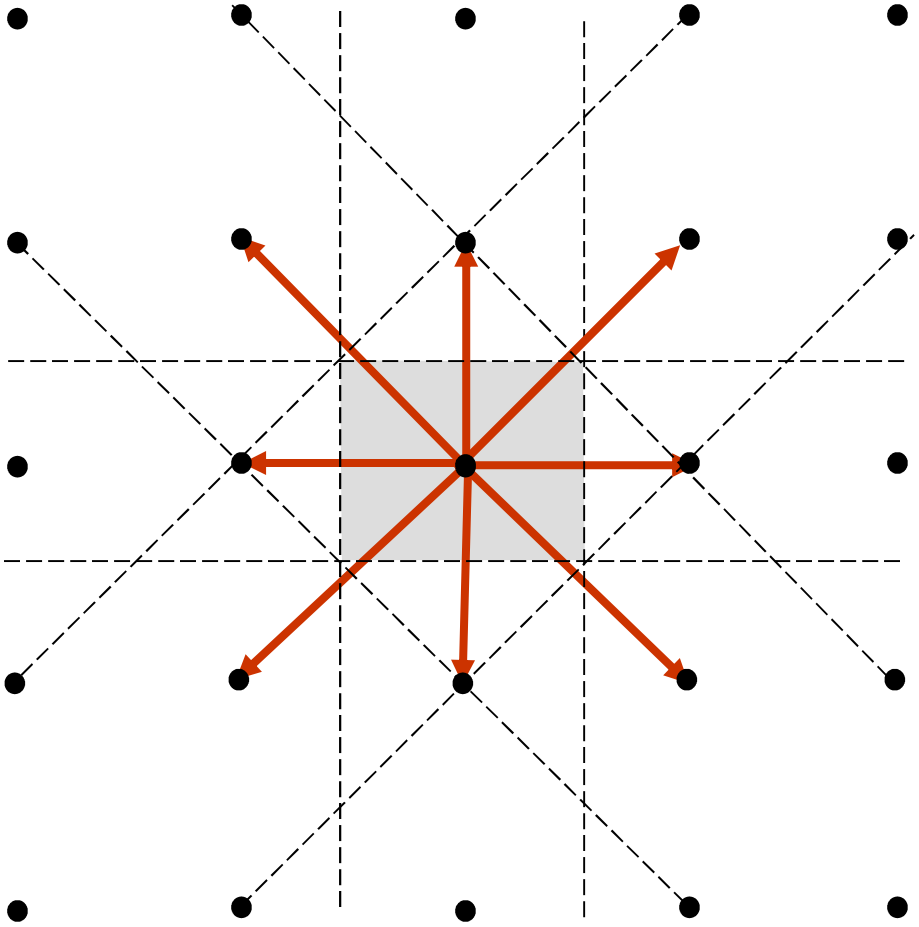
Diffraction

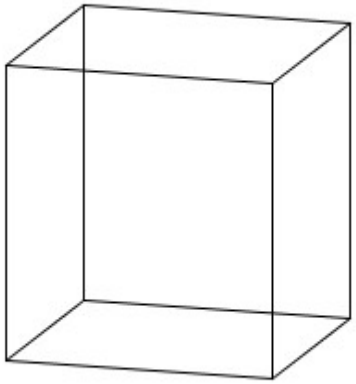
Brillouin zones

Leon Brillouin

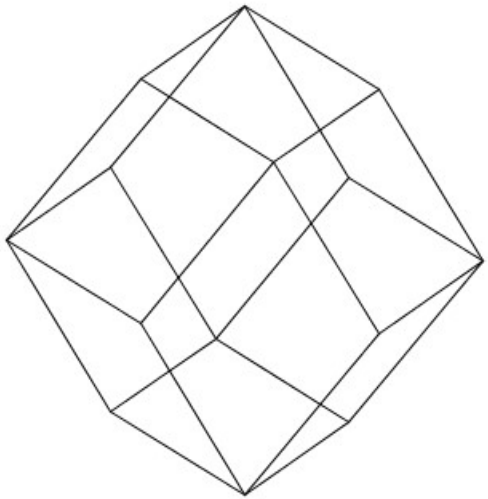


1st Brillouin zone consists of the *k*-states around the origin that can be reached without crossing a plane.

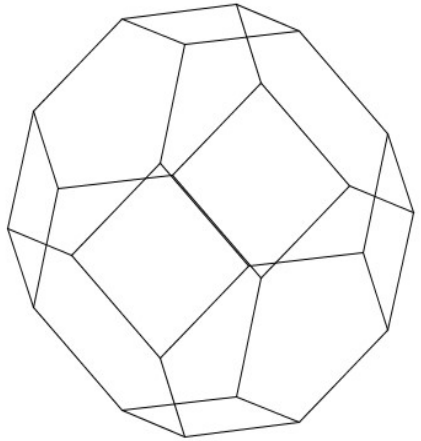
1st Brillouin zones



sc



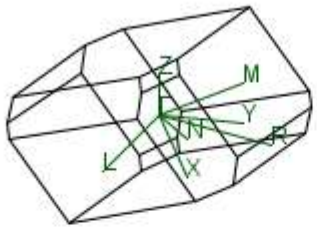
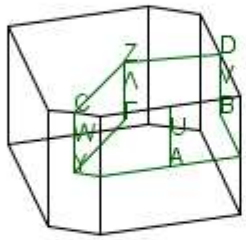
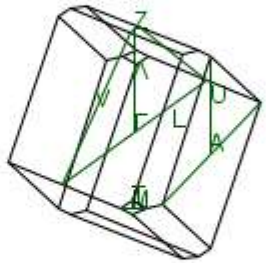
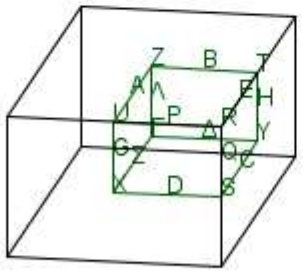
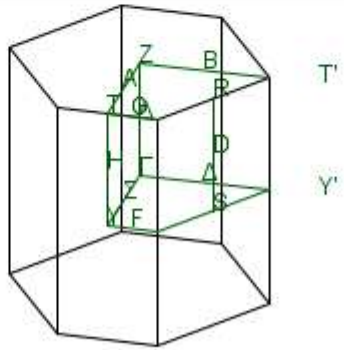
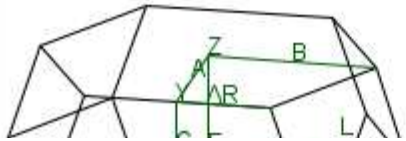
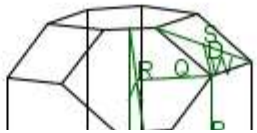
bcc



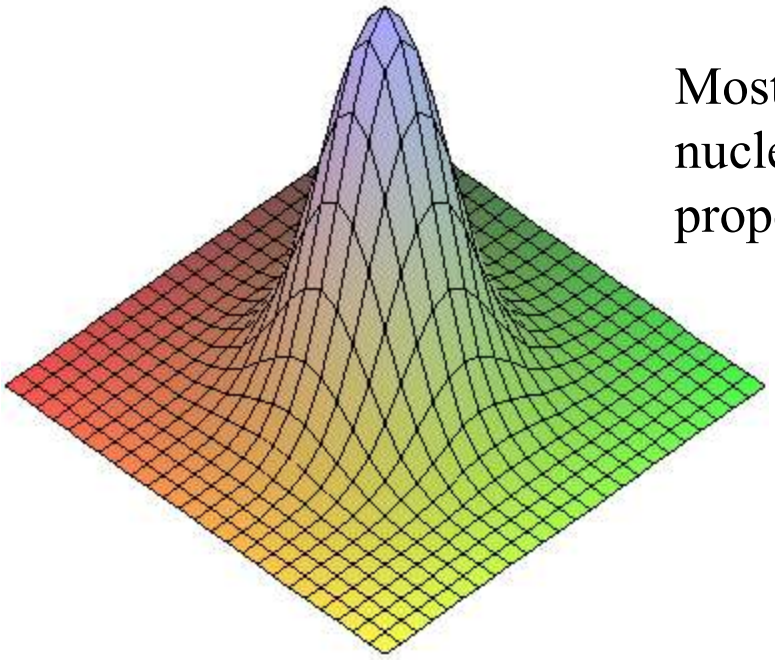
fcc

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

Brillouin zones

Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	 Triclinic	
Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$ $\beta = \gamma = 90°$	 Monoclinic simple	 Monoclinic Base centered
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	 Orthorhombic simple	 Base centered
		

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.

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

Approximately a Gaussian centered at r_j

Electron density

Write the electron density as a Fourier series

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

Translation vector

position of atom j of the basis

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

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

1

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

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

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

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

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

sum over the basis

position of atom *j* of the basis

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Section 4.3.2. Parameterizations of electron atomic scattering factors

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$s = G$

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

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

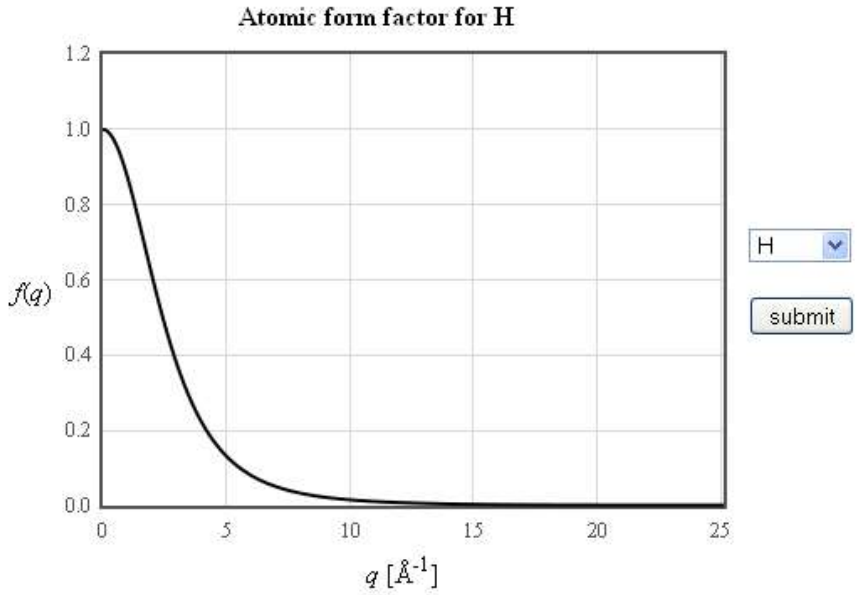
Element	Z	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5
H	1	0.0349	0.1201	0.1970	0.0573	0.1195	0.5347	3.5867	12.3471	18.9525	38.6269
He	2	0.0317	0.0838	0.1526	0.1334	0.0164	0.2507	1.4751	4.4938	12.6646	31.1653
Li	3	0.0750	0.2249	0.5548	1.4954	0.9354	0.3864	2.9383	15.3829	53.5545	138.7337
Be	4	0.0780	0.2210	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

Atomic form factors

In the range of scattering vectors between $0 < q < 25$ Å^{-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.



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
H1-	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

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

submit

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

Primitive reciprocal lattice vectors

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

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	$\lvert\vec{G}\rvert$ Å^{-1}	$\lvert n_{\vec{G}}\rvert$	$\lvert n_{\vec{G}}\rvert^2$	$\mathrm{Re}\{n_{\vec{G}}\}$	$\mathrm{Im}\{n_{\vec{G}}\}$
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

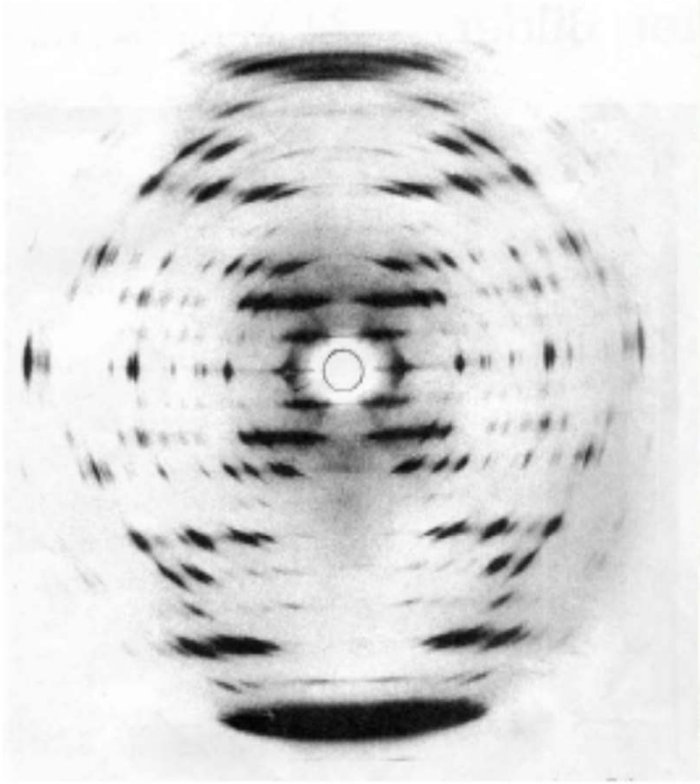
Structure factor

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

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

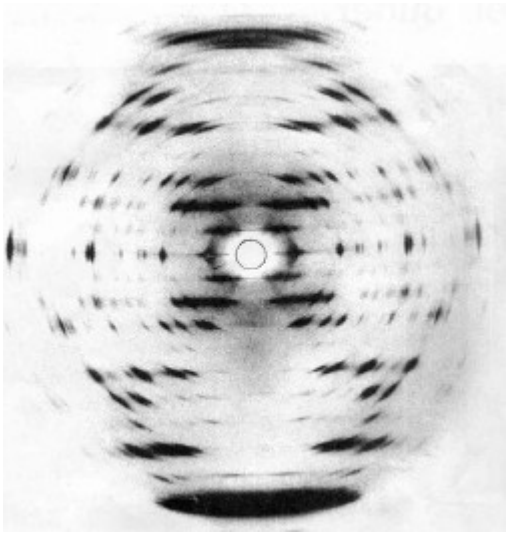
crystal structure solution

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 |
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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
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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

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

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

Sum over basis

position of atom j of the basis

Compare $|n_G|^2$ to the measurements

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.

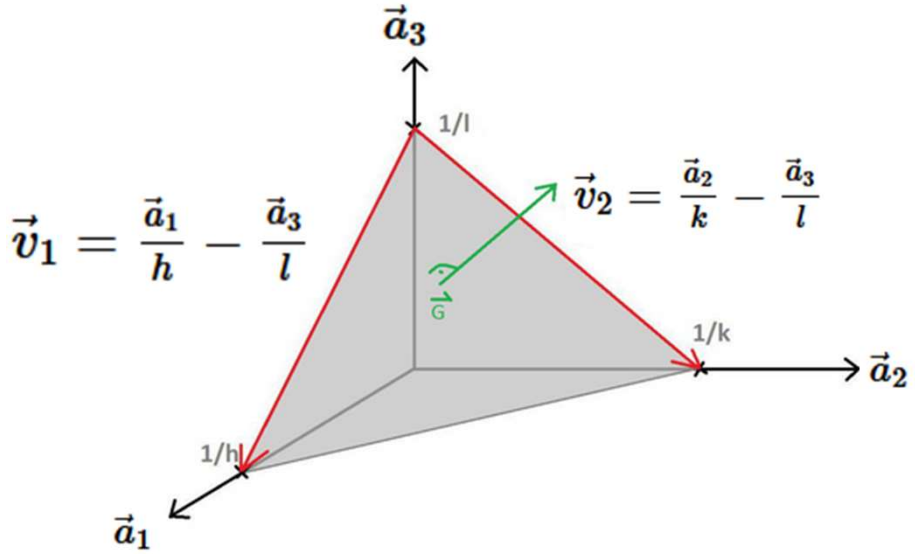
Solid State Physics, Ibach and Lüth

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

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

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

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



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

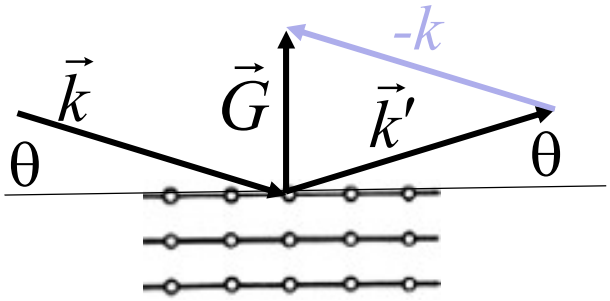
$$\vec{v}_1 \cdot \vec{G}_{hkl} = \left(\frac{1}{h} h\vec{b}_1 \cdot \vec{a}_1 - \frac{1}{l} l\vec{a}_3 \cdot \vec{b}_3\right) = 2\pi - 2\pi = 0$$

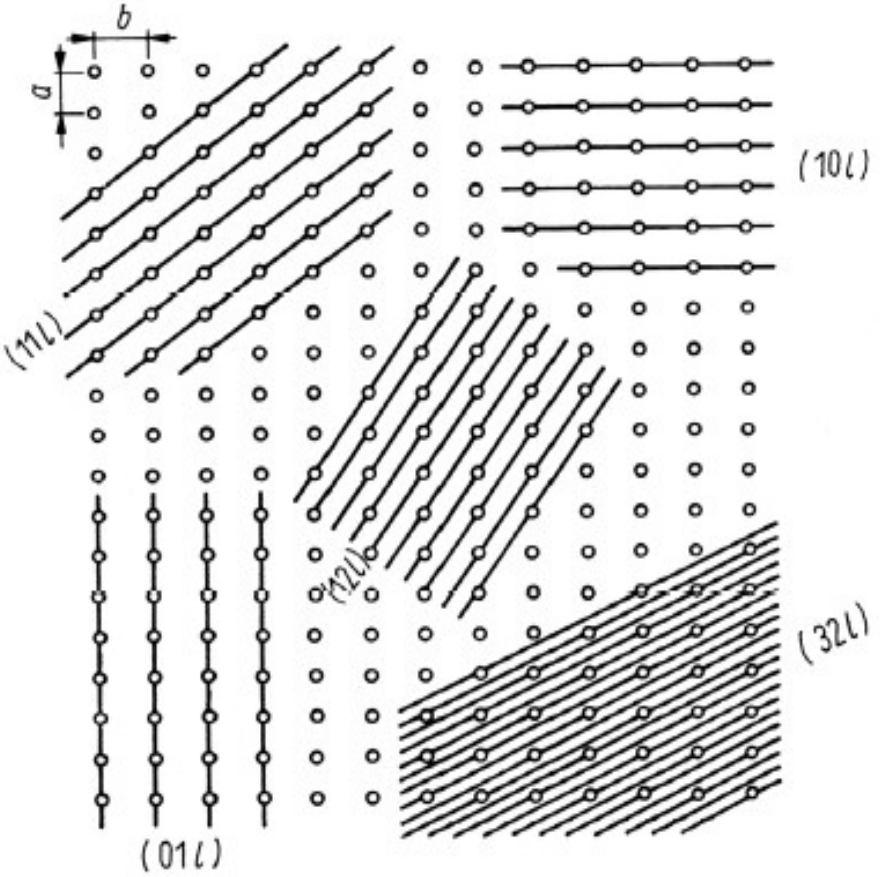
$$\vec{v}_2 \cdot \vec{G}_{hkl} = \left(\frac{1}{k} k\vec{a}_2 \cdot \vec{b}_2 - \frac{1}{l} l\vec{b}_3 \cdot \vec{a}_3\right) = 2\pi - 2\pi = 0$$

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

x-ray diffraction

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



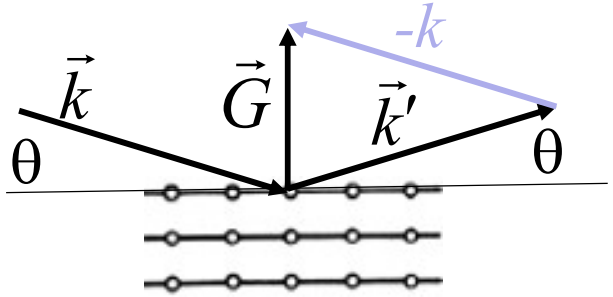


$$\left|\vec{G}_{hkl}\right| = \frac{2\pi}{d_{hkl}}$$

distance between the net planes

x-ray diffraction

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



$$\left|\vec{G}_{hkl}\right| = \left|\Delta\vec{k}\right| = 2\left|\vec{k}\right| \sin\theta$$

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

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

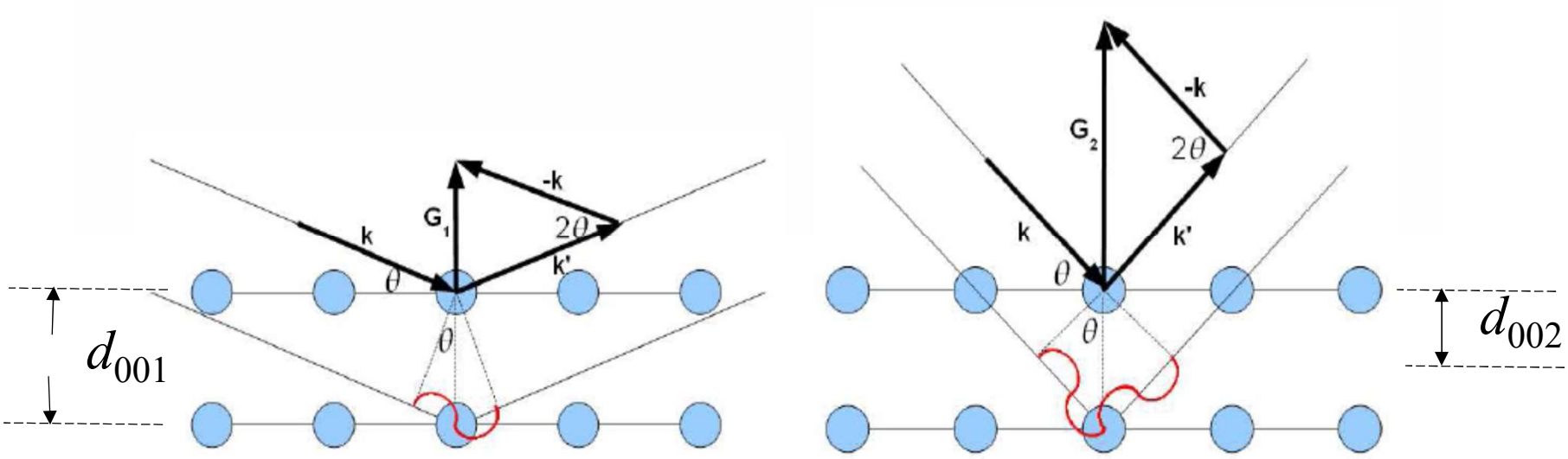
$$\frac{2\pi}{d_{hkl}} = 2\frac{2\pi}{\lambda}\sin\theta$$

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

Bragg and Laue conditions

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

Laue condition: $\Delta\vec{k} = \vec{G} \quad \Leftrightarrow \quad 2d_{hkl}\sin\theta = \lambda$

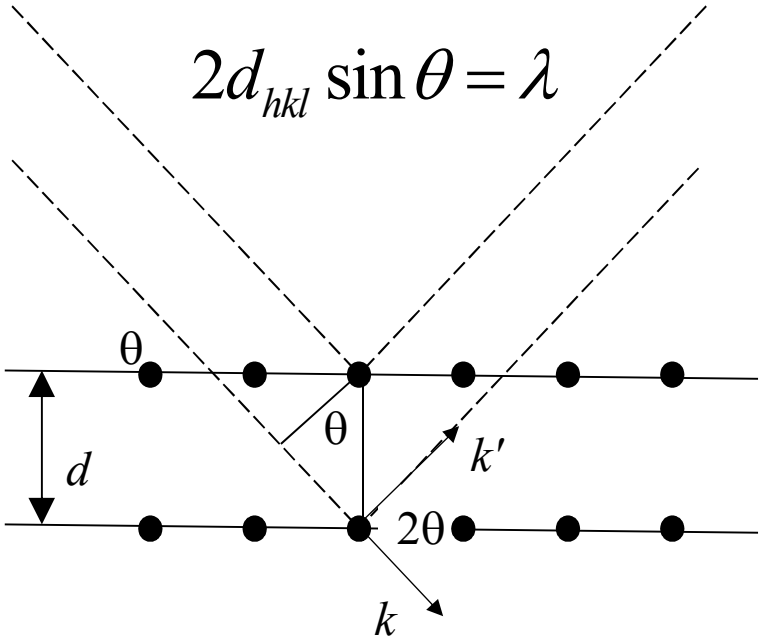


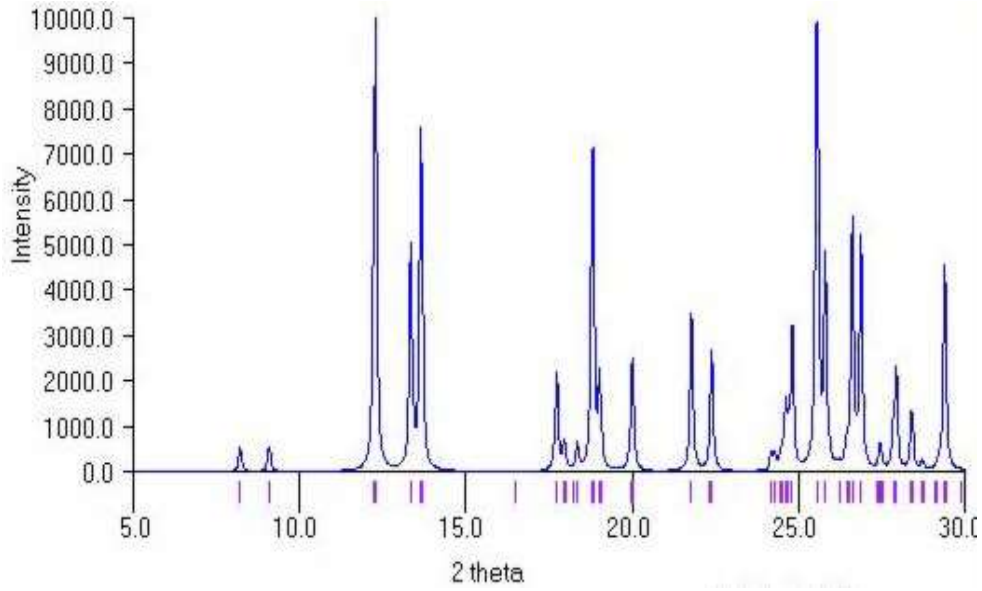
$n = 1 \Leftrightarrow 001$

$n = 2 \Leftrightarrow 002$

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.

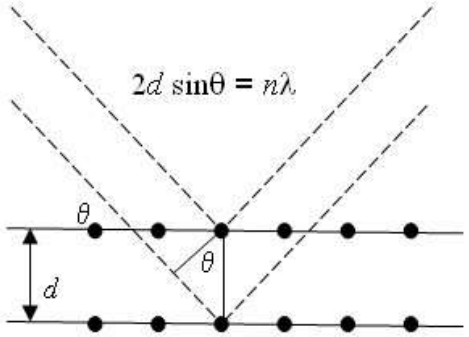




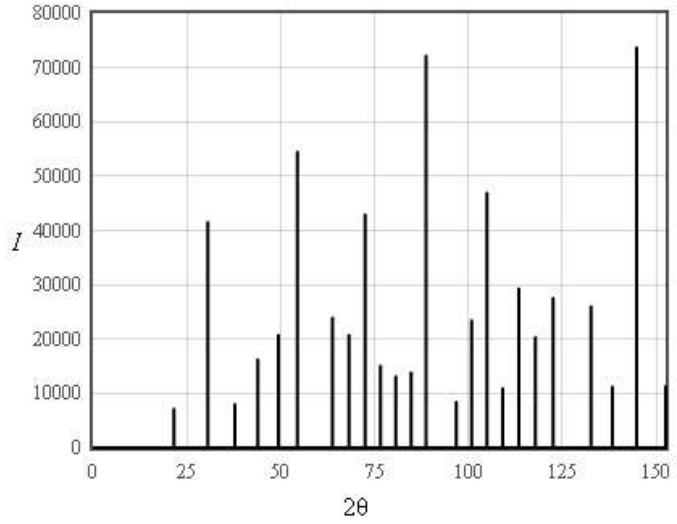
X-rays: Bragg diffraction

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 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:

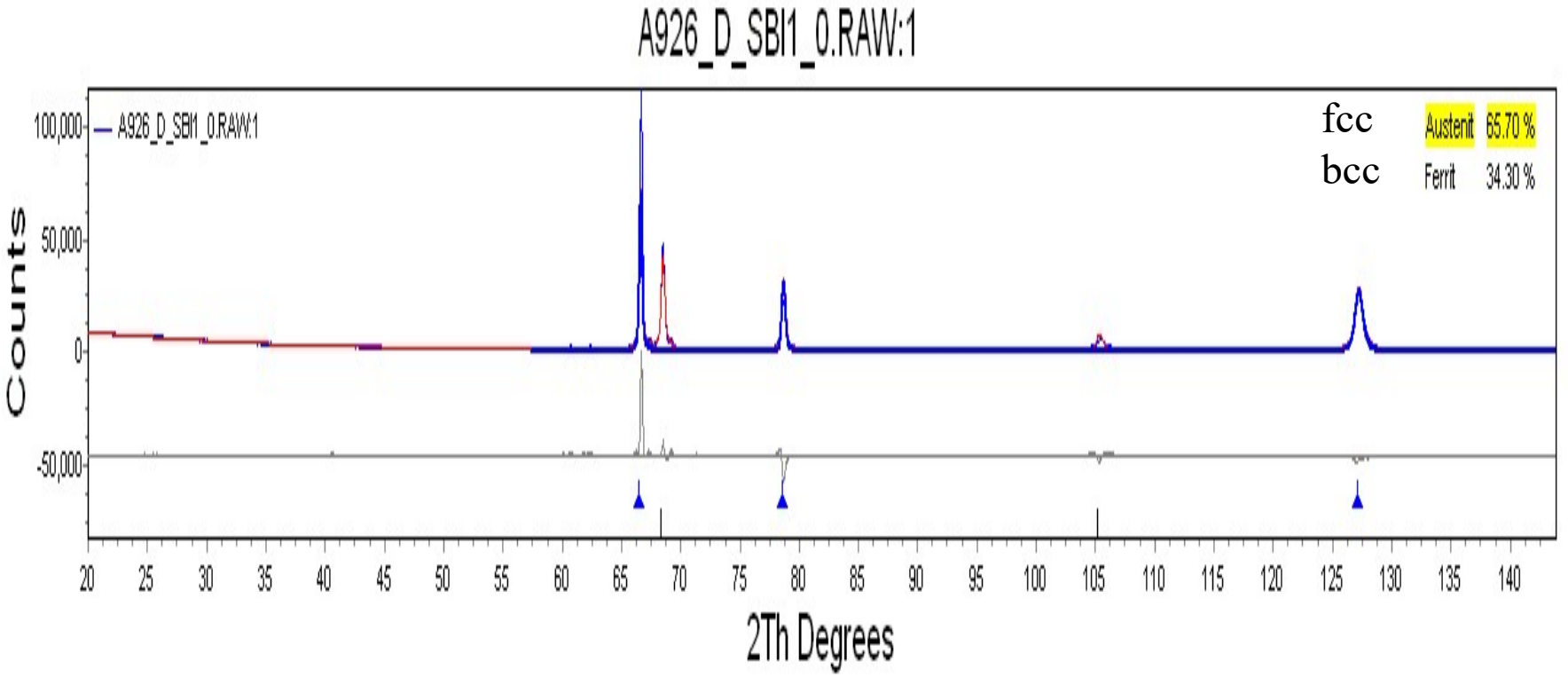
The positions of the atoms are given in fractional coodinates between -1 and 1.

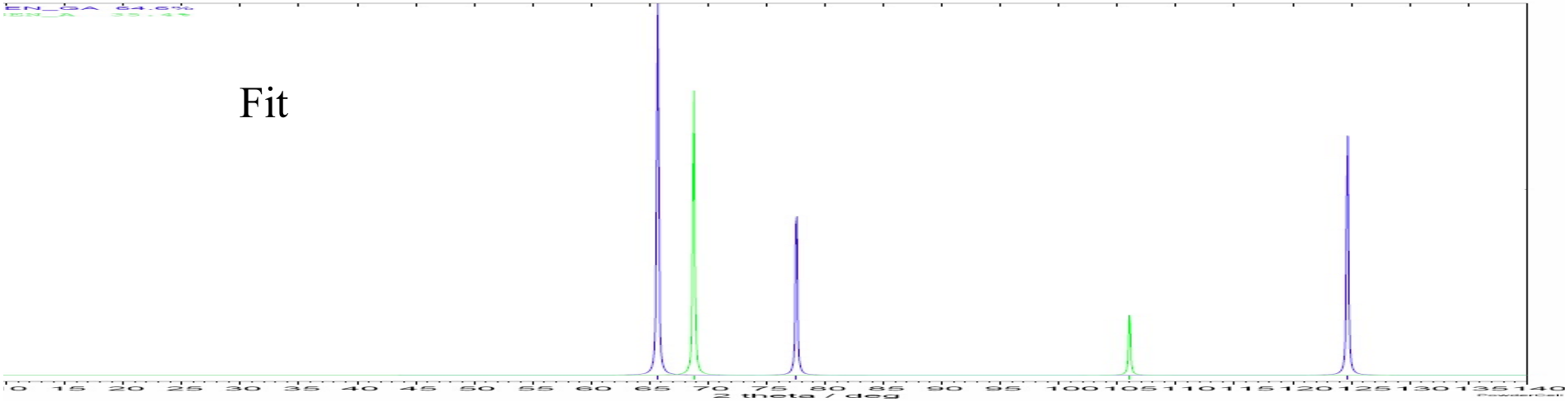
Cs1+	0	$\vec{a}_1$ +	0	$\vec{a}_2$ +	0	$\vec{a}_3$
Cl1-	0.5	$\vec{a}_1$ +	0.5	$\vec{a}_2$ +	0.5	$\vec{a}_3$
		$\vec{a}_1$ +		$\vec{a}_2$ +		$\vec{a}_3$
		$\vec{a}_1$ +		$\vec{a}_2$ +		$\vec{a}_3$
		$\vec{a}_1$ +		$\vec{a}_2$ +		$\vec{a}_3$

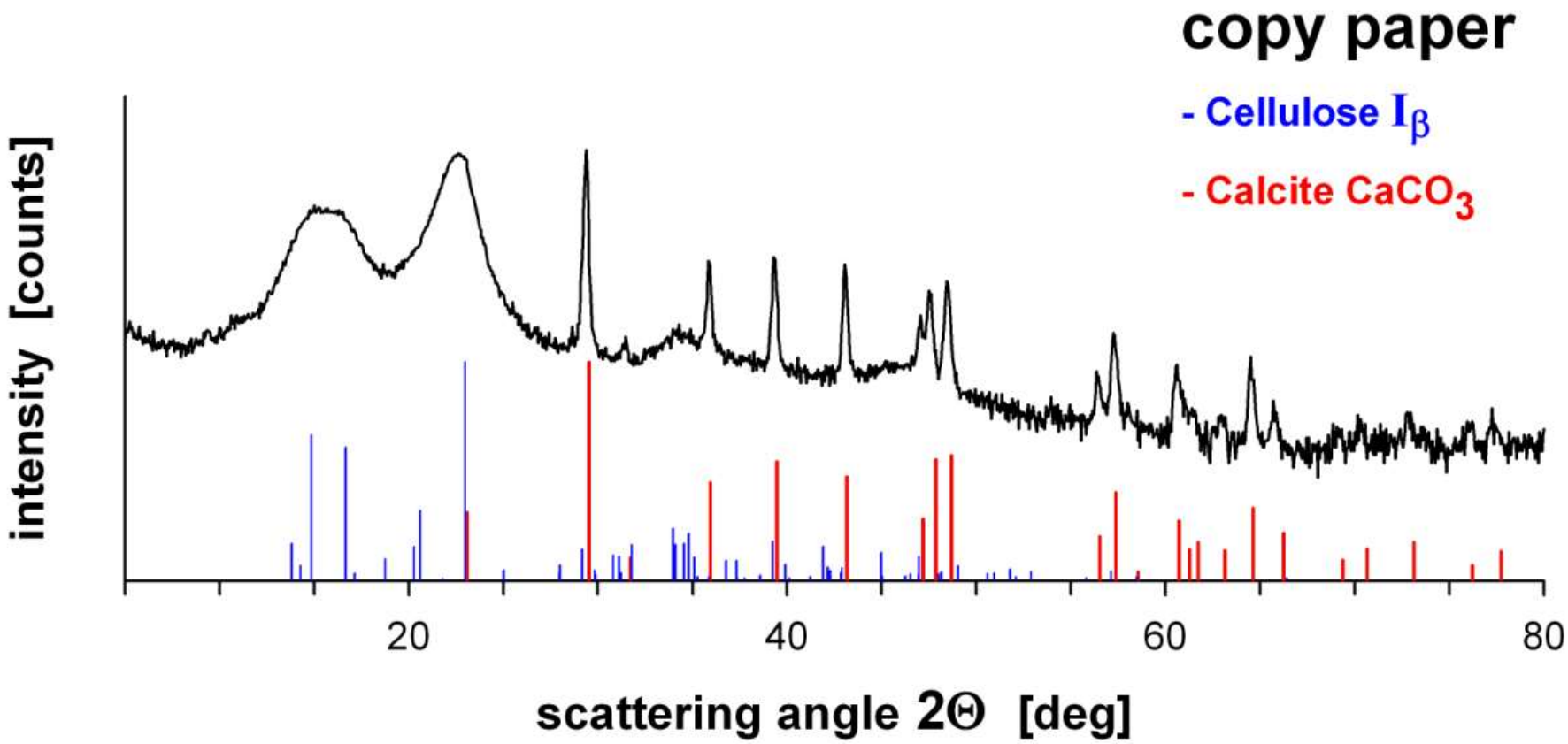
X-ray wavelength λ [Å] = 1.540598 Cu Kα

submit

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


A926_D_SBI1_0.RAW:1
A926_D_SBI1_0.RAW:1
fcc
bcc
Austenit 65.70 %
Ferrit 34.30 %
Counts
100,000
50,000
0
-50,000
20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140
2Th Degrees


Fit
2 theta / deg


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

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	Alnaperboei			
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 (permalink)

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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.
```

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
Release 2024: 1186076 material data sets

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

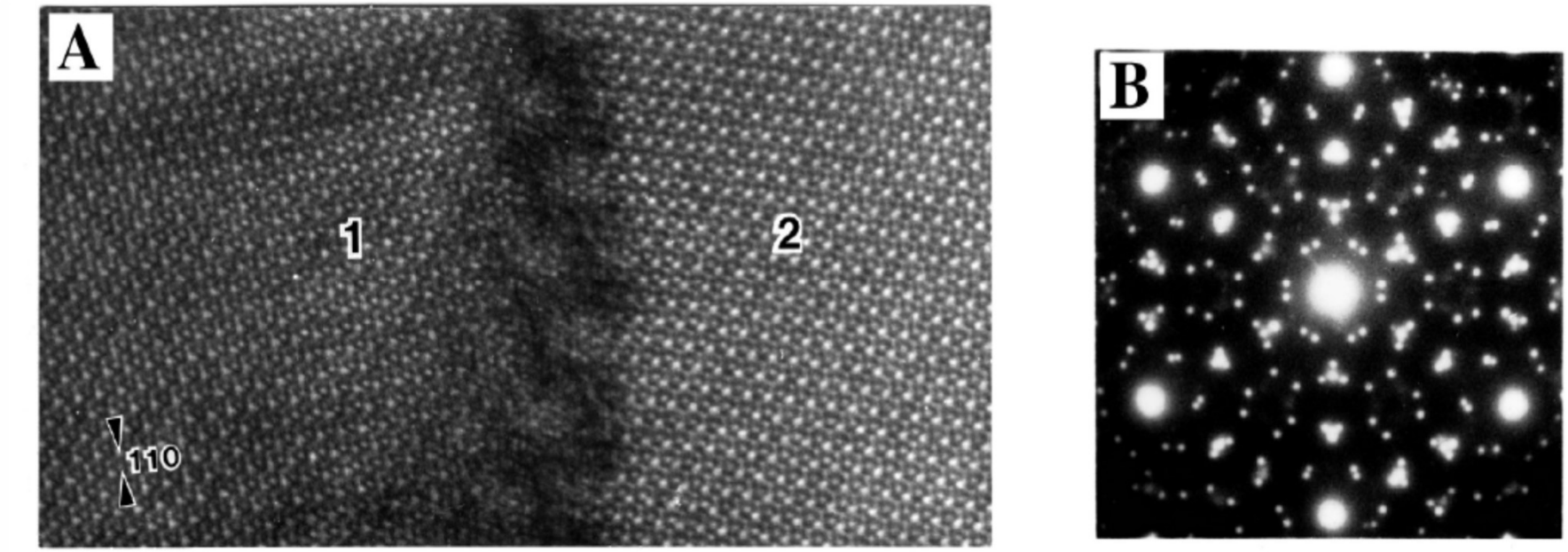
Particle beams

Particles moving in vacuum have the following energy-momentum relation.

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

If λ is much smaller than the distance between atoms, you can generate a diffraction pattern.

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.

Electron diffraction

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

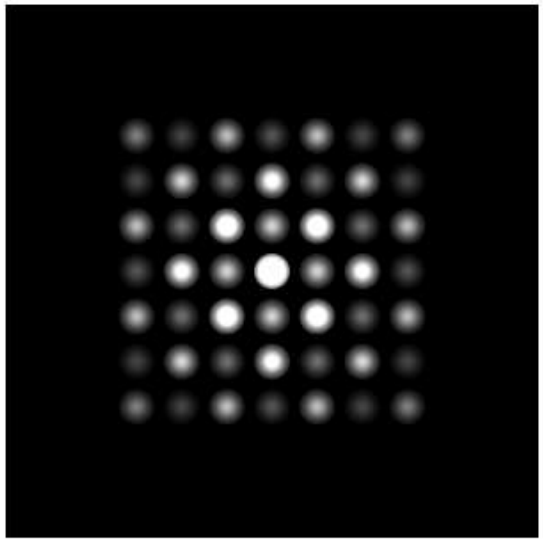
$$n_{\vec{G}} = \frac{1}{V}\sum_j f_j\left(\vec{G}\right)e^{-i\vec{G}\cdot\vec{r}_j} = \frac{1}{V}\sum_j f_j\left(\vec{G}\right)\left(\cos\left(\vec{G}\cdot\vec{r}_j\right) - i\sin\left(\vec{G}\cdot\vec{r}_j\right)\right)$$

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

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.

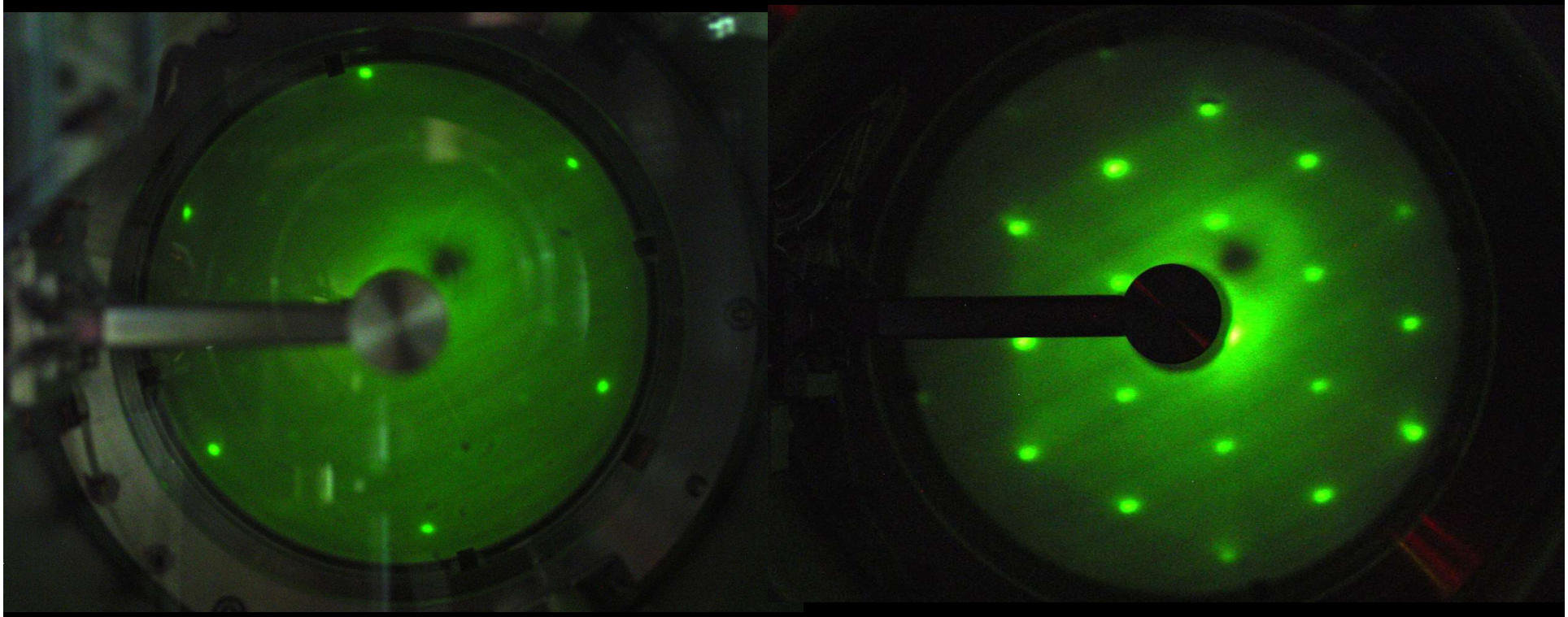
Pb	0	$\vec{a}_1+$	0	$\vec{a}_2+$	0	$\vec{a}_3$
Ti	0.5	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0.5	$\vec{a}_1+$	0	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0.5	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0	$\vec{a}_3$
		$\vec{a}_1+$		$\vec{a}_2+$		$\vec{a}_3$
		$\vec{a}_1+$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

submit

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

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

Energy of the electron beam: 100 [eV]

Primitive lattice vectors:

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

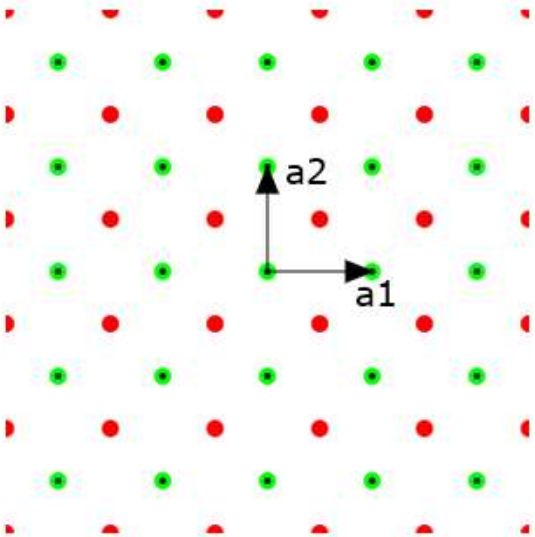
$\vec{a}_2 =$ 0 $\hat{x} +$ 4.12E-10 $\hat{y}$ [m]

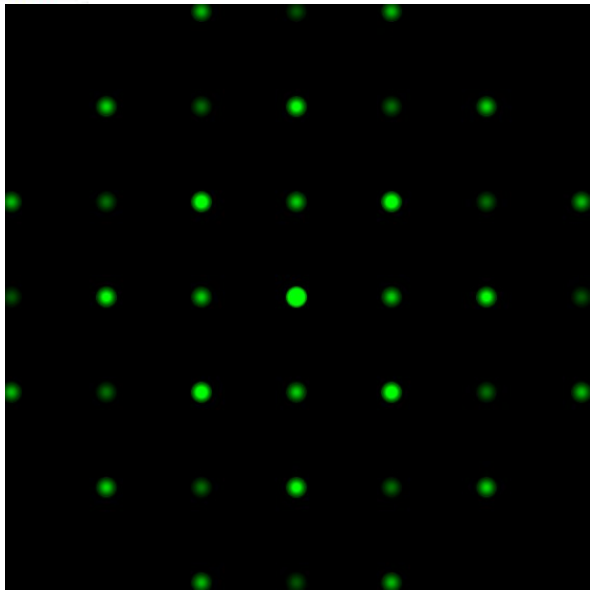
Basis:

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





Forbidden reflections

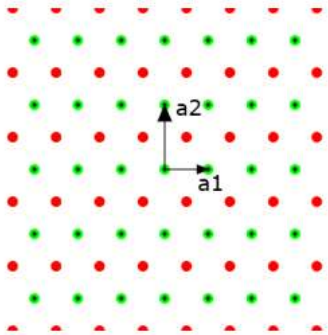
Primitive lattice vectors:

$\vec{a}_1 =$ 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	$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	

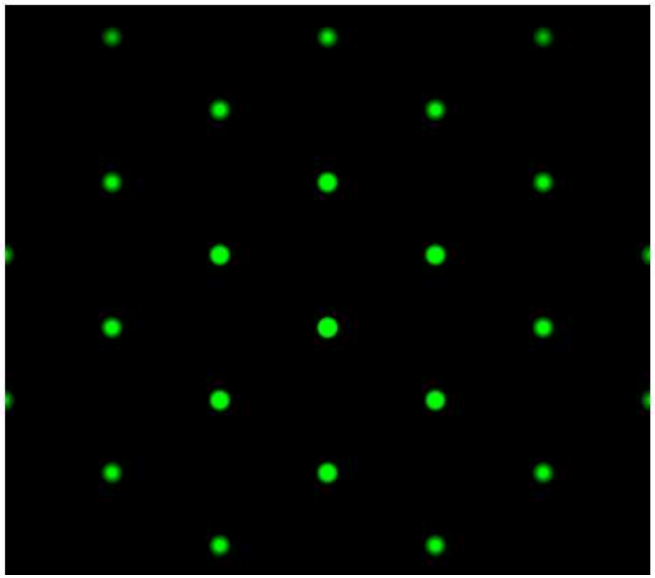
submit



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

$$n_{u.c.}(\vec{r}) = \sum_j Z_j \delta(\vec{r} - \vec{r}_j)$$

Primitive reciprocal lattice vectors

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

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

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

$$n_{\vec{G}} = \sum_j Z_j \exp(-i\vec{G} \cdot \vec{r}_j)$$

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

hkl	$\|\vec{G}\|$ Å^{-1}	$\|n_{\vec{G}}\|$	$\|n_{\vec{G}}\|^2$	Re$\{n_{\vec{G}}\}$	Im$\{n_{\vec{G}}\}$
000	0.000	75.94	5767	75.94	0.000
0-10	4.549e-10	37.87	1434	-37.87	0.02201
010	4.549e-10	37.87	1434	-37.87	-0.02201
0-20	9.098e-10	38.17	1457	-38.17	0.04379
020	9.098e-10	38.17	1457	-38.17	-0.04379
0-30	1.365e-9	75.94	5767	75.94	-0.1318
030	1.365e-9	75.94	5767	75.94	0.1318
0-3-1	1.212	0.3909	0.1528	0.02780	0.3899
0-31	1.212	0.3914	0.1532	-0.02727	0.3904
0-2-1	1.212	42.85	1836	-7.648	42.16
0-21	1.212	42.74	1827	7.551	42.07
0-1-1	1.212	43.01	1850	7.610	-42.33
0-11	1.212	42.96	1845	-7.561	-42.29
00-1	1.212	8.896e-8	7.914e-15	-1.573e-8	8.756e-8
001	1.212	8.896e-8	7.914e-15	-1.573e-8	-8.756e-8
01-1	1.212	42.96	1845	-7.561	42.29
011	1.212	43.01	1850	7.610	42.33
02-1	1.212	42.74	1827	7.551	-42.07
021	1.212	42.85	1836	-7.648	-42.16
03-1	1.212	0.3914	0.1532	-0.02727	-0.3904

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.