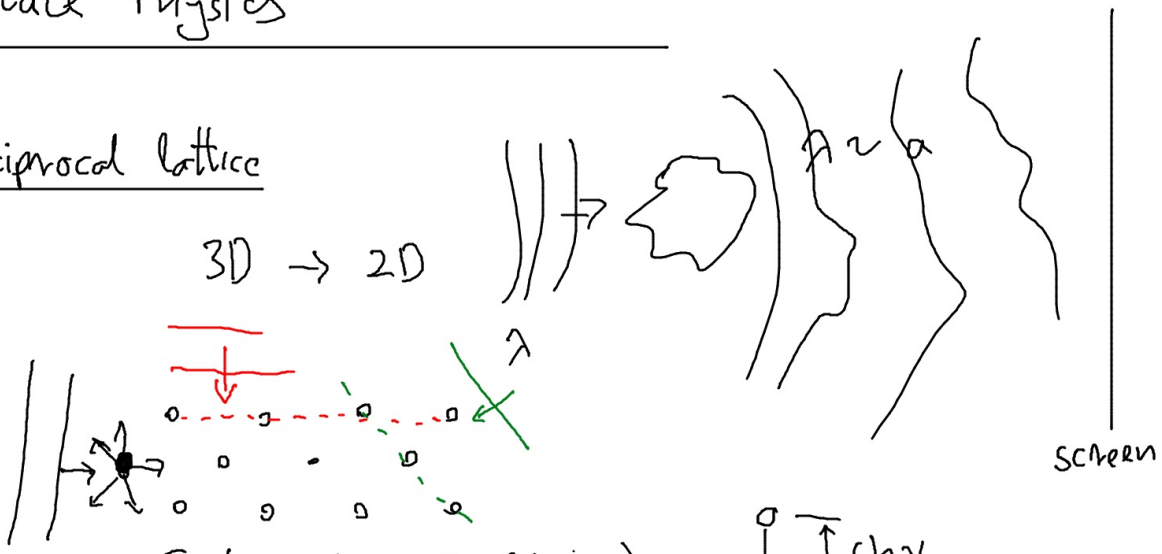
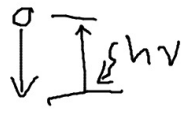
Solid State Physics

Reciprocal lattice

3D → 2D



Electro Magnetic wave $\underline{E}(t,\underline{r})$, $\underline{B}(t,\underline{r})$



lattice planes

electron beam $\lambda = \frac{h}{p}$

plane wave ↓

$$\underline{E}(t,\underline{r}) = \underline{E}_0 e^{i(\omega t - \underline{k}\underline{r})}$$

$$E(t,x) = E_0 \sin(\underline{\omega t - kx})$$ (phase)

$t_0 \ni \omega t_0 - k x_0 = 0$

$\boxed{\omega t - k x = 0}$

$\underline{k}$ direction the w. travels

$|\underline{k}| = \frac{2\pi}{\lambda}$ wave vector

$x = \frac{\omega}{k} t$

$$\underline{R} = \sum_{i=1}^{3} n_i \underline{a}_i \qquad n_i = 0, \pm 1, \pm 2 \ldots$$

$e^{i\varphi} = \cos\varphi + i \sin\varphi$

$e^{i(\omega t - \underline{k}\underline{r})}$ ... $\underline{R}$

$\underline{r}_1, \underline{r}_2$ equivalent point, i.e.

$\underline{r}_1$ $\underline{r}_2 = \underline{r}_1 + \underline{R}_{1,2}$ → $e^{i\underline{k}\underline{r}_1} = e^{i\underline{k}(\underline{r}_1 + \underline{R}_{1,2})}$

if

$e^{i\underline{k}\underline{r}_1} = e^{i\underline{k}\underline{r}_1} \cdot e^{i\underline{k}\underline{R}_{1,2}}$

if $e^{i\underline{K}\underline{R}} = 1 \Rightarrow \boxed{\underline{K}\underline{R} = 2\pi}$ as $e^{i2\pi} = 1$

Δ = distance of lattice planes

let $\underline{R} = \underline{a}_1 \Rightarrow \underline{b}_1 \underline{a}_1 = 2\pi$ ($\underline{b}_1 \equiv K$ for $\underline{a}_1$)

$\underline{a}_1\ \underline{a}_2\ \underline{a}_3 \leftrightarrow \underline{b}_1, \underline{b}_2, \underline{b}_3$ where $\underline{b}_n \cdot \underline{a}_n = 2\pi$

direct lattice — reciprocal lattice

then

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

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

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

but

$$\underline{a}_1 (\underline{a}_2 \times \underline{a}_3) = \underline{a}_2 (\underline{a}_3 \times \underline{a}_1) = \underline{a}_3 (\underline{a}_1 \times \underline{a}_2)$$

notation $\underline{a}_1 \underline{a}_2 \underline{a}_3$ ← volume of cell

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

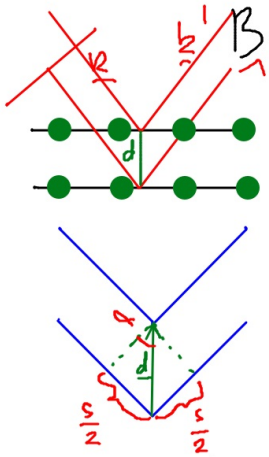
$$\underline{K} = h \underline{b}_1 + k \underline{b}_2 + l \underline{b}_3$$

$$\underline{K}\,\underline{R} = 2\pi \cdot \underbrace{(n_1 h + n_2 k + n_3 l)}_{\text{integer}}$$

lattice planes in reciprocal lattice

plane wave

phase is constant



Bragg formula

condition of constructive interference:

$s = 2 \cdot d \cdot \sin\alpha = n \cdot \lambda$

path difference

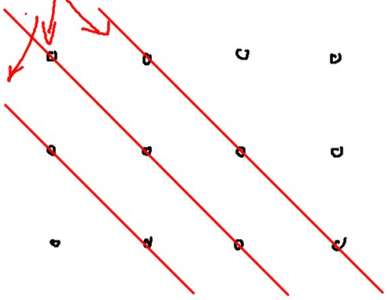
$|\underline{k}| = \frac{2\pi}{\lambda}$

$h_1 k_1 l$

$\underline{g}_{hkl} = h \cdot \underline{b}_1 + k \underline{b}_2 + l \underline{b}_3$

determines a lattice plane

equivalent lattice planes



$h, k, l = 0, \pm 1, \ldots$

infinite number of equivalent lattice planes

Miller indeces (indexes ☺)

describes **all equivalent** lattice planes in direct lattice and directions in reciprocal lattice

Direction in rec. l. $g_{hkl} = h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3$ notation: [hkl]

equivalent dir.: <hkl>

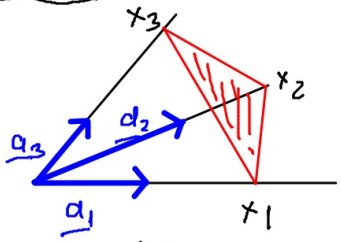
Lattice planes.

notation: (h k l) example (123) → h=1, k=2, l=3

(1$\bar{2}$3) h=1, k=-2, l=3

if any of these is >9 use commas

method of determination:



(non cartesian system of base vectors)

$x_1 = \alpha \underline{a}_1$

$x_2 = \beta \underline{a}_2$ α, β, γ integers, or ∞ if no intersections

$x_3 = \gamma \underline{a}_3$ with the corresponding axis

take the reciprocals: $\left(\frac{1}{\alpha} \frac{1}{\beta} \frac{1}{\gamma}\right)$ using the lowest common denominator A:

then $\frac{1}{\alpha} = \frac{h}{A}$, $\frac{1}{\beta} = \frac{k}{A}$, $\frac{1}{\gamma} = \frac{l}{A}$ ⇒ use the numerators only:

(h, k, l) ⇒ (h k l)

if a plane goes through the origin select another equivalent plane.

(can't divide by 0) {hkl} ← each equivalent numbers for this example:

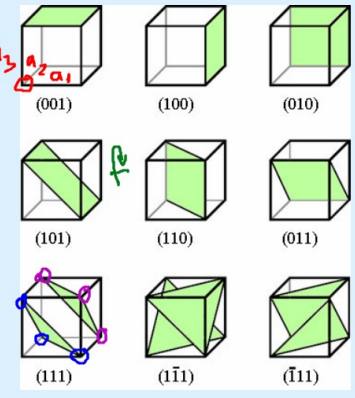
(001) equivalent with (100) and (010)

so {100} means any of these

Problem 37. a unit cell

Draw all 9 lattice planes and determine the Miller indexes in a simple cubic Bravais lattice.

Solution: 2 90° 3 90° SC



{100}

{101}

{111}

α = ∞
β = ∞
γ = 1
α = 1
β = ∞
γ = 1
a = 1
b = 1
γ = 1

$\frac{1}{1} \frac{1}{\infty} \frac{1}{1}$

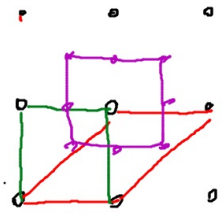
(1 0 1)

{1 $\bar{1}$ 1}

(Where is the origin of the 3 lattice vectors in the cubes?)

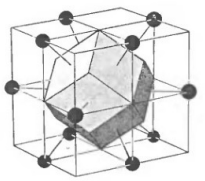
special cell in reciprocal lattice: primitive
primitive

$\underline{b}_1, \underline{b}_2, \underline{b}_3$ unit cells

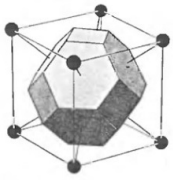


primitive cell

Wigner-Seitz cell or Brillouin-zone



fcc



bcc

direct lattice		reciprocal lattice
sc	→	sc
fcc	→	bcc
bcc	→	fcc

$\underline{g}_{hkl} \perp (hkl)$

↑ select the shortest one

$$|\underline{g}_{hkl}| = d_{hkl} = \sqrt{h^2 b_1^2 + k^2 b_2^2 + l^2 b_3^2}$$

↑ distance $= \sqrt{h^2 \left(\frac{2\pi}{a_1}\right)^2 + k\left(\frac{2\pi}{a_2}\right)^2 + l\left(\frac{2\pi}{a_3}\right)^2}$

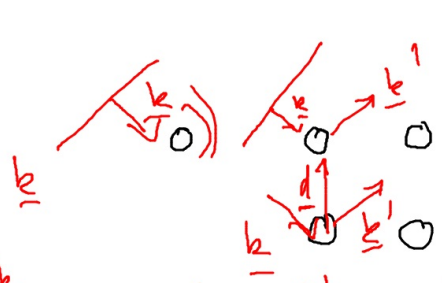
$$|\underline{g}_{hkl}| = 2\pi \sqrt{\left(\frac{h}{a_1}\right)^2 + \left(\frac{k}{a_2}\right)^2 + \left(\frac{l}{a_3}\right)^2}$$

reciprocal lattice is the Fourier transform of the direct lattice

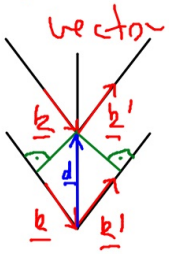
Bragg's formula works – why

crystal = point lattice + basis

Laue-formulas



$|\underline{k}| = |\underline{k}'|$ ⇒ elastic process



$\underline{n} := \frac{\underline{k}}{|\underline{k}|}$ $\quad \underline{n}' := \frac{\underline{k}'}{|\underline{k}'|} = \frac{\underline{k}'}{|\underline{k}|}$

$s = \underline{d}\,(\underline{n}' - \underline{n}) = m \cdot \lambda \qquad m = 1, 2, \dots$

$\underline{d}\,(\underline{k}' - \underline{k}) = 2\pi \cdot m$

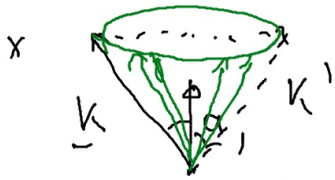
$|\underline{k}| = \frac{2\pi}{\lambda}$

$\Delta \underline{k} \equiv \underline{K}$

for any $\underline{K}$, even for $\underline{K} = \underline{a}_1, \dots$

Laue cond.

$$\underline{a}_1 \underline{K} = 2\pi h$$
$$\underline{a}_2 \underline{K} = 2\pi k$$
$$\underline{a}_3 \underline{K} = 2\pi l$$



$\underline{a}_1 \cdot \underline{K} = \text{const}$ on a cone

Experimental methods

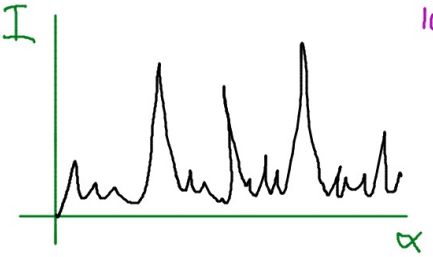
ATM, AFM + E.M. waves

what kind of E.M. X-rays ($\lambda \sim$ nm)

what can we vary? λ, orientation

1. use $\lambda_1 < \text{every } \lambda < \lambda_2$ — Laue-method — orientation of known
   fixed orientation — film
   diffraction curves for each λ

2. λ and rotate crystal — identify unknown crystals
   for λ



3. powder (microcrystals) — Debye-Scherrer — lattice parameters
   fixed λ