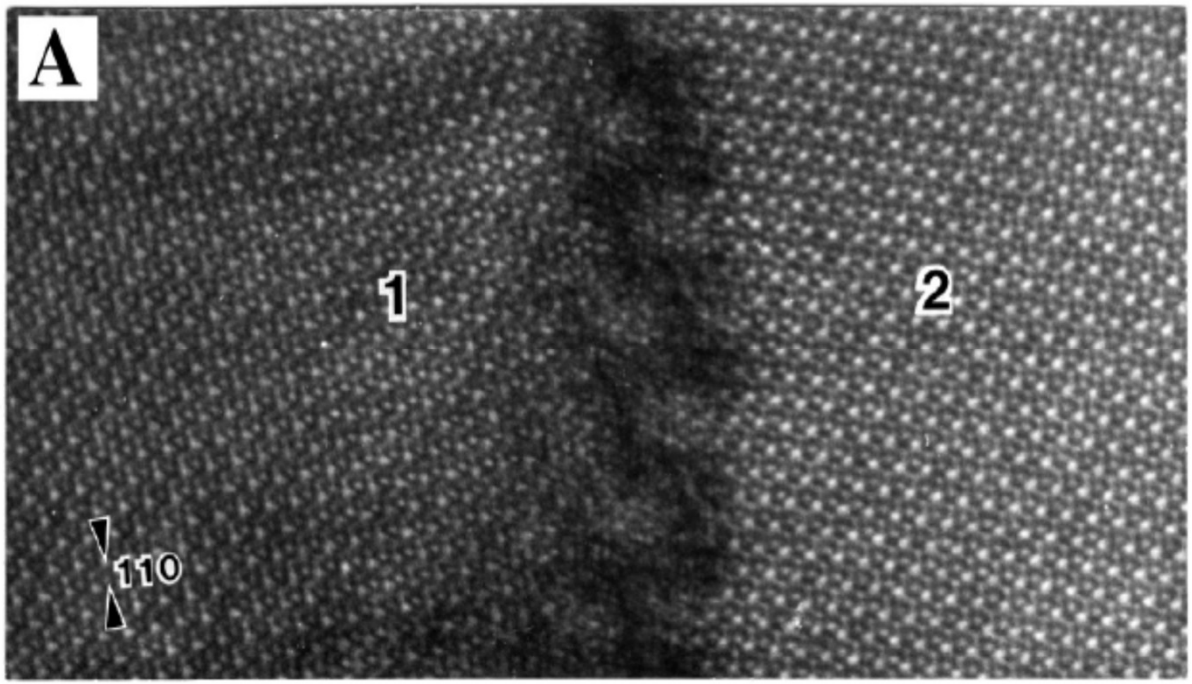
Powder diffraction

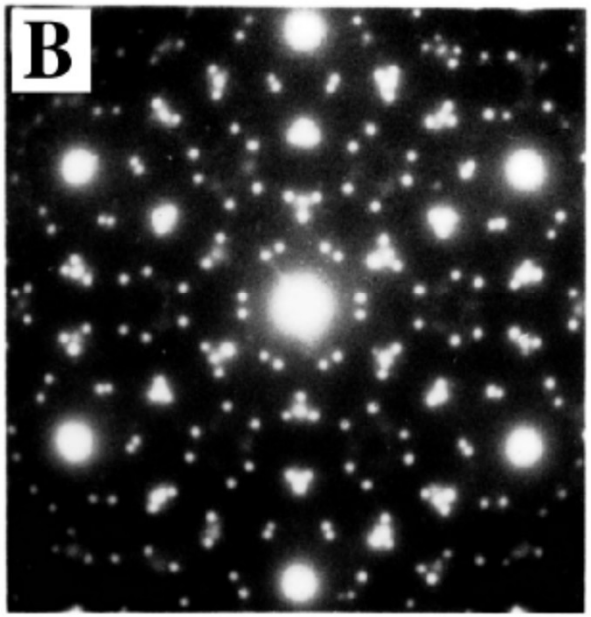
Phase identification
Every crystal has a specific "fingerprint" given by the positions and intensities of the diffraction peaks. The composition of a multi-phase specimen can be determined by fitting its diffraction pattern to the diffraction patterns of pure crystals which can be looked up in a database.

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.

Electron diffraction in a TEM





The wavelength of the electrons is typically much smaller than the lattice spacing. The diffraction peaks in the plane perpendicular to *k* are observed.

$$eV = \frac{mv^2}{2} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Electron diffraction

In electron diffraction, the intensity of a diffraction peak at reciprocal lattice vector $\vec{G}$ is the square of the structure factor, $n_{\vec{G}}$.

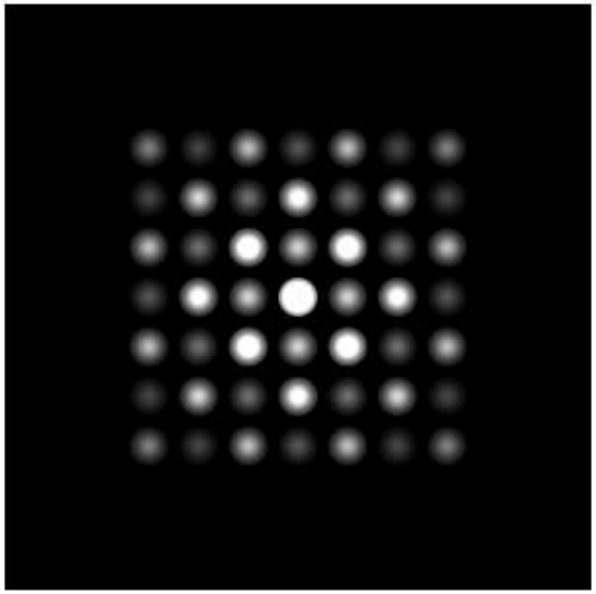
$$n_{\vec{G}} = \frac{1}{V}\sum_j f_j\left(\vec{G}\right)e^{-i\vec{G}\cdot\vec{r}_j} = \frac{1}{V}\sum_j f_j\left(\vec{G}\right)\left(\cos\left(\vec{G}\cdot\vec{r}_j\right) - i\sin\left(\vec{G}\cdot\vec{r}_j\right)\right)$$

Here V is the volume of the primitive unit cell, j sums over the atoms in the basis, $\vec{r}_j$ are the positions of the atoms in the basis, and $f_j\left(\vec{G}\right)$ are the electron atomic form factors evaluated at $\vec{G}$.

The form below calculates the electron structure factors based on this formula. The crystal structure is specified by providing the primitive lattice vectors and the positions of the atoms in the basis. A basis of up to five atoms can be calculated. The script first calculates the primitive reciprocal lattice vectors and from them calculates the reciprocal lattice vectors $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$.

On this page, the direction of the incoming electrons is given in terms of the primitive lattice vectors in reciprocal space, $H\vec{b}_1 + K\vec{b}_2 + L\vec{b}_3$. Usually the direction of the incoming electrons are given in terms of the conventional lattice vectors. Be aware that the [100] is a (usually) different direction if primitive lattice vectors are used than if conventional lattice vectors are used.

H: 1 *K*: 0 *L*: 0



[010] →

Primitive lattice vectors:

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

Basis:

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

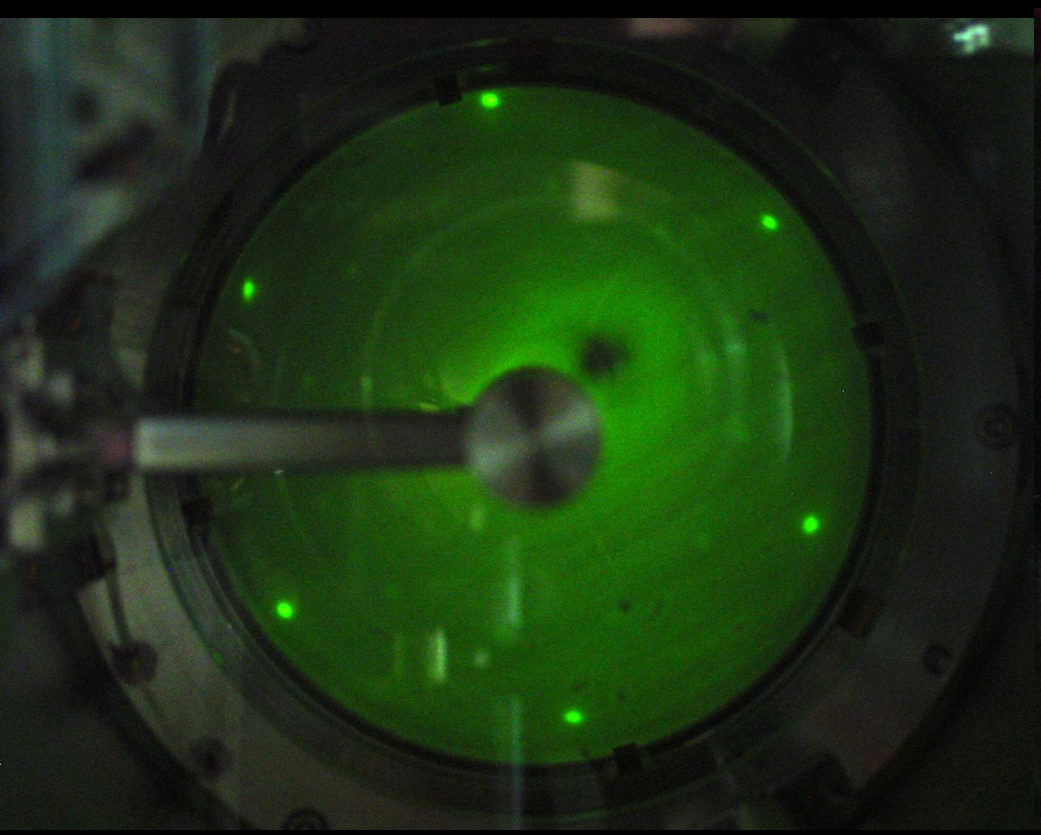
Cs	0	$\vec{a}_1 +$	0	$\vec{a}_2 +$	0	$\vec{a}_3$
Cl	0.5	$\vec{a}_1 +$	0.5	$\vec{a}_2 +$	0.5	$\vec{a}_3$
		$\vec{a}_1 +$		$\vec{a}_2 +$		$\vec{a}_3$
		$\vec{a}_1 +$		$\vec{a}_2 +$		$\vec{a}_3$
		$\vec{a}_1 +$		$\vec{a}_2 +$		$\vec{a}_3$

submit

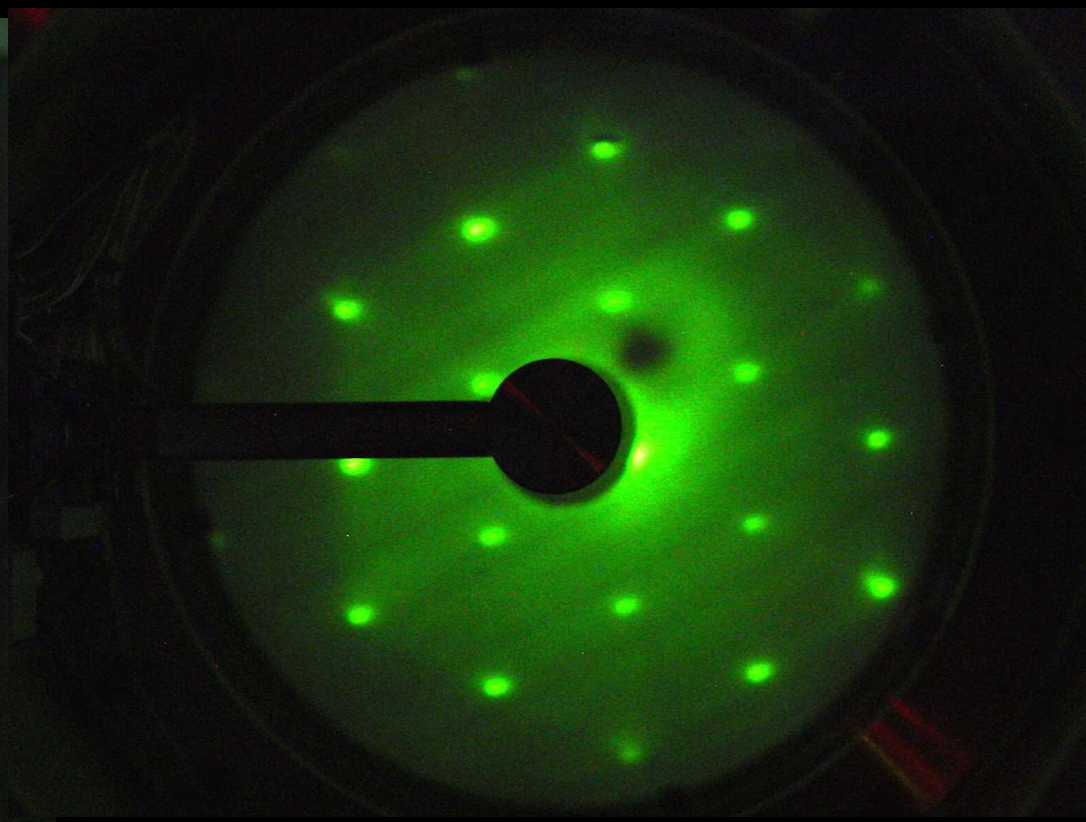
LEED

Low Energy Electron Diffraction

$100\ \text{V} \rightarrow k \sim 5 \times 10^{10}\ \text{m}^{-1}$



Clean Pd (111)



Pd (111) + 0.3 ML VO_x

LEED is surface sensitive

LEED

Energy of the electron beam: 100 [eV]

Primitive lattice vectors:

$\vec{a}_1 =$ 4.12E-10 $\hat{x} +$ 0 $\hat{y}$ [m]

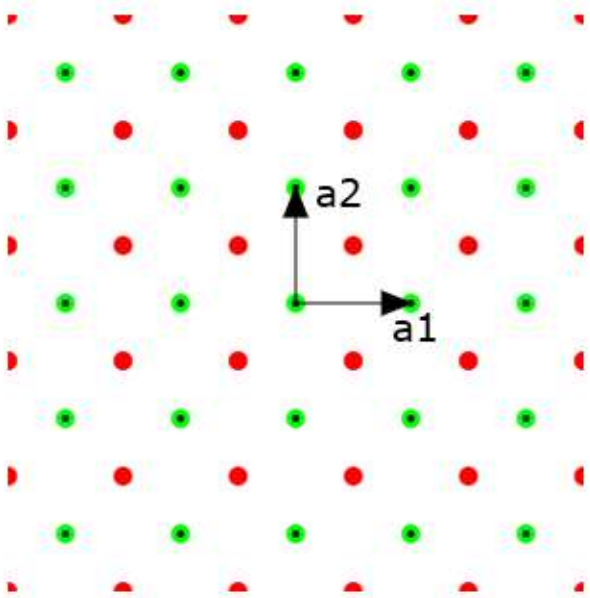
$\vec{a}_2 =$ 0 $\hat{x} +$ 4.12E-10 $\hat{y}$ [m]

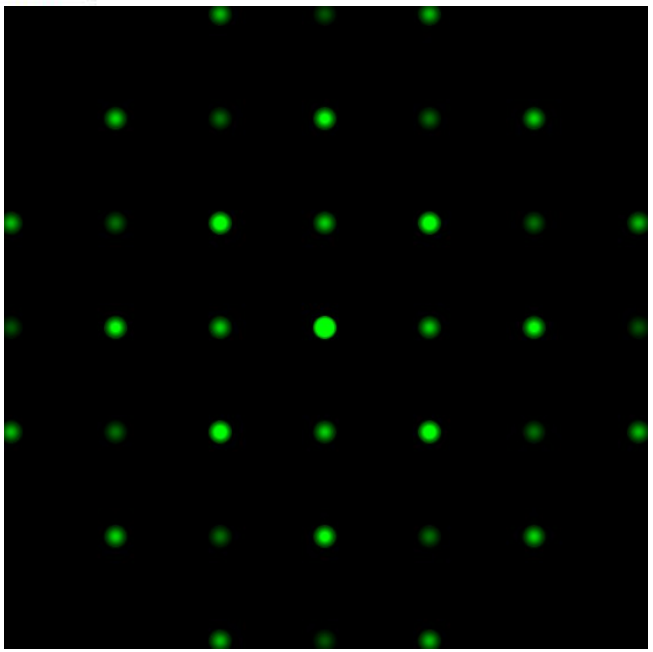
Basis:

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

Cs	0	$\vec{a}_1 +$	0	$\vec{a}_2$	
Cl	0.5	$\vec{a}_1 +$	0.5	$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	

submit





http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/atomicformfactors/LEED.php

Neutron diffraction

Typically a nuclear reactor is used as the neutron source

There are different atomic form factors for neutrons than for x-rays.

Determine the positions of H in biological samples.

Can for example distinguish between Fe and Co which have similar atomic form factors for x-rays.

Structure factor for neutrons

The structure factor for neutrons can be calculated with the following formula,

$$F_{\vec{G}} = \sum_j b_j e^{-i\vec{G}\cdot\vec{r}_j} = \sum_j b_j \left(\cos\left(\vec{G}\cdot\vec{r}_j\right) - i\sin\left(\vec{G}\cdot\vec{r}_j\right)\right).$$

where $\vec{r}_j$ defines the position of the atom j and $\vec{G}$ is the reciprocal lattice vector. $\vec{b}_j$ is called the neutron scattering length, it depends on the spin-state of the neutron-nucleus system and the isotope the neutron is scattered from. The scattering lengths can be looked up at the NIST Center for Neutron Research.

The form below calculates the neutron structure factors. The script first calculates the reciprocal lattice vectors and from them calculates the reciprocal lattice vectors $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$. The structure factors are calculated for a few reciprocal lattice vectors and listed in a table.

Primitive lattice vectors:

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

Basis:
The positions of the atoms are given in fractional coodinates between -1 and 1.

Pb	0	$\vec{a}_1+$	0	$\vec{a}_2+$	0	$\vec{a}_3$
Ti	0.5	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0.5	$\vec{a}_1+$	0	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0.5	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0	$\vec{a}_3$
		$\vec{a}_1+$		$\vec{a}_2+$		$\vec{a}_3$
		$\vec{a}_1+$		$\vec{a}_2+$		$\vec{a}_3$
		$\vec{a}_1+$		$\vec{a}_2+$		$\vec{a}_3$

submit

Forbidden reflections

Primitive lattice vectors:

$\vec{a}_1 =$ 4.12E-10 $\hat{x} +$ 0 $\hat{y}$ [m]

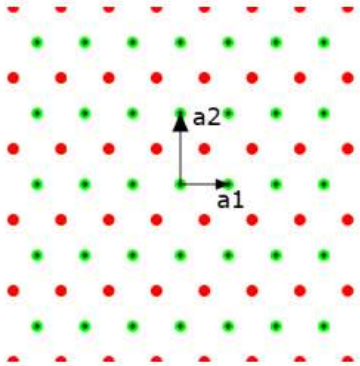
$\vec{a}_2 =$ 0 $\hat{x} +$ 6.12E-10 $\hat{y}$ [m]

Basis:

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

C	0	$\vec{a}_1 +$	0	$\vec{a}_2$	
C	0.5	$\vec{a}_1 +$	0.5	$\vec{a}_2$	
	0.2	$\vec{a}_1 +$	0.3	$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	

submit



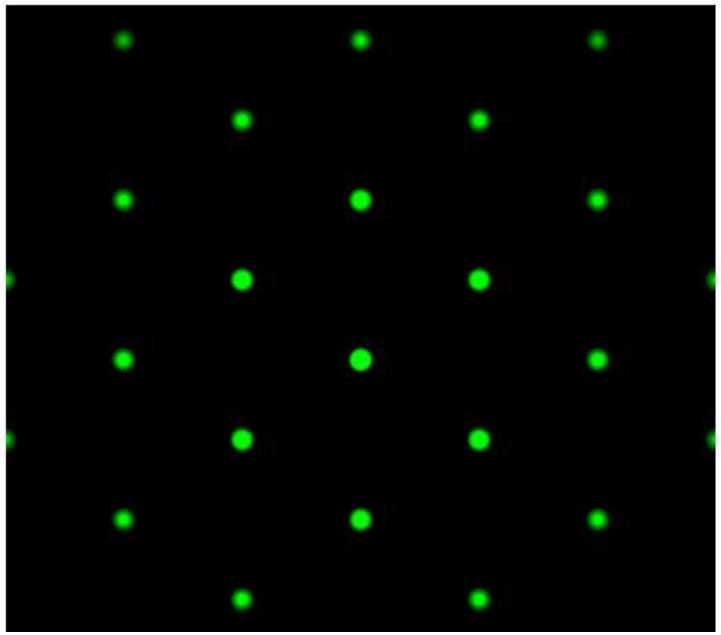
Primitive reciprocal lattice vectors

$\vec{b}_1 = 2\pi \frac{R\,\vec{a}_2}{\vec{a}_1 \cdot R\,\vec{a}_2} =$1.525e+10 $\hat{k}_x +$ 0.000 $\hat{k}_y$ [m^{-1}]

$\vec{b}_2 = 2\pi \frac{R\,\vec{a}_1}{\vec{a}_1 \cdot R\,\vec{a}_2} =$ 0.000 $\hat{k}_x +$ -1.027e+10 $\hat{k}_y$ [m^{-1}]

with $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

Low Energy
Electron Diffraction



Forbidden reflections

Primitive reciprocal lattice vectors

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 3.939\ \hat{k}_x + \text{-}2.275\text{e+}10\ \hat{k}_y + 0.000\ \hat{k}_z\ [\text{m}^{-1}]$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 3.939\ \hat{k}_x + 2.275\ \hat{k}_y + 0.000\ \hat{k}_z\ [\text{m}^{-1}]$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0.000\ \hat{k}_x + 0.000\ \hat{k}_y + 1.212\text{e+}10\ \hat{k}_z\ [\text{m}^{-1}]$$

Structure factors

The value of $|S_{\vec{G}}|$ 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 are proportional to $|S_{\vec{G}}|^2$. Note that elements with more electrons produce stronger diffraction intensities.

hkl	$\lvert\vec{G}\rvert$ Å^{-1}	$\lvert S_{\vec{G}}\rvert$	$\lvert S_{\vec{G}}\rvert^2$	Re$\{S_{\vec{G}}\}$	Im$\{S_{\vec{G}}\}$
000	0.000	51.97	2701	51.97	0.000
-100	1.553	0.000	0.000	0.000	0.000
0-10	1.553	0.000	0.000	0.000	0.000
00-1	1.553	0.000	0.000	0.000	0.000
001	1.553	0.000	0.000	0.000	0.000
010	1.553	0.000	0.000	0.000	0.000
100	1.553	0.000	0.000	0.000	0.000
-1-10	2.196	0.000	0.000	0.000	0.000
-10-1	2.196	0.000	0.000	0.000	0.000
-101	2.196	0.000	0.000	0.000	0.000
-110	2.196	0.000	0.000	0.000	0.000
0-1-1	2.196	0.000	0.000	0.000	0.000
0-11	2.196	0.000	0.000	0.000	0.000
01-1	2.196	0.000	0.000	0.000	0.000
011	2.196	0.000	0.000	0.000	0.000
1-10	2.196	0.000	0.000	0.000	0.000
10-1	2.196	0.000	0.000	0.000	0.000

Atomic beams

Hydrogen and Helium are used for diffraction studies

$$E = \tfrac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

Low energies can be used for delicate samples.
Measure the surface like LEED.

For the exam

- You should know the diffraction condition $\Delta\vec{k} = \vec{G}$ and be able to explain how the reciprocal lattice vectors can be determined in an experiment.
- Given the wavelength of the x-rays, you should be able to tell which diffraction peaks will occur in an experiment. This can be determined with the Ewald sphere.
- You should be able to explain how the Bravais lattice and the size of the unit cell can be determined from the measured reciprocal lattice vectors.
- You should know how to calculate structure factors from the atomic form factors and know that the square of the structure factors is proportional to the intensity of the diffraction peaks.
- You should know how the intensity of the diffraction peaks can be used to determine the basis of the crystal structure. (The basis is the pattern of atoms that are repeated at every Bravais lattice site to create the crystal.)
- Diffraction will occur if the incoming $\vec{k}$ vector falls on a Brillouin zone boundary. You should know how to construct the Brillouin zones of a crystal.
- The Bravais lattice points always fall on netplanes. The distance between two adjacent netplanes is $d_{hkl} = \frac{2\pi}{|\vec{G}_{hkl}|}$.

  You should be able to define netplanes and lattice planes. Lattice planes are specified by coprime integers h, k, and l, which are the same as the Miller indices.
- Diffraction can be explained in terms of reflections from lattice planes. In this interpretation, the diffraction condition can be written $n\lambda = 2d_{hkl}\sin\theta$ where h, k, and l are coprime, λ is the wavelength and n is a nonnegative integer.
- You should be able to explain: powder diffraction, electron diffraction, LEED, and neutron diffraction.