MSE-238
Structure of Materials

Week 6 – crystallography IV

Spring 2025

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General Outline

- introduction and reminder of atomic bonds, crystals – week 1

Part I: crystallography - weeks 2-6

- packing of spheres, constructing crystal structure
- crystal lattice and symmetry operations
- mathematical description of the lattice, Miller indices
- reciprocal space

Part II: characterization – week 6-8

- diffraction
- scattering

BREAK 18.4. & 25.4.

Part III: amorphous & hierarchical structures – week 9-12

- glasses
- polymers
- biological and hybrid materials

Recap – week 13

General Outline (adapted)

- introduction and reminder of atomic bonds, crystals – week 1

Part I: crystallography - weeks 2-6

- packing of spheres, constructing crystal structure week 2
- crystal lattice and symmetry operations week 3
- mathematical description of the lattice, Miller indices week 4
- reciprocal space (&diffraction) week 6
- characterization I: diffraction week 7
- diffraction & recap of crystallography week 8

BREAK 18.4. & 25.4.

Part III: amorphous & hierarchical structures – week 9-12

- glasses
- polymers
- Characterization II: scattering
- biological and hybrid materials

Recap – week 13

Overview today

- Reminder of crystallography I-III
- Diffraction on planes of crystals
- Reciprocal lattice
- d-spacing of planes
- Young's double slit experiment and Bragg's law
- Laue's condition: connection between diffraction and reciprocal lattice
- Diffraction as Fourier Transform of the crystal (=lattice & motif)

- Hammond Chapter 6-8
- Jens Als-Nielsen & Des McMorrow "Elements of Modern X-ray Physics" Chapter 5

CsCl

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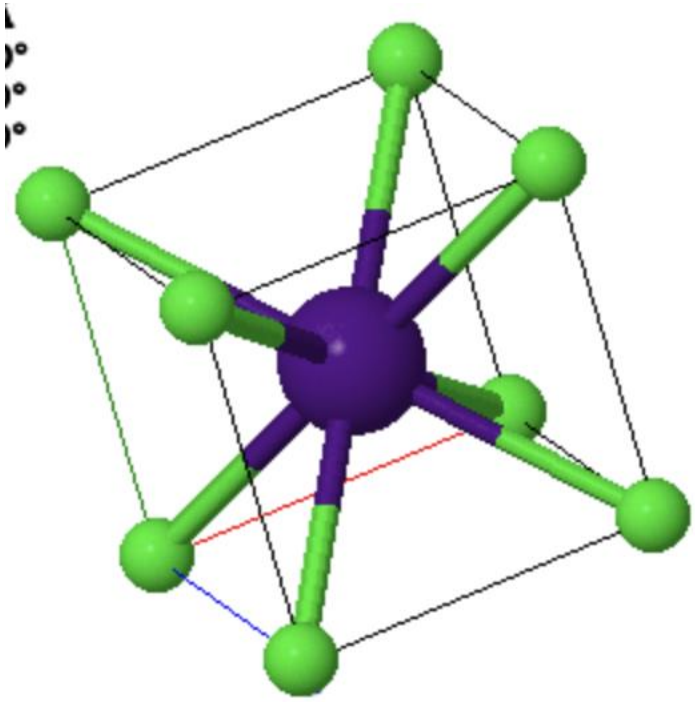

CsCl

CsCl

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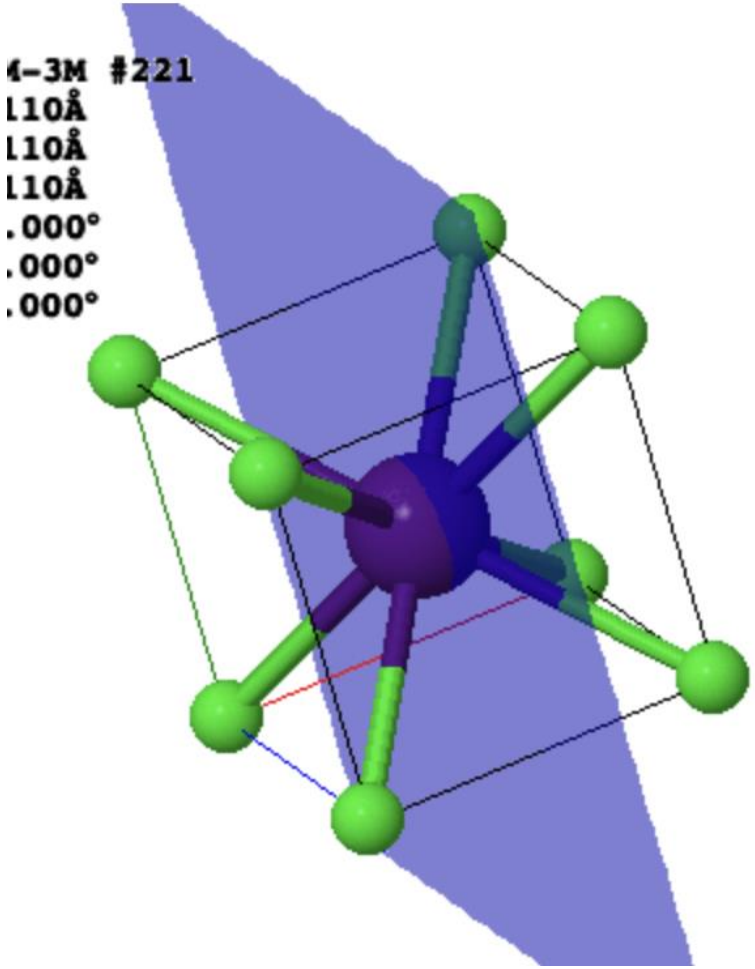
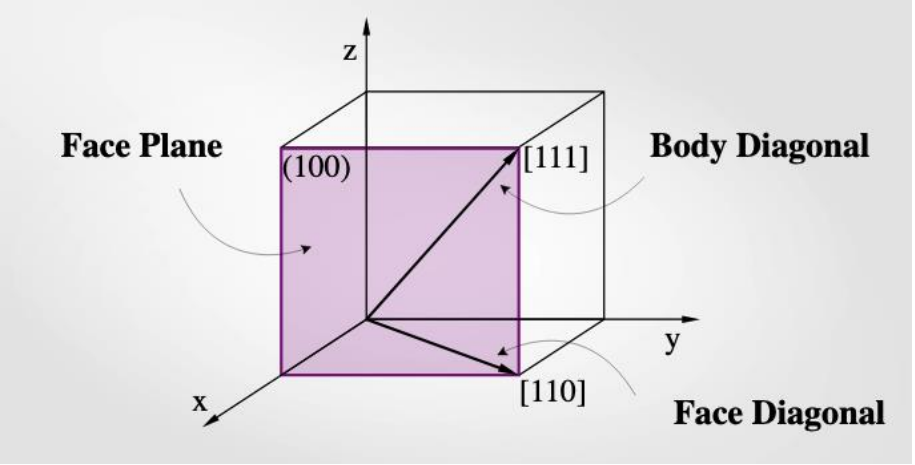


Summary of notations

(h, k, l) is for points. Remember to use the negative sign (-*h*) instead of bar sign ($\bar{h}$) and **don't** reduce fractions–these rules apply to directions and planes.

[hkl] is for a specific direction.
<hkl> is for a family of directions.

(hkl) is for a specific plane. Remember about reciprocal (inverse) space in planes!
{hkl} is for a family of planes.



NaCl

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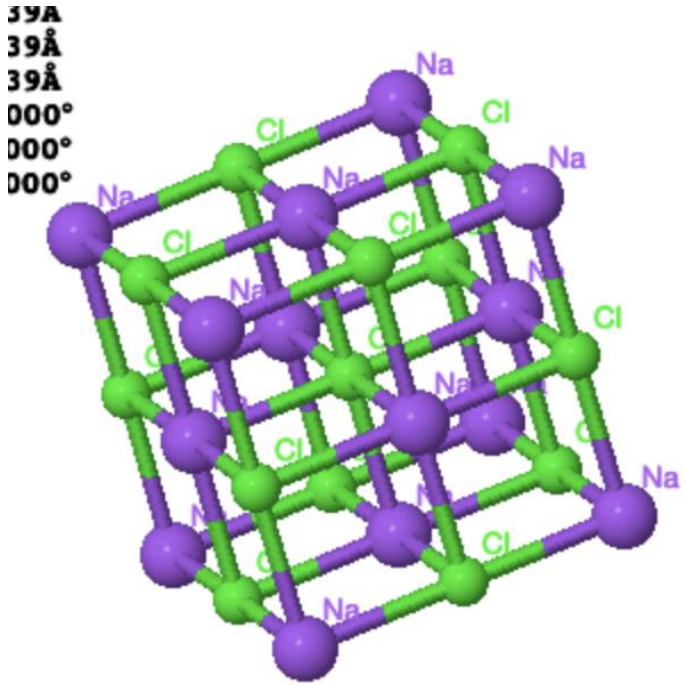

NaCl

NaCl

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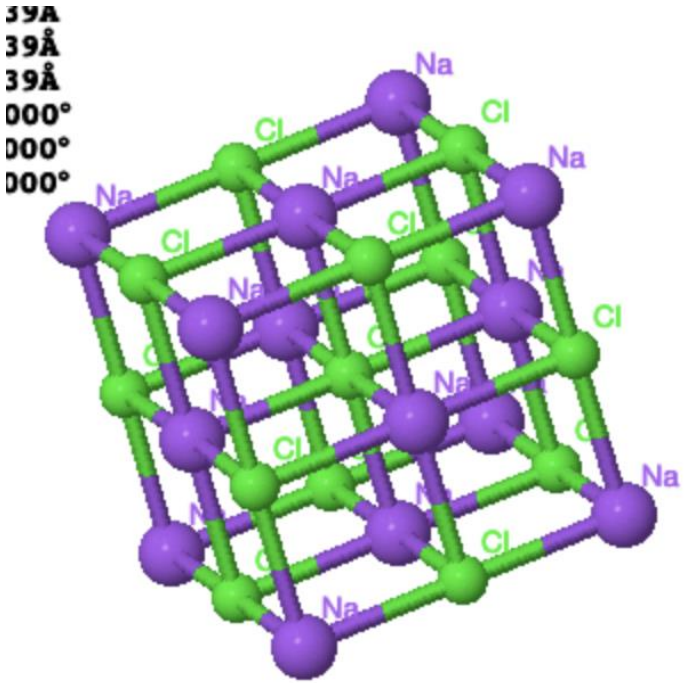
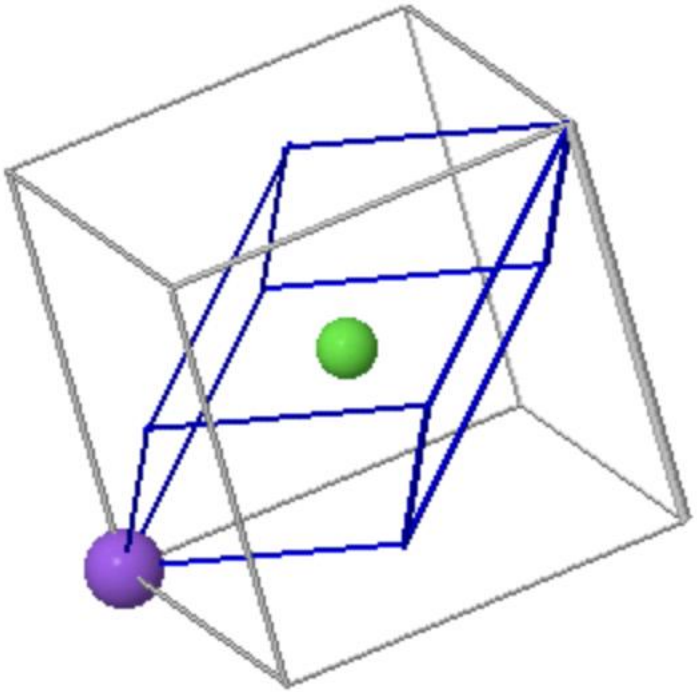


conventional unit cell



primitive unit cell

Ionic crystals: Interstitial sites

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- ionic radius ratio: $\rho = \frac{r_+}{r_-}$

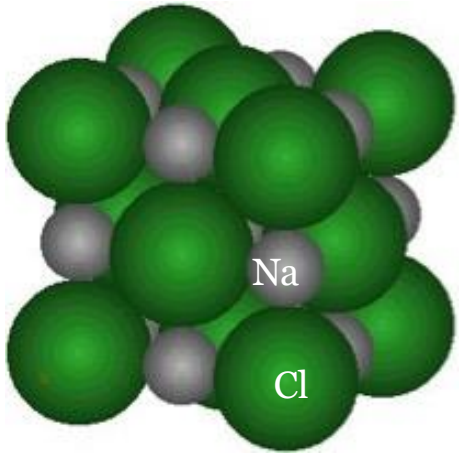
Which ionic radius is larger: Na or Cs?

NaCl

Na Cl

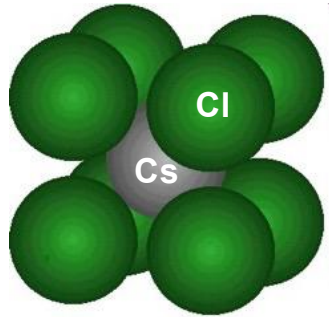
R_{Na+} = 1.02 Å

R_{Cl-} = 1.81 Å



For $0.4142 < \rho < 0.7320$:

CsCl



Cs Cl

R_{Cs+} = 1.67 Å

R_{Cl-} = 1.81 Å

- For $0.7320 < \rho < 1$:

Diamond

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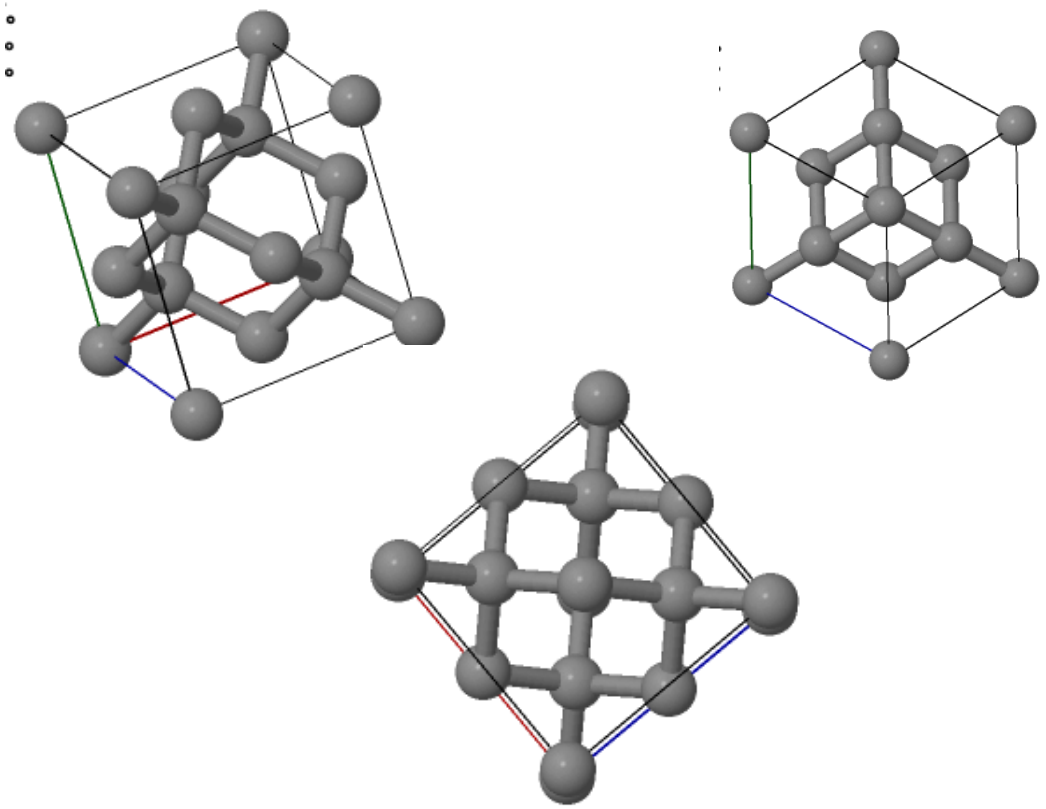

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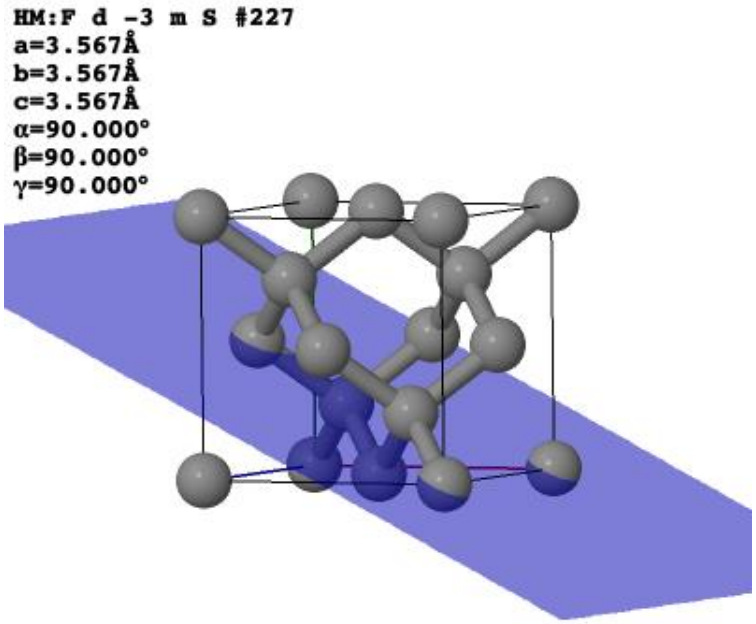

(120) plane

what is the atom configuration in the (100) plane of diamond?

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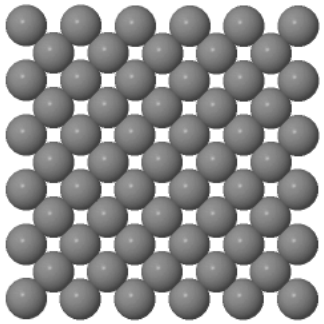
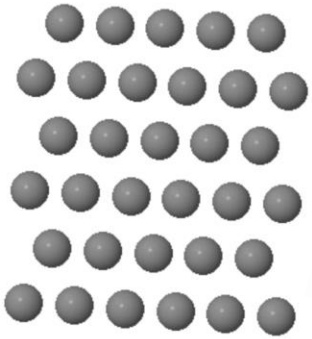


(100)



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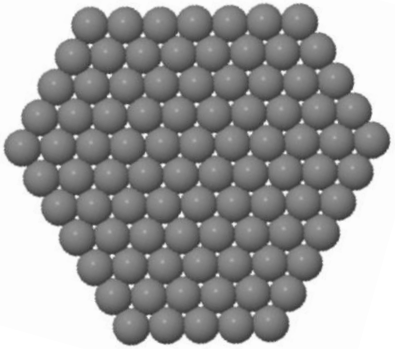

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Diamond and Zincblende (ZnS)

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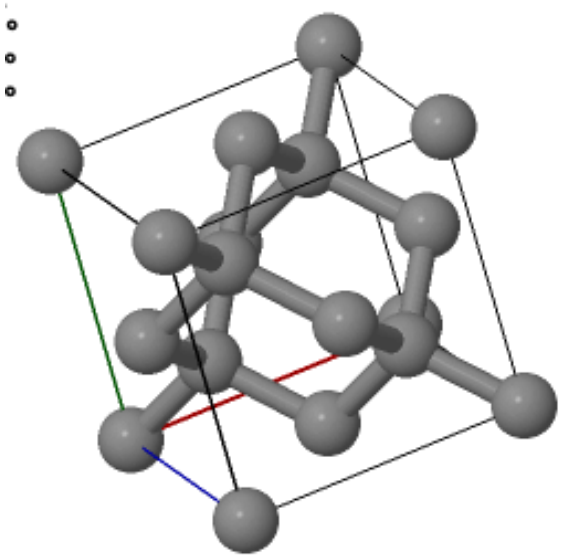
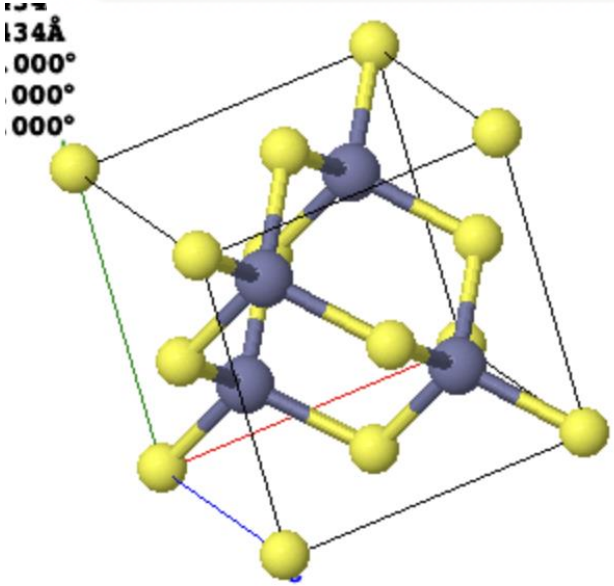
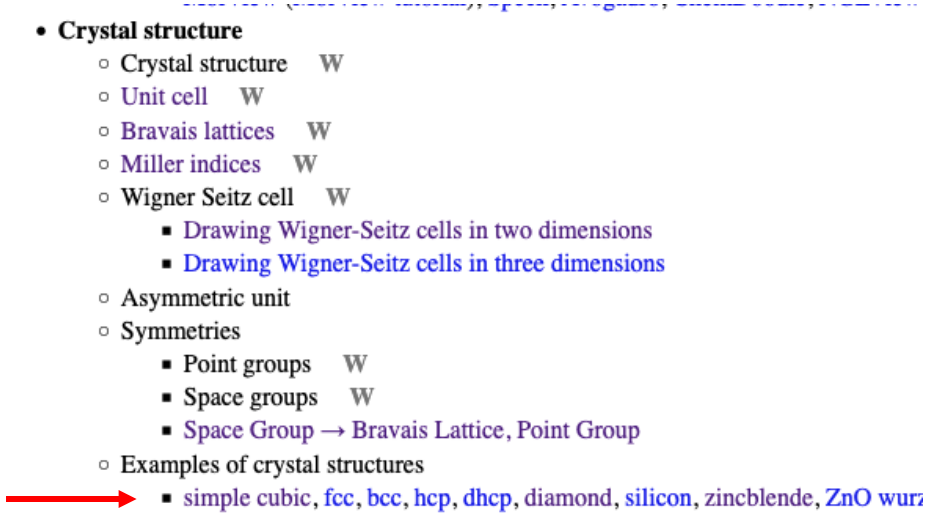


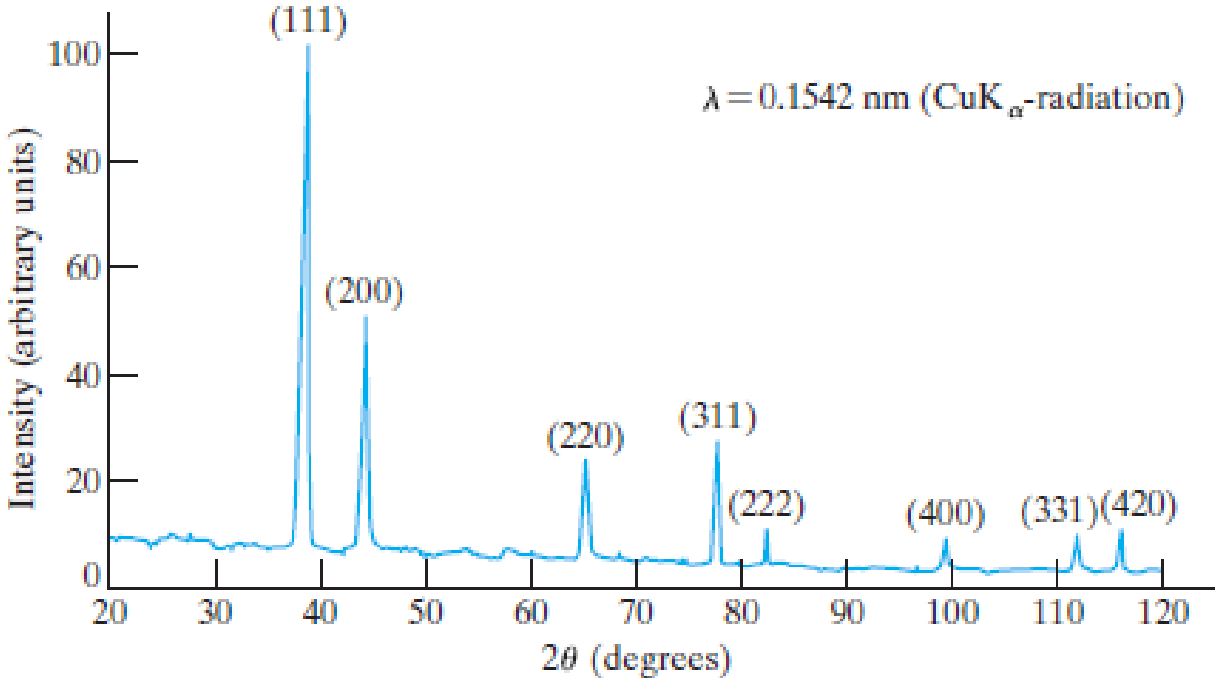


crystal system	cubic	cubic
Bravais lattice	fcc	fcc
motif	C-C	Zn-S

https://lampz.tugraz.at/~hadley/ss1/skriptum/outline.php for some nice visualization and interactive plots!



X-ray diffraction: crystal planes



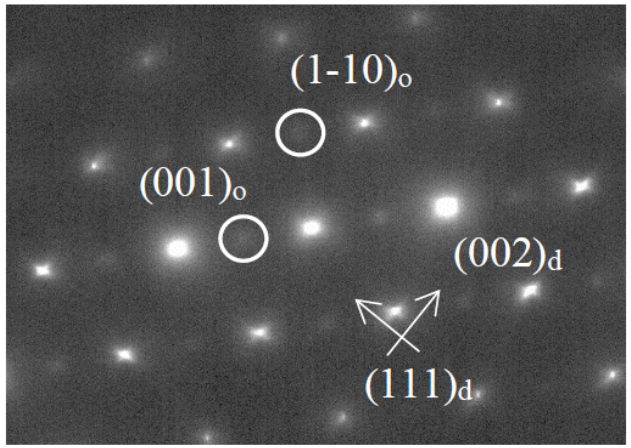
Diffraction pattern of Al (FCC crystal)

An X-ray diffraction pattern reflects the lattice and symmetry of the crystalline material.

The diffraction peaks are indexed, these indices tell you which crystal planes are reflecting the X-rays

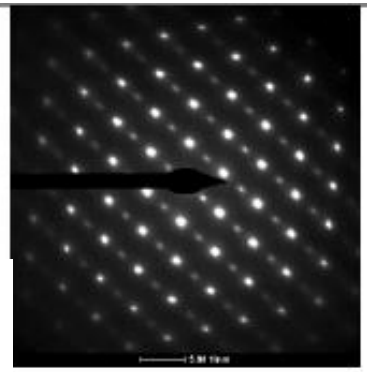
Electron diffraction: crystal planes

beam falls in parallel to the [110] zone axis.

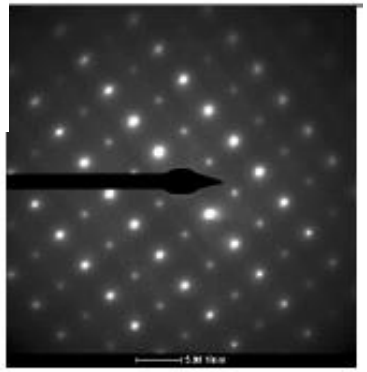


Images of same sample with incident electron beam parallel to other crystallographic directions

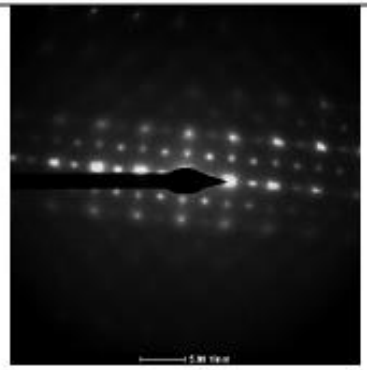
[110]



[112]



[001]



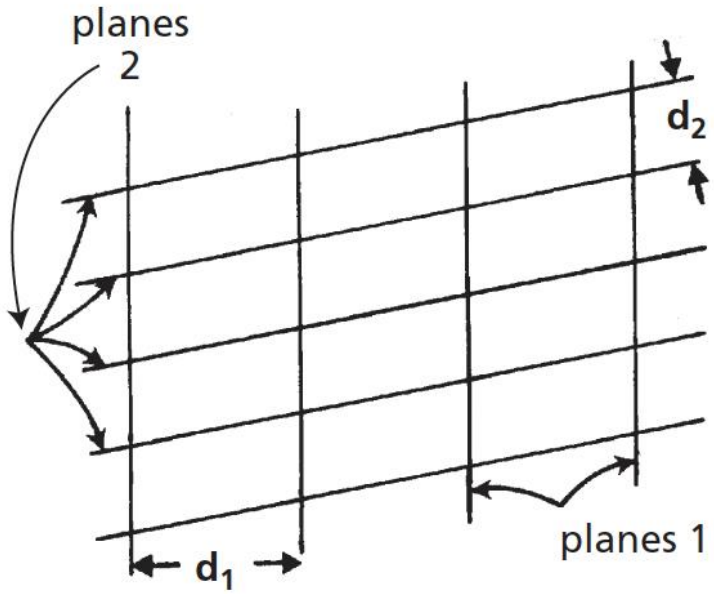
Depending on how the sample is oriented relative to the incoming beam, the diffraction pattern will be different and allow to recognize the symmetry of the crystal

Au alloy

Reciprocal lattice and diffraction

- the electron diffraction patterns or the X-ray diffraction patterns are simply sections through the reciprocal lattice of a crystal—the pattern of spots on the screen or area detector and the pattern of reciprocal lattice points in the corresponding plane or section through the crystal are identical.
- which section of the 3D reciprocal lattice is probed is defined by the Ewald sphere (as will be discussed in coming weeks)

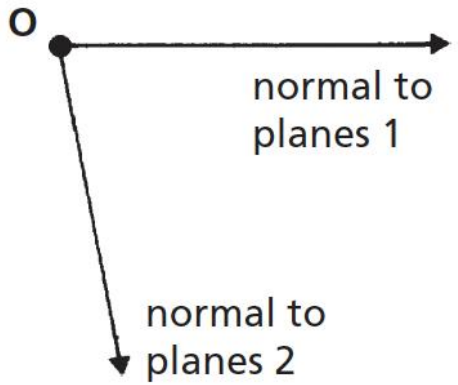
Reciprocal lattice vectors



(a)

two families of planes with d-spacing d_1 and d_2

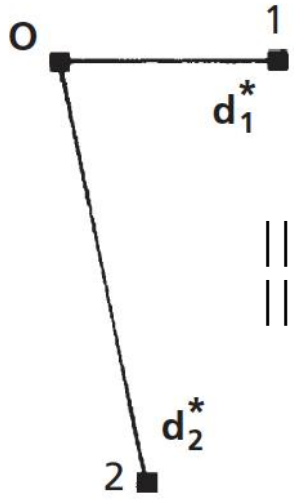
direction normal to plane



(b)

normals to the family of planes from common origin O

length inversely proportional to lattice spacing d



$||\mathbf{d}_1^*|| = C/d_1$

$||\mathbf{d}_2^*|| = C/d_2$

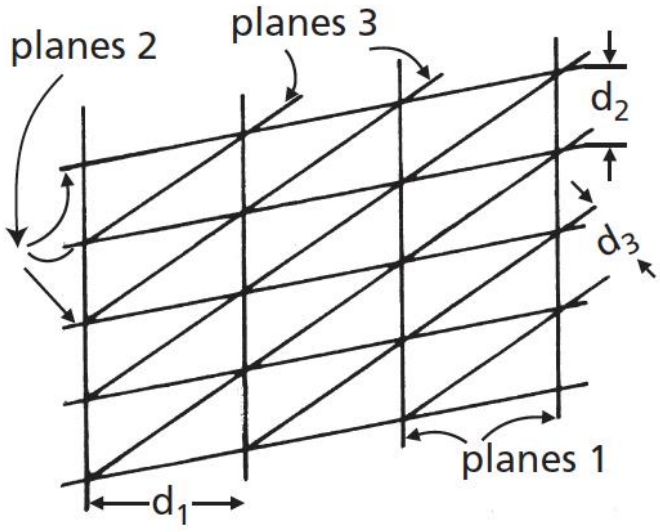
$C = 2\pi$

(c)

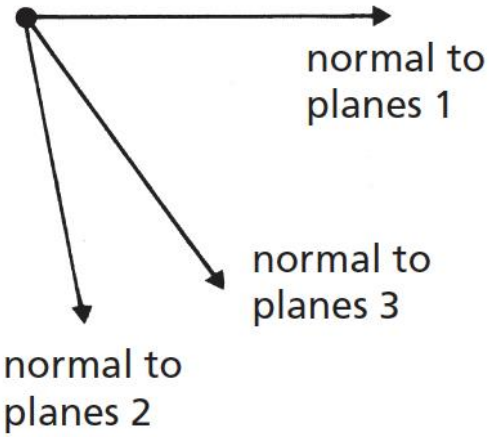
reciprocal (lattice) vectors

longer vector for smaller d-spacing

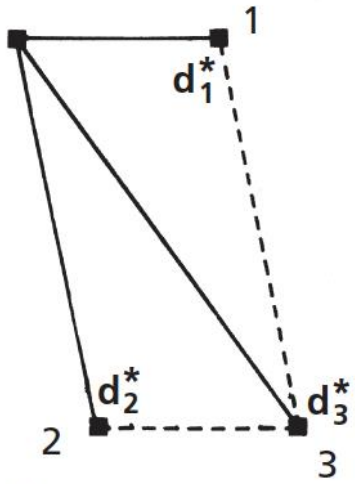
Reciprocal lattice



(a)



(b)

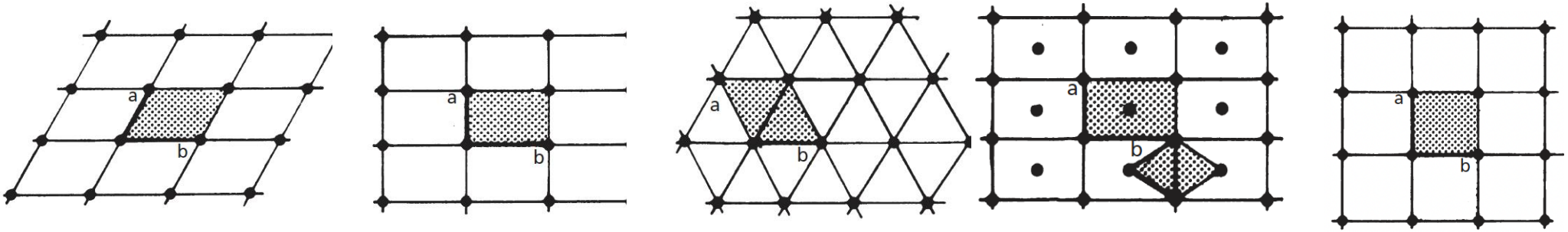


(c)

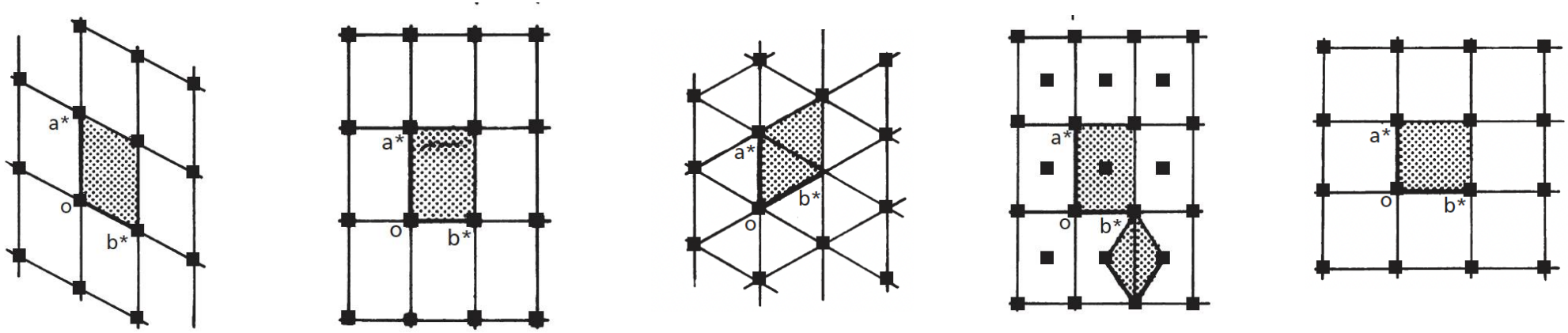
scale in reciprocal space is 1/length
$Å^{-1}$, or nm

third family of planes, the reciprocal vectors start to form a grid or lattice

The five plane lattices and their corresponding reciprocal lattice



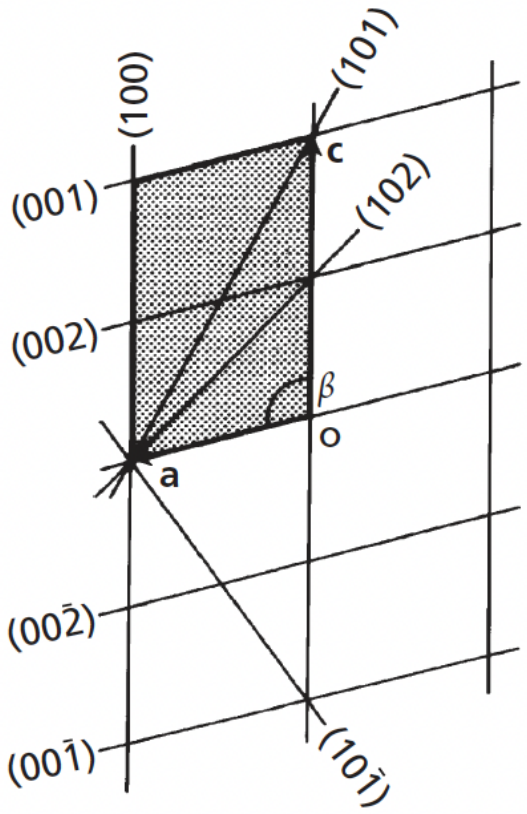
unit cell specified by lattice vectors **a** and **b**



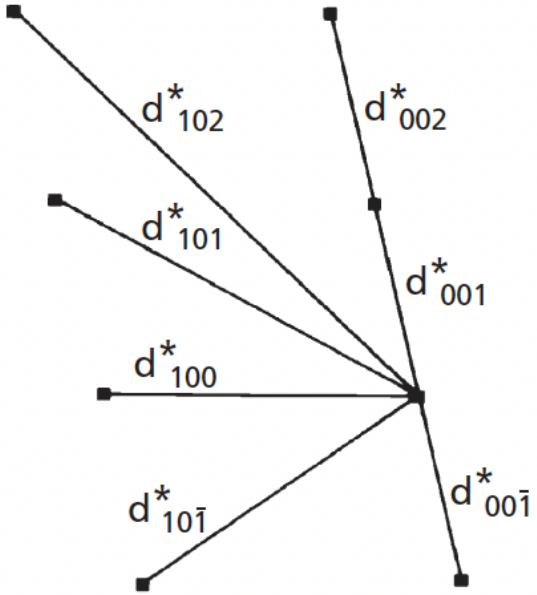
unit cell specified by reciprocal lattice vectors **a*** and **b***

Reciprocal lattice

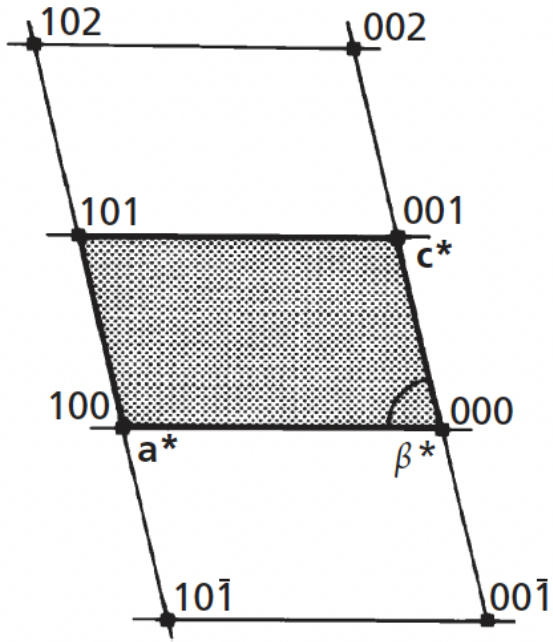
Plan of a monoclinic P unit cell perpendicular to the y-axis



planes (hok)



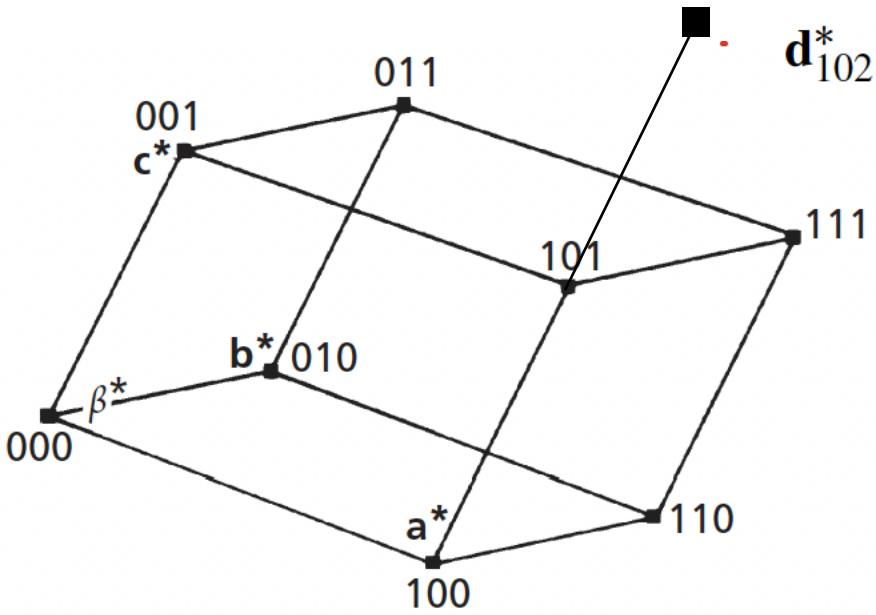
Note that **a*** and **c*** are not parallel to **a** and **c**, respectively, because the normals to the (100) and (001) planes in the monoclinic lattice are not parallel to **a** and **c**, respectively.



$$\mathbf{a}^* = \mathbf{d}^*_{100} \quad \text{and} \quad ||\mathbf{a}^*|| = 2\pi/d_{100}$$

$$\mathbf{c}^* = \mathbf{d}^*_{001} \quad \text{and} \quad ||\mathbf{c}^*|| = 2\pi/d_{001}$$

Reciprocal lattice



The reciprocal lattice unit cell of a monoclinic P crystal defined by reciprocal lattice vectors **a***, **b*** and **c***

for the (102) planes:

$$\mathbf{d}^*_{102} = 1\mathbf{a}^* + 0\mathbf{b}^* + 2\mathbf{c}^*$$

for the (hkl) planes:

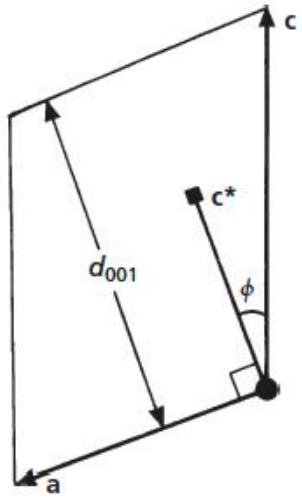
$$\mathbf{d}^*_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*.$$

plane indices are components of the $\mathbf{d}^*_{hkl}$ vector

direct lattice vector: directions are its components

$$\mathbf{r}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

Reciprocal lattice



Plan of a monoclinic unit cell perpendicular to the y-axis

c* is perpendicular to both **a** and **b**, which means their dot products are zero

$\mathbf{c^*} \cdot \mathbf{a} = 0$ and $\mathbf{c^*} \cdot \mathbf{b} = 0$

$\mathbf{c^*} \cdot \mathbf{c} = cc^* \cos\phi$

with $||\mathbf{c}^*|| = 2\pi/d_{001}$ and from drawing: $c \cos\phi = d_{001}$

$\mathbf{c^*} \cdot \mathbf{c} = 2\pi d_{001}/d_{001} = 2\pi$

does we have:

$\vec{a^*}.\ \vec{a} = 2\pi$ $\quad$ $\vec{b^*}.\ \vec{a} = 0$ $\quad$ $\vec{c^*}.\ \vec{a} = 0$

$\vec{a^*}.\ \vec{b} = 0$ $\quad$ $\vec{b^*}.\ \vec{b} = 2\pi$ $\quad$ $\vec{c^*}.\ \vec{b} = 0$

$\vec{a^*}.\ \vec{c} = 0$ $\quad$ $\vec{b^*}.\ \vec{c} = 0$ $\quad$ $\vec{c^*}.\ \vec{c} = 2\pi$

We have a new basis new basis (O, **a***, **b***, **c***) in which a vector $\mathbf{N^*_{hkl}} = h\mathbf{a^*} + k\mathbf{b^*} + l\mathbf{c^*}$ is perpendicular to the plane (hkl)

If we consider any vector in the direct space $\boldsymbol{R} = r_1\boldsymbol{a} + r_2\boldsymbol{b} + r_3\boldsymbol{c}$ and one in the reciprocal space $\boldsymbol{N^*} = n_1\boldsymbol{a^*} + n_2\boldsymbol{b^*} + n_3\boldsymbol{c^*}$, we have:

$$\boldsymbol{R} \cdot \boldsymbol{N^*} = r_1 n_1 \boldsymbol{a} \cdot \boldsymbol{a^*} + r_2 n_2 \boldsymbol{b} \cdot \boldsymbol{b^*} + r_3 n_3 \boldsymbol{c} \cdot \boldsymbol{c^*} = 2\pi(r_1 n_1 + r_2 n_2 + r_3 n_3)$$

→ an integer

Reciprocal lattice – Notations…

- A note on Notations:
- the reciprocal space vector (which points from one reciprocal lattice point to some other reciprocal lattice point) is called
- $\mathbf{d}^*_{hkl}$
- $\mathbf{N}^*$

or in diffraction literature often

- **G** or **K**

$\mathbf{a}^* \cdot \mathbf{a} = \mathbf{b}^* \cdot \mathbf{b} = \mathbf{c}^* \cdot \mathbf{c} = C$, C a constant

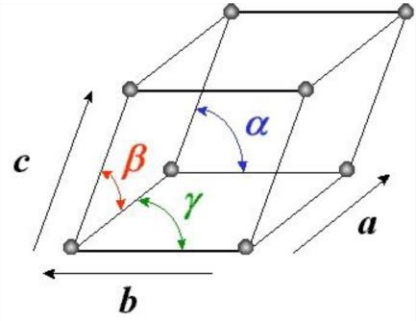
Often C is often noted as 2π (and we will see soon why it is very convenient to do so) in some text books (including Hammond) C= 1

Find the reciprocal space vectors from direct lattice vectors

find **a*** which is orthogonal to **b** and **c** → cross product!
and fullfills **a** · **a*** = 2π

Reminder Volume:

$$\mathbf{V} = (\vec{a}, \vec{b}, \vec{c}) = \vec{a} \cdot (\vec{b} \times \vec{c}) = \vec{b} \cdot (\vec{c} \times \vec{a}) = \vec{c} \cdot (\vec{a} \times \vec{b})$$



$$\mathbf{a}^* = (\boldsymbol{b} \times \boldsymbol{c}) \frac{2\pi}{V}$$

$$\mathbf{a} \cdot \mathbf{a}^* = \mathbf{a} \cdot (\boldsymbol{b} \times \boldsymbol{c}) \frac{2\pi}{V} = 2\pi$$

so we can find the reciprocal space vectors by:

$$\vec{a}^* = 2\pi \frac{\vec{b} \times \vec{c}}{V} \qquad \vec{b}^* = 2\pi \frac{\vec{c} \times \vec{a}}{V} \qquad \vec{c}^* = 2\pi \frac{\vec{a} \times \vec{b}}{V}$$

For cubic structure

primitive cubic:

$V = a^3$ $\quad \mathbf{a} = a\mathbf{x}$ $\quad \mathbf{b} = a\mathbf{y}$ $\quad \mathbf{c} = a\mathbf{z}$

$$\mathbf{a}^* = \frac{2\pi}{V}(\boldsymbol{b} \times \boldsymbol{c})$$

$$\mathbf{a}^* = \frac{2\pi}{a^3}\begin{pmatrix}0\\a\\0\end{pmatrix} \times \begin{pmatrix}0\\0\\a\end{pmatrix} = \frac{2\pi}{a^3}\begin{pmatrix}a^2\\0\\0\end{pmatrix} = \frac{2\pi}{a}\mathbf{x} = \frac{2\pi}{a^2}\mathbf{a} \quad \text{and} \quad \mathbf{b}^* = = \frac{2\pi}{a}\mathbf{y}$$

$$\mathbf{c}^* = = \frac{2\pi}{a}\mathbf{z}$$

→ another cubic
→ $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ are parallel to $\mathbf{a}, \mathbf{b}, \mathbf{c}$

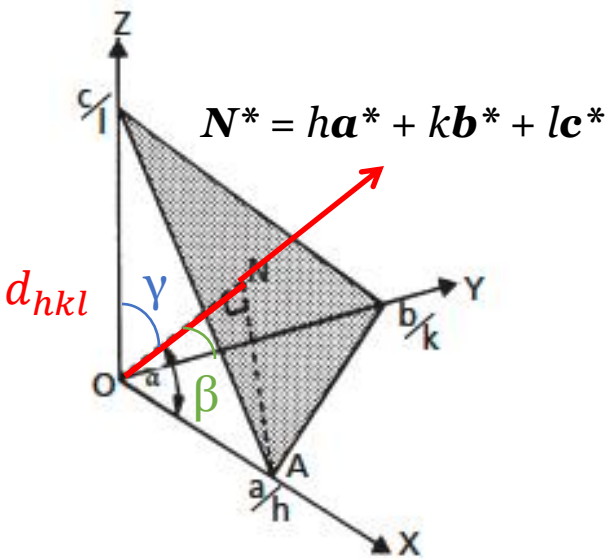
face-centred cubic reciprocal lattice (cubic F) for the body-centred cubic (direct) lattic (cubic I)

reciprocal lattice of the face-centred cubic lattice is body-centred

Distances between (hkl) planes

The reciprocal space formalism facilitates the derivation of the interplane distance of parallel (hkl) planes.

$$\boldsymbol{OA} = \frac{1}{h}\boldsymbol{a} \qquad \boldsymbol{OB} = \frac{1}{k}\boldsymbol{b} \qquad \boldsymbol{OC} = \frac{1}{l}\boldsymbol{c}$$



distance $d_{(hkl)}$ is the projection of **OA** (or **OB** or **OC**) onto the normal of the plane → the scalar product

now we have the reciprocal lattice vector $\mathbf{N}^*_{(hkl)}$ which is perpendicular to the (hkl) plane

does we can now calculate the distance by projection of OA onto the unit vector along $\mathbf{N}^*_{(hkl)}$

$$d_{(hkl)} = \boldsymbol{OA} \cdot \frac{\boldsymbol{N}^*_{(\boldsymbol{hkl})}}{\left\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\right\|}$$

as we have seen before, for any vector (e.g. **OA**) in real space it holds

$$\boldsymbol{OA} \cdot \boldsymbol{N}^*_{(\boldsymbol{hkl})} = \boldsymbol{OB} \cdot \boldsymbol{N}^*_{(\boldsymbol{hkl})} = \boldsymbol{OC} \cdot \boldsymbol{N}^*_{(\boldsymbol{hkl})} = 2\pi * \text{integer}$$

$$\boxed{d_{(hkl)} = \frac{2\pi}{\left\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\right\|}}$$

- Calculate the reciprocal lattice vectors $\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*$ and the vector $\boldsymbol{N}^*_{(\boldsymbol{hkl})}$
- Find the norm of $\boldsymbol{N}^*_{(\boldsymbol{hkl})}$ -→ find the distance.

Distance between (hkl) planes: cubic system

$$d_{(hkl)} = \frac{2\pi}{\|\boldsymbol{N}^*_{(\boldsymbol{hkl})}\|}$$

$$||\mathbf{N}^*_{(hkl)}|| = \sqrt{(h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*) \cdot (h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*)}$$

for crystals with orthogonal axis, for example cubic
also reciprocal basis is orthogonal $\mathbf{a}^* \cdot \mathbf{b}^* = 0$ etc.

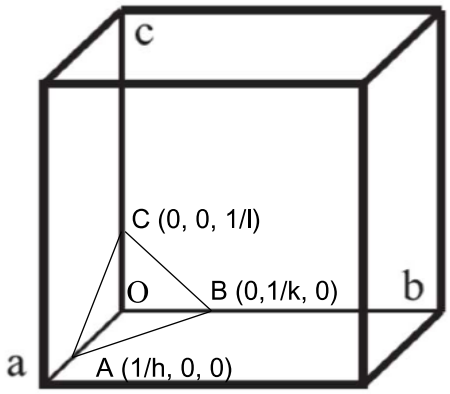
$$||\mathbf{N}^*_{(hkl)}|| = \sqrt{h\boldsymbol{a}^* \cdot h\boldsymbol{a}^* + k\boldsymbol{b}^* \cdot k\boldsymbol{b}^* + l\boldsymbol{c}^* \cdot l\boldsymbol{c}^*)}$$

as we have seen before for cubic $\mathbf{a}^* = \frac{2\pi}{a}\mathbf{x}$ $\mathbf{b}^* = \frac{2\pi}{a}\mathbf{y}$ $\mathbf{c}^* = \frac{2\pi}{a}\mathbf{z}$

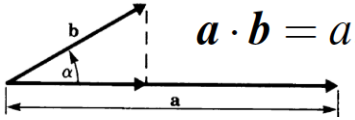
orthonormal basis → norm of vector as square root of components

$$||\mathbf{N}^*|| = \sqrt{\left(\frac{2\pi}{a}h\right)^2 \left(\frac{2\pi}{a}k\right)^2 + \left(\frac{2\pi}{a}l\right)^2} = 2\pi\frac{\sqrt{h^2+k^2+l^2}}{a} \qquad d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

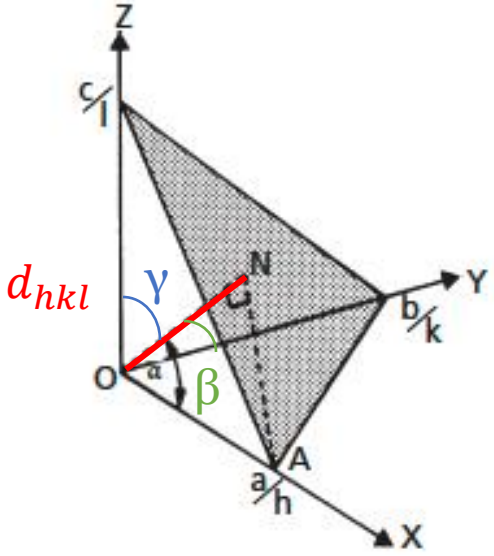
Reminder distance in direct lattice



- The plane parallel to the plane (ABC) and passing through the origin O is a crystal plane belonging to the family of planes $\{hkl\}$.
- Assuming that the distance between two (hkl) planes is the same for all consecutive planes, this distance is given by ***ON,*** which is the projection of the vector ***OA*** on the normal to the plane
- $ON = d_{(hkl)} = \boldsymbol{OA} \cdot \boldsymbol{n_{hkl}}$



$\boldsymbol{a} \cdot \boldsymbol{b} = ab\cos\alpha$



$$\text{OA}\cos\alpha = \text{ON} \quad \text{or} \quad (a/h)\cos\alpha = d_{hkl} \quad \text{or} \quad \cos\alpha = \left(\frac{h}{a}\right) d_{hkl}.$$

$$\cos\beta = \left(\frac{k}{b}\right) d_{hkl} \quad \text{and} \quad \cos\gamma = \left(\frac{l}{c}\right) d_{hkl}.$$

For orthogonal axes $\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$ (Pythagoras' theorem),

$$\left(\frac{h}{a}\right)^2 d_{hkl}^2 + \left(\frac{k}{b}\right)^2 d_{hkl}^2 + \left(\frac{l}{c}\right)^2 d_{hkl}^2 = 1.$$

For a cubic crystal $a = b = c$, $\dfrac{1}{d_{hkl}^2} = \dfrac{h^2 + k^2 + l^2}{a^2}$. $d_{(hkl)} = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$

→ for cubic both works, for non-orthogonal lattice it is much easier in the reciprocal space

Distance between (hkl) planes

$$d_{(hkl)} = \frac{2\pi}{\left\| \boldsymbol{N}^*_{(\boldsymbol{hkl})} \right\|}$$

$$||\mathbf{N}^*_{(hkl)}|| = \sqrt{(h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*) \cdot (h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*)}$$

watch out, **a***, **b*** and **c*** are not orthogonal to each other for many of the crystal lattices!
but the reciprocal space lattice helps to get back some orthogonality since we defined **a*** to be orthogonal to **a** and **b** etc.

→ exercise to calculate for hexagonal lattice

Distances betweek (hkl) planes

– Monoclinic:

$$d_{hkl} = \frac{1}{\sqrt{\left(\frac{h^2}{a^2} + \frac{l^2}{c^2} - \frac{2\,hl}{a\,c}\cos\beta\right)\frac{1}{\sin^2\beta} + \frac{k^2}{b^2}}}$$

– Orthorhombic:

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

–Tetragonal:

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}}}$$

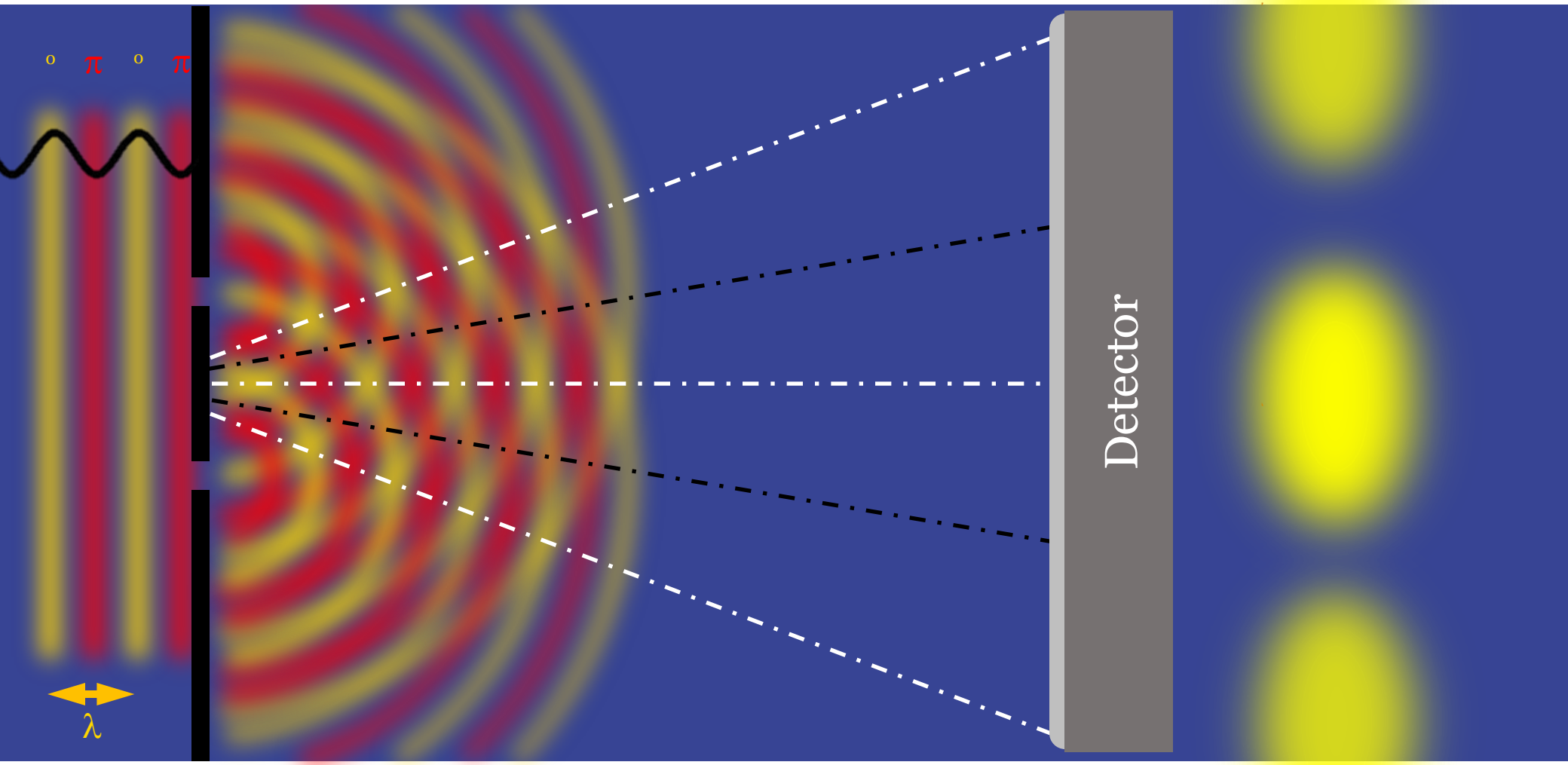
– Hexagonal:

$$d_{hkl} = \frac{1}{\sqrt{\frac{4}{3\,a^2}(h^2 + k^2 + hk) + \frac{l^2}{c^2}}}$$

– Cubic:

$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$

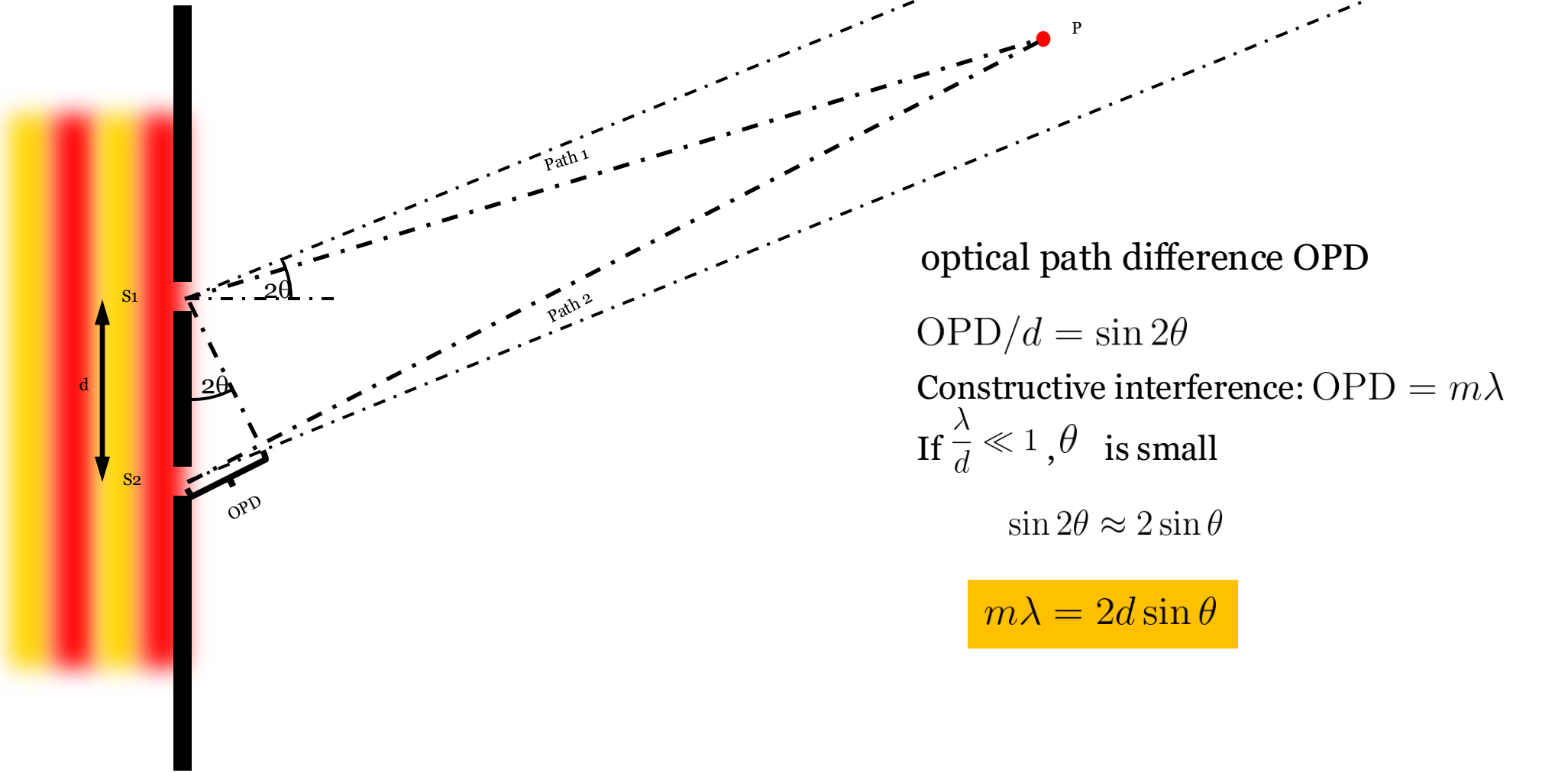
Young's double slit experiment



to get such an interference pattern we need a wavelength that is of the order of the distance between the slits.

by Phil Willmott

Young's double slit experiment



optical path difference OPD

$\mathrm{OPD}/d = \sin 2\theta$

Constructive interference: $\mathrm{OPD} = m\lambda$

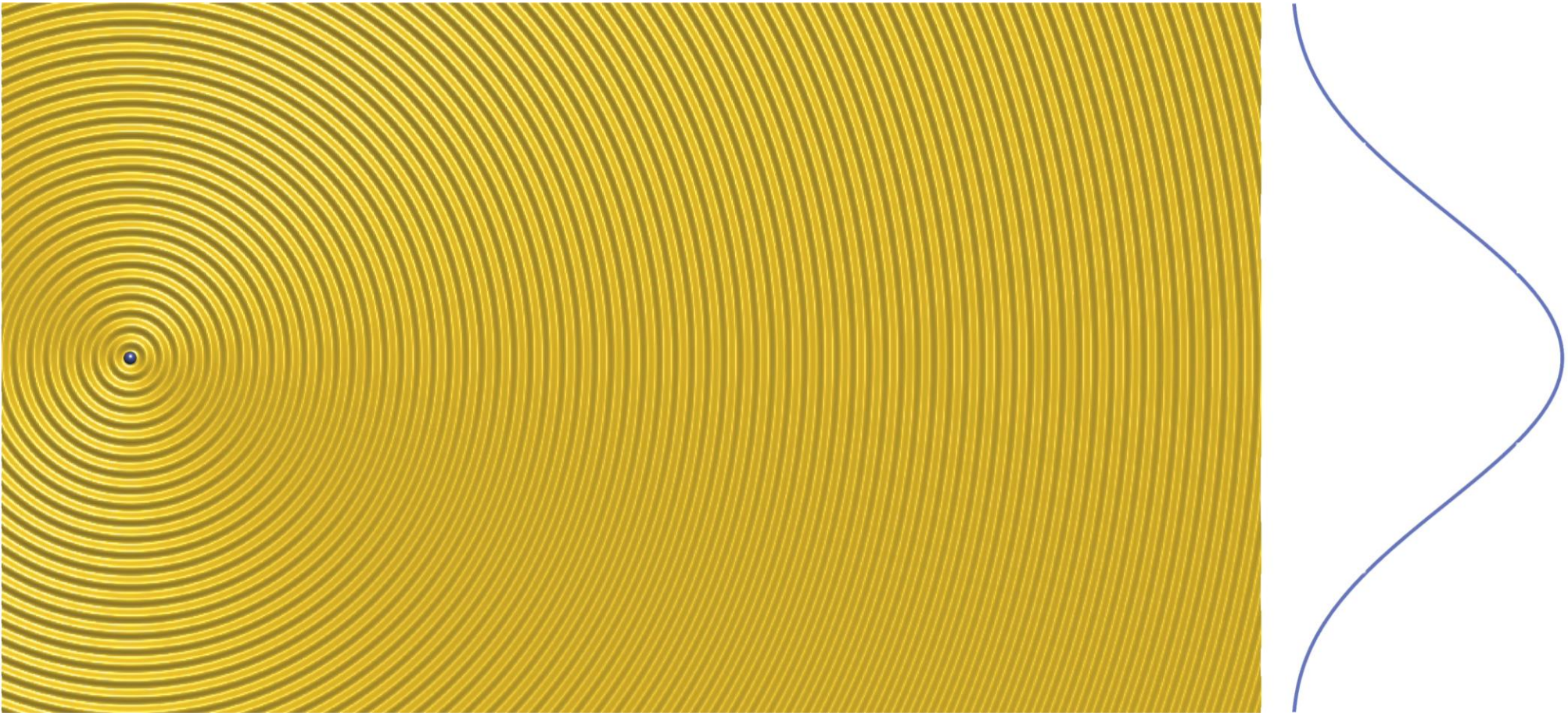
If $\frac{\lambda}{d} \ll 1$, θ is small

$$\sin 2\theta \approx 2 \sin \theta$$

$$m\lambda = 2d \sin \theta$$

by Phil Willmott

Young's double slit experiment



$$m\lambda = 2d\sin\theta$$

distance between two scattering centers or slits increases
the angle between maxima become narrower

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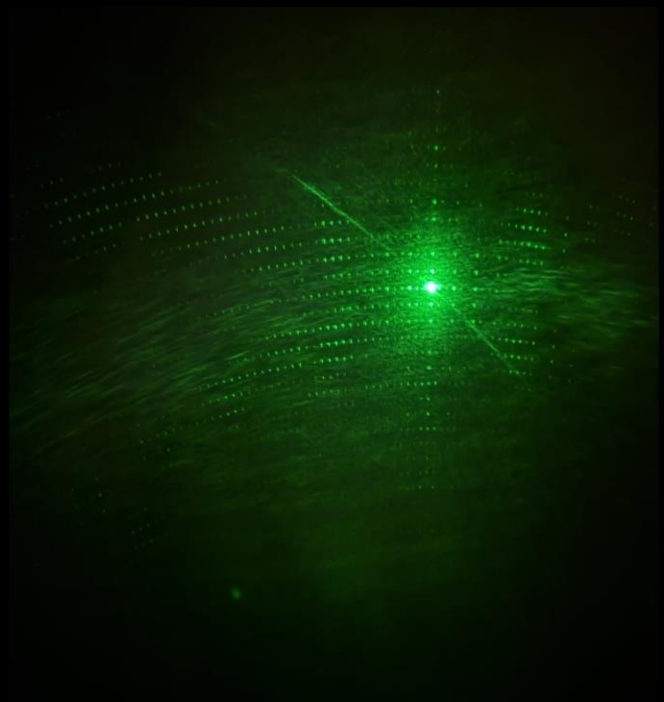
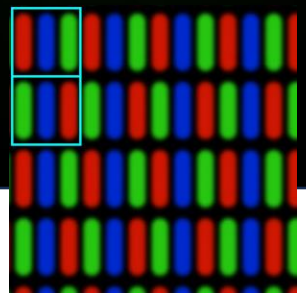
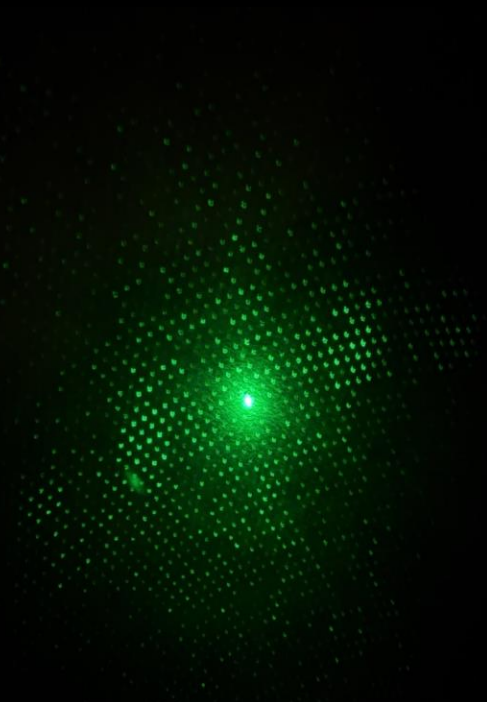
Diffraction from phone display

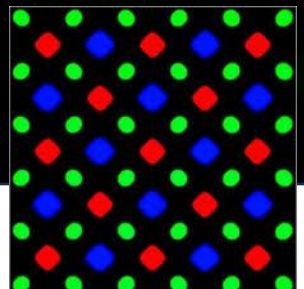
a)



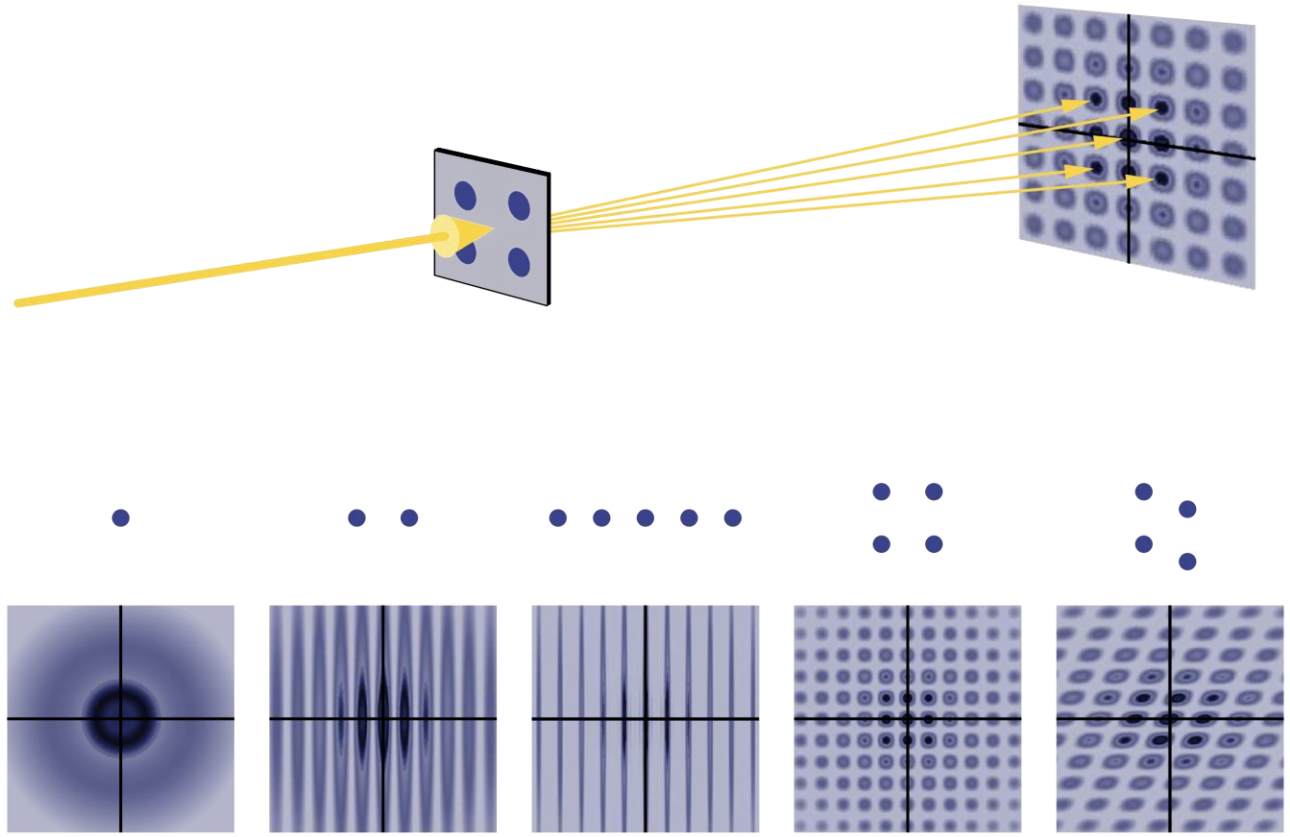


b)





Crystal instead of double slit



to get such an interference pattern we need a wavelength that is of the order of the distance between the slits.

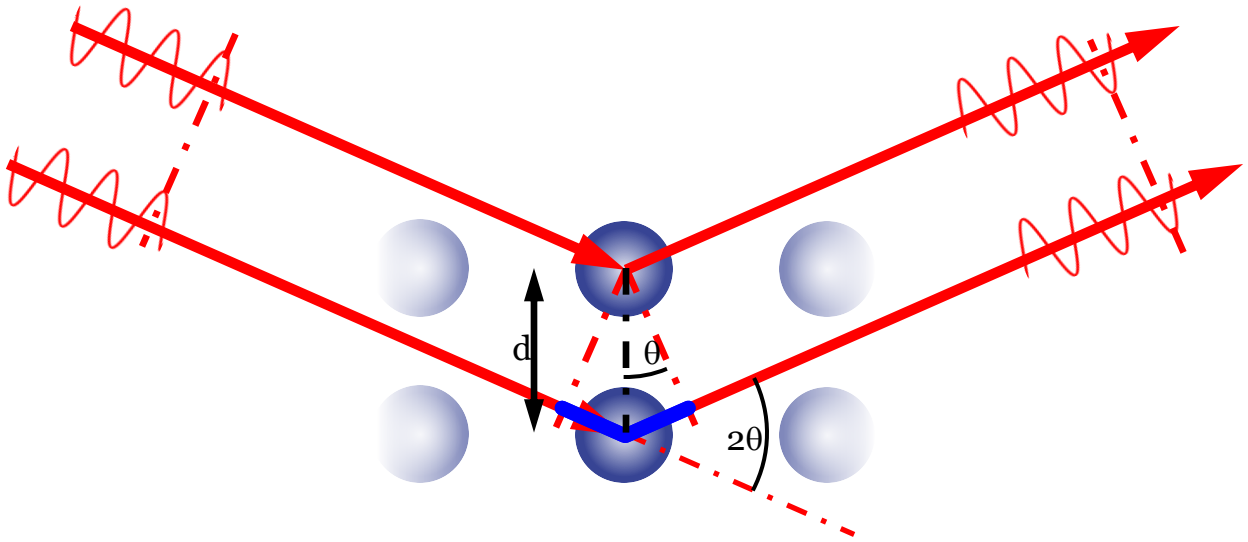
by Phil Willmott

Which radiation?

visible light will not be a good probe since the wavelength is 400nm-700nm, which is much bigger than the distance between the atoms, typically of the order of a few 10^{-10}m. For instance,
- the lattice parameter of the element Ni is 3.6 10^{-10}m,
- the size of an atom is about 1.4 10^{-10}m.

	Energy	wavelength
Neutrons	1 – 5 meV (cold) 25 – 50 meV (thermal)	9 - 4 A 1.8 – 1.3 A
Xrays	100keV 40 keV 5 keV	0.12 A (hard Xrays) 0.31 A 2.48 A (soft Xrays)
Electrons	200 keV	0.025 A

Bragg's law



Again, $m\lambda = 2d\sin\theta$ or $\lambda = 2d_{hkl}\sin\theta$

→ exercise 4

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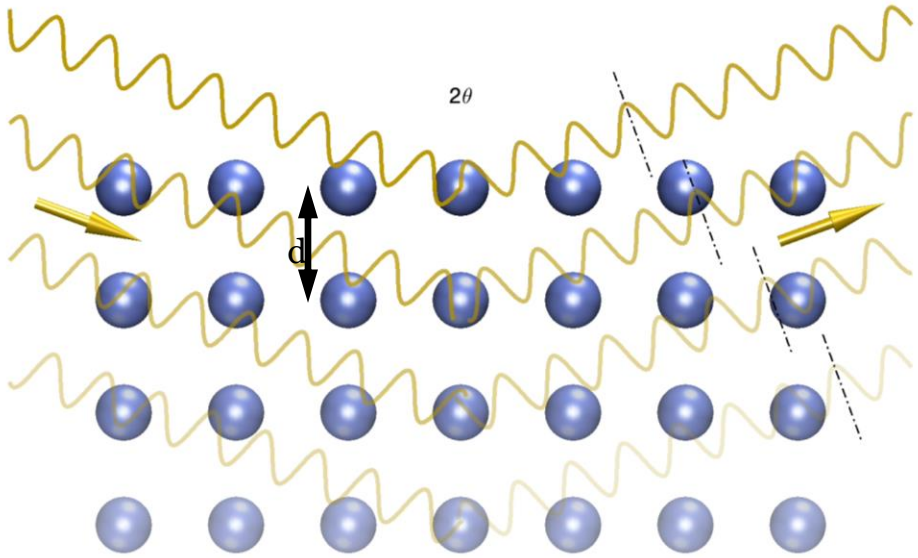
Bragg's law



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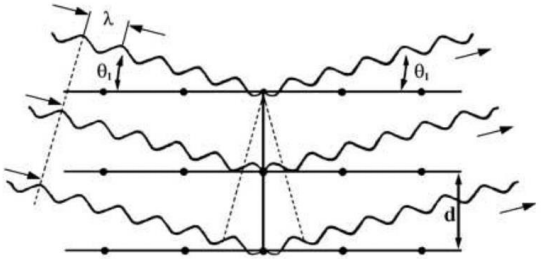
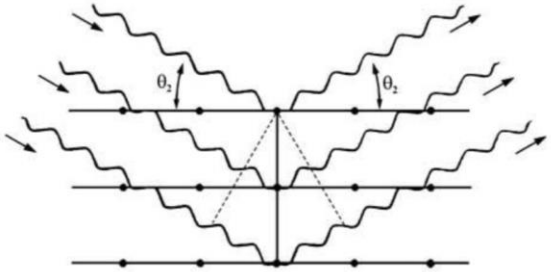
Bragg's law

higher orders m (or n):





$$m\lambda = 2d\sin\theta$$

$$\lambda = 2d_{hkl}\sin\theta$$ what happened to m?

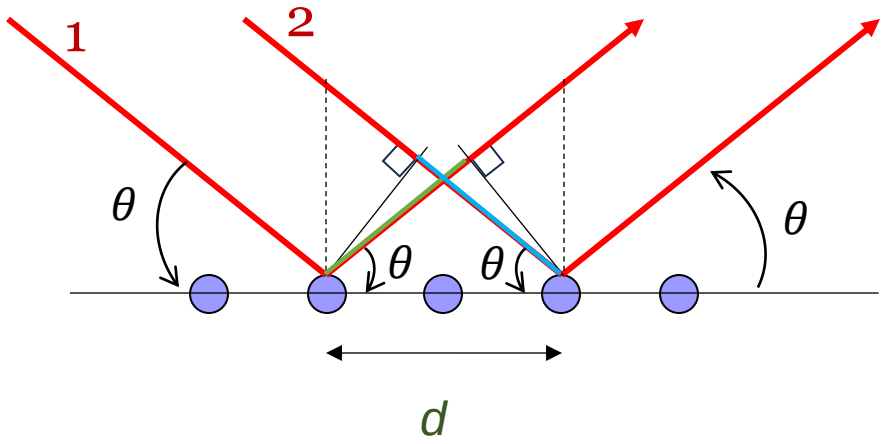
it usually is incorporated into (hkl)

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

$$\lambda = 2\left(\frac{d_{hkl}}{n}\right)\sin\theta = 2d_{nh\,nk\,nl}\sin\theta$$

for example third order reflection of the plane (111) is represented as a first order of the plane (333)

Bragg's law



$$\Delta L = d_2 - d_1 = 0$$

$$d_2 = d\cos(\theta)$$
$$d_1 = d\cos(\theta)$$

only atoms on different planes can scatter out of phase! So we can consider entire planes as scatterers.
geometrical view, simple expression

what if we look at a crystal as a three-dimensional lattice with atoms located in a certain motif? We can look at the lattice as a 3D diffraction grating → view of Max von Laue (1912)

Reminder complex numbers

Designation	Formulae
Imaginary unit j Imaginary number η	$j^2 = -1$ $\eta = \mathrm{j}y$ (y real)
Complex number z in arithmetic form Complex conjugate	$z = x + \mathrm{j}y \quad (x, y \text{ real})$ $x =$ real part $y =$ imaginary part $z^* = x - \mathrm{j}y$
Complex numbers in polar form Transformation $(x, y) \leftrightarrow (r, \alpha)$	$z = r(\cos\alpha + \mathrm{j}\sin\alpha)$ $\left.\begin{array}{l} x = r\cos\alpha \\ y = r\sin\alpha \end{array}\right\} \quad \left.\begin{array}{l} r = \sqrt{x^2 + y^2} \\ \tan\alpha = y/x \end{array}\right\}$
Complex number in exponential form Euler's formula	$z = re^{\mathrm{j}\alpha}$ $e^{\mathrm{j}\alpha} = \cos\alpha + \mathrm{j}\sin\alpha$
Exponential form for cosine and sine functions	$\cos\alpha = \frac{1}{2}(e^{\mathrm{j}\alpha} + e^{-\mathrm{j}\alpha}) = \cosh \mathrm{j}\alpha$ $\sin\alpha = \frac{1}{2\mathrm{j}}(e^{\mathrm{j}\alpha} - e^{-\mathrm{j}\alpha}) = \frac{1}{\mathrm{j}}\sinh \mathrm{j}\alpha$
Periodicity of complex numbers	$z = re^{\mathrm{j}\alpha}$ $= re^{\mathrm{j}(\alpha + 2k\pi)} \quad (k = \pm 1, \pm 2, \pm 3, \cdots)$

Reminder complex numbers

Designation	Formulae
Multiplication and division in exponential form	$z_1 = r_1 e^{j\alpha_1}, z_2 = r_2 e^{j\alpha_2}$ $z_1 z_2 = r_1 r_2 e^{j(\alpha_1+\alpha_2)}$ $\frac{z_1}{z_2} = \frac{r_1}{r_2} e^{j(\alpha_1-\alpha_2)}$
Raising to a power and extracting roots in exponential form	$z = r e^{j\alpha}$ $z^n = r^n e^{jn\alpha}$ $\sqrt[n]{z} = \sqrt[n]{r} e^{j[(\alpha+2\pi k)/n]}\ (k = 0, \pm 1, \pm 2, \cdots)$
Multiplication and division in polar form	$z_1 = r_1(\cos\alpha_1 + j\sin\alpha_1)$ $z_2 = r_2(\cos\alpha_2 + j\sin\alpha_2)$ $z_1 z_2 = r_1 r_2[\cos(\alpha_1+\alpha_2) + j\sin(\alpha_1+\alpha_2)]$ $\frac{z_1}{z_2} = \frac{r_1}{r_2}[\cos(\alpha_1-\alpha_2) + j\sin(\alpha_1-\alpha_2)]$
Raising to a power and extracting roots in polar form	$z = r(\cos\alpha + j\sin\alpha)$ $z^n = r^n[\cos n\alpha + j\sin n\alpha]$ $\sqrt[n]{z} = \sqrt[n]{r}\left[\cos\left(\frac{\alpha}{n} + \frac{2\pi k}{n}\right) + j\sin\left(\frac{\alpha}{n} + \frac{2\pi k}{n}\right)\right]$ $(k = 0, \pm 1, \pm 2, \cdots)$

Reminder complex numbers

- The polar form : $z = rcos\theta + irsin\theta = re^{i\theta}$
- The relation $e^{i\theta} = cos\theta + isin\theta$ is called the Euler relation
- Link with the algebraic form:

$$r = \sqrt{x^2 + y^2} \text{ and } \tan\theta = \frac{y}{x} \qquad cos\theta = \frac{x}{\sqrt{x^2+y^2}} \text{ and } \sin\theta = \frac{y}{\sqrt{x^2+y^2}}$$

- Remember that $e^{i\theta}$ is periodic ! So:

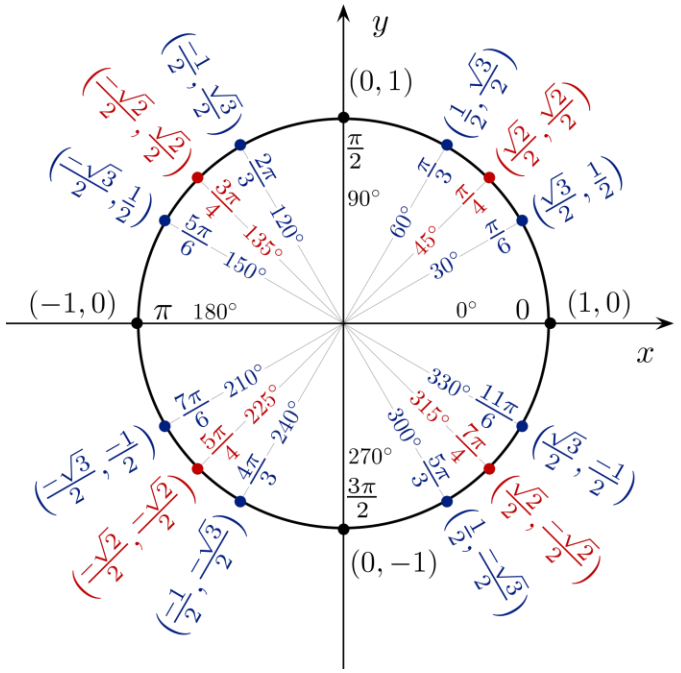
$$e^{i\theta} = e^{i(\theta+2p\pi)}, p \in \mathbb{Z}$$

- $\left|e^{i\theta}\right| = 1 = \sqrt{x^2 + y^2}$, with

$x = cos\theta$ and y= $sin\theta$

So the x coordinate are the cosine of the angle;
The y coordinates are the sine of the angle.

Example: $\cos\left(\frac{\pi}{3}\right) = \frac{1}{2}$; $\sin\left(\frac{\pi}{3}\right) = \frac{\sqrt{3}}{2}$



Plane wave equation

$$\psi(\boldsymbol{r},t) = Ae^{i\Phi} = Ae^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_0)} = A'e^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} \quad \psi(\boldsymbol{r},t) = A\cos(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_0)$$

$\boldsymbol{r}$ is the position vector (x,y,z)
t is the time
Φ the (total) phase
A is the amplitude of the wave (in electromagnetism often noted as $\boldsymbol{E}_o$, the electric field amplitude)

A' is the complex amplitude $A' = e^{i\phi}$
which includes the phase shift ϕ_0

$\mathbf{k}$ is the wave vector $\boldsymbol{k} = \frac{2\pi}{\lambda}\hat{n}$
λ is the wave length, $\hat{n}$ a unit vector pointing in the direction of propagation

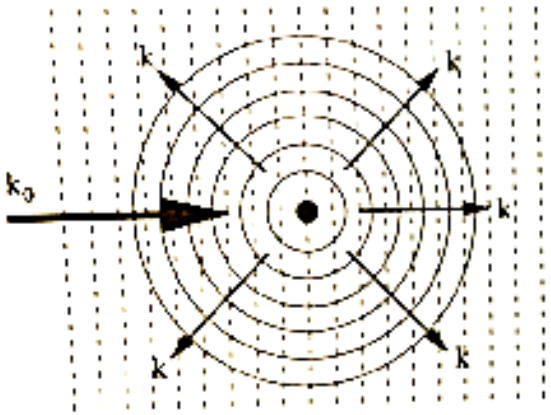
ω is the angular frequency, with $\omega = 2\pi f$

Laue's condition

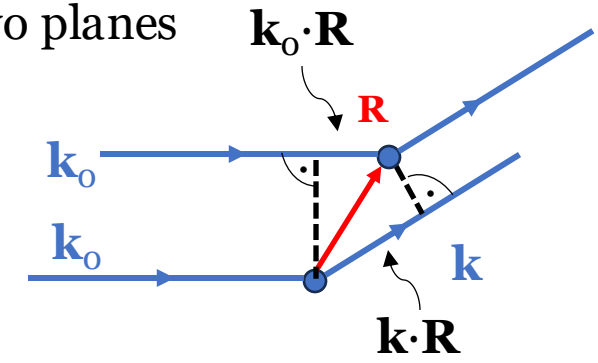
- scattering of an electromagnetic plane wave

$\vec{E} = \overrightarrow{E_0} e^{i(\boldsymbol{k}.\boldsymbol{r}-\omega t)}$ where $\boldsymbol{k}$ is the wave vector on a crystal, $|\mathbf{k}|=2\pi/\lambda$, $\omega = 2\pi/T$

- consider simplified crystal where motif = 1 atom, located at lattice points
- each atom acts like an independent source that scatters the incoming light in different directions



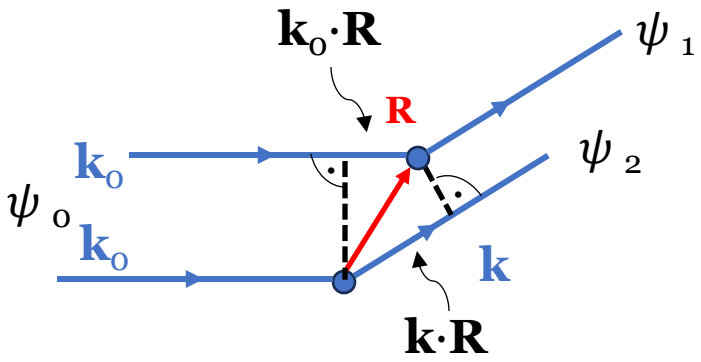
look at any 2 points on the lattice, not two planes



- diffraction peaks will be observed in directions that the rays scattered from all lattice points interfere constructively

Laue's condition

two (random) lattice points on the crystal lattice
any lattice vector $\boldsymbol{R} = r_1\boldsymbol{a} + r_2\boldsymbol{b} + r_3\boldsymbol{c}$



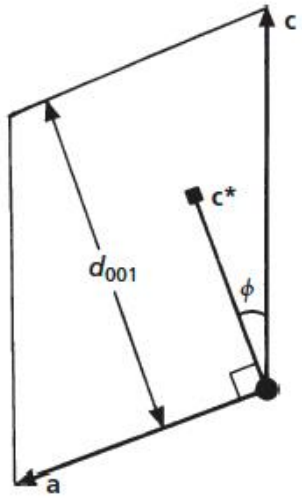
$$\psi = \psi_1 + \psi_2$$

$$\psi(\boldsymbol{r}, t) = Ae^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_0)}$$

there is constructive interference if the phase of ψ_1 and ψ_2 are the same, or an integer of 2π

$$\boldsymbol{k}\cdot\boldsymbol{R} - \omega t = \boldsymbol{k_0}\cdot\boldsymbol{R} - \omega t + 2\pi N$$
$$(\boldsymbol{k} - \boldsymbol{k_0})\cdot\boldsymbol{R} = 2\pi N$$

Reciprocal lattice



Plan of a monoclinic unit cell perpendicular to the y-axis

c* is perpendicular to both **a** and **b**, which means their dot products are zero

$\mathbf{c}^* \cdot \mathbf{a} = 0$ and $\mathbf{c}^* \cdot \mathbf{b} = 0$

$\mathbf{c}^* \cdot \mathbf{c} = cc^* \cos\phi$

with $|\mathbf{c}^*| = 2\pi/d_{001}$ and from drawing: $c \cos\phi = d_{001}$

$\mathbf{c}^* \cdot \mathbf{c} = 2\pi d_{001}/d_{001} = 2\pi$

does we have:

c* is perpendicular to both **a** and **b**, which means their dot products are zero

$\mathbf{c}^* \cdot \mathbf{a} = 0$ and $\mathbf{c}^* \cdot \mathbf{b} = 0$

$\mathbf{c}^* \cdot \mathbf{c} = cc^* \cos\phi$

with $|\mathbf{c}^*| = 2\pi/d_{001}$ and from drawing: $c \cos\phi = d_{001}$

$\mathbf{c}^* \cdot \mathbf{c} = 2\pi d_{001}/d_{001} = 2\pi$

We have a new basis new basis (O, **a***, **b***, **c***) in which a vector $\mathbf{N}^*_{\mathbf{hkl}} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ is perpendicular to the plane (hkl)

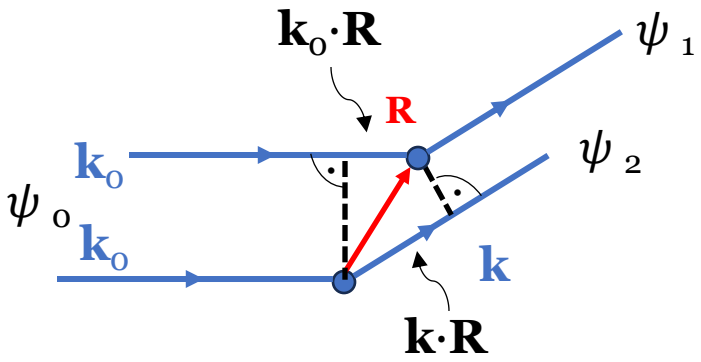
If we consider any vector in the direct space $\boldsymbol{R} = r_1\boldsymbol{a} + r_2\boldsymbol{b} + r_3\boldsymbol{c}$ and one in the reciprocal space $\boldsymbol{N}^* = n_1\boldsymbol{a}^* + n_2\boldsymbol{b}^* + n_3\boldsymbol{c}^*$, we have:

$$\boldsymbol{R} \cdot \boldsymbol{N}^* = r_1 n_1 \boldsymbol{a} \cdot \boldsymbol{a}^* + r_2 n_2 \boldsymbol{b} \cdot \boldsymbol{b}^* + r_3 n_3 \boldsymbol{c} \cdot \boldsymbol{c}^* = 2\pi(r_1 n_1 + r_2 n_2 + r_3 n_3)$$

an integer

Laue's condition

two (random) lattice points on the crystal Bravais lattice
any lattice vector $\boldsymbol{R} = r_1\boldsymbol{a} + r_2\boldsymbol{b} + r_3\boldsymbol{c}$



$$\psi = \psi_1 + \psi_2$$

$$\psi(\boldsymbol{r}, t) = A' e^{i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)}$$

there is constructive interference if the phase of ψ_1 and ψ_2 are the same, or an integer of 2π

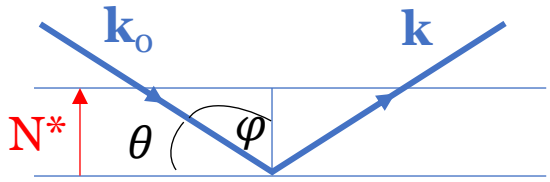
$$\boldsymbol{k}\cdot\boldsymbol{R} - \omega t = \boldsymbol{k_0}\cdot\boldsymbol{R} - \omega t + 2\pi N$$
$$(\boldsymbol{k} - \boldsymbol{k_0})\cdot\boldsymbol{R} = 2\pi N$$

this is fullfilled if
$$\boldsymbol{k} - \boldsymbol{k_0} = \mathbf{N}^*$$

$\boldsymbol{R} \in \mathcal{D}$ the (direct) Bravais lattice
$\mathbf{N}^* \in \mathcal{R}$ the reciprocal lattice

→ Laue's condition: for constructive interference, the difference between incident wave vector $\boldsymbol{k_o}$ and scattered wave vector $\boldsymbol{k}$ must be a reciprocal lattice vector $\mathbf{N}^*$

Laue's condition and Bragg's law



$\boldsymbol{k} - \boldsymbol{k_0} = \mathbf{N}^*$

$\boldsymbol{k_0} = \boldsymbol{k} - \mathbf{N}^*$

$\|\boldsymbol{k}_0\|^2 = \|\boldsymbol{k}\|^2 - 2\,\|\boldsymbol{k}\|\,\|\mathbf{N}*\|\cos\varphi + \|\mathbf{N}*\|^2$

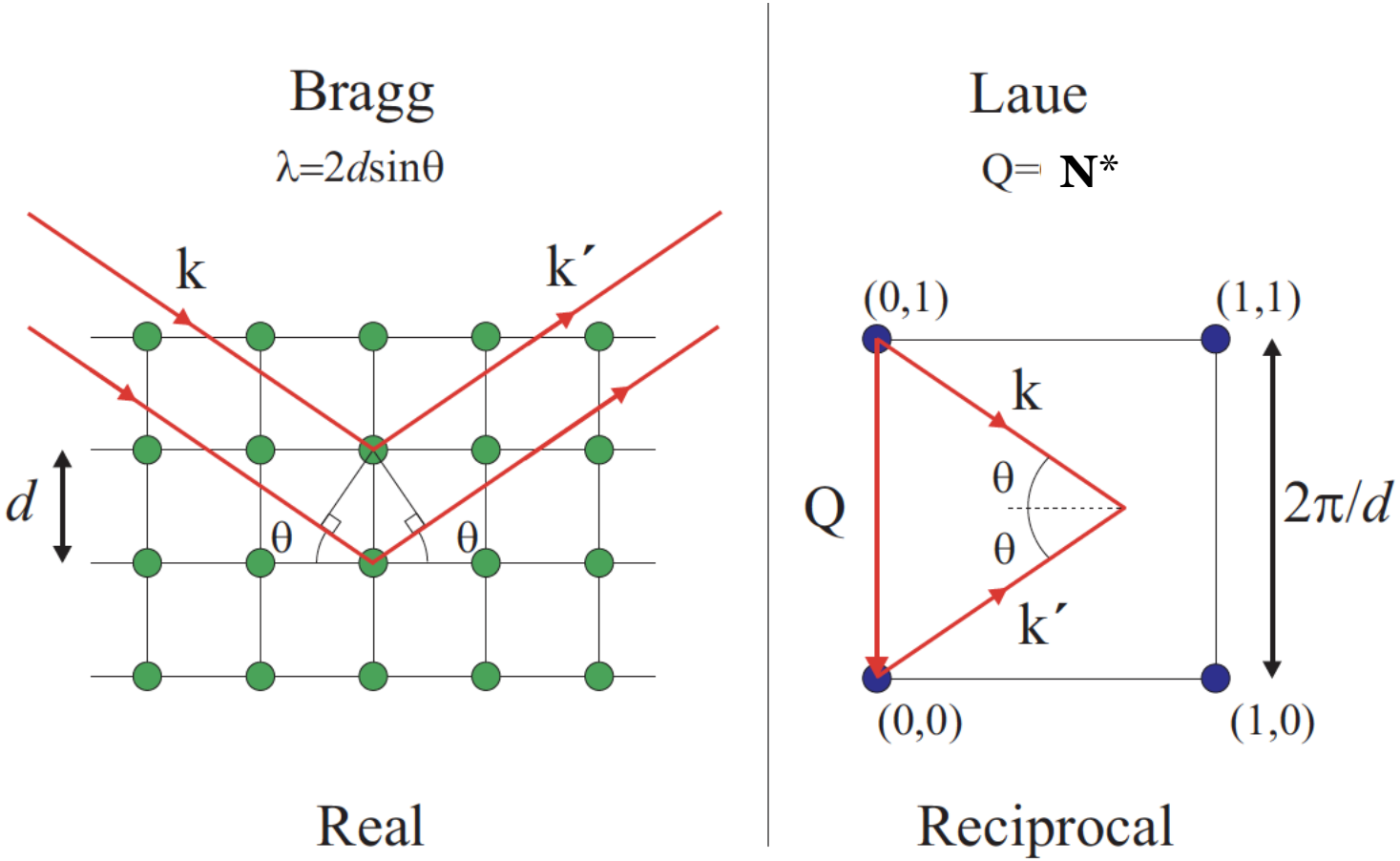
$$\cos\left(\frac{\pi}{2} - \theta\right) = \sin\theta$$

wave only changes direction, thus $\|\boldsymbol{k}_0\| = \|\boldsymbol{k}\| = \frac{2\pi}{\lambda}$

and using $\|\mathbf{N}*\| = \frac{2\pi}{d}$

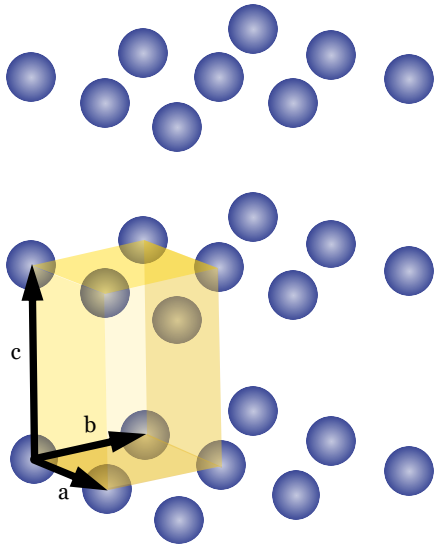
→ $\lambda = 2d_{hkl}\sin\theta$

Laue's condition and Bragg's law



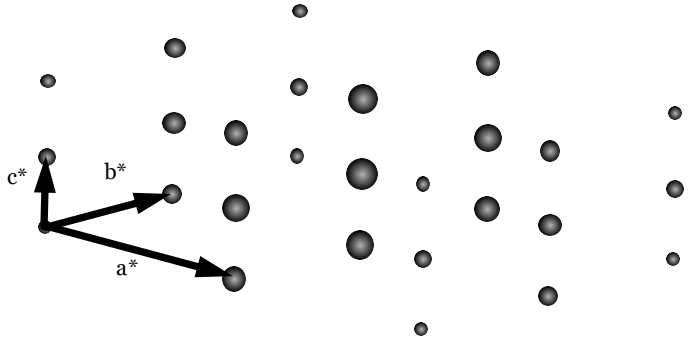
Reciprocal space lattice → diffraction pattern

The reciprocal lattice represents the framework and components of the diffraction pattern



e.g. a < b < c

Real space



a* > b* > c*

Reciprocal space

The reciprocal lattice is the Fourier transform of the direct lattice!

The spacings between peaks in reciprocal lattice (a*, b*, c*) are inversely proportional to the corresponding dimensions in real space (a, b, c)

Summary

- Definition of recirprocal lattice
- Relation between direct lattice and reciprocal lattice
- Distances betweek crystallographic planes with reciprocal lattice
- Basics of diffraction: Young's double slit experiments
- Diffraction on a crystal
- Bragg's law
- Laue condition and the connection of reciprocal lattice to diffraction