project:

R-1

Reciprocal Lattice

In $d=1$ we considered k which give $e^{ikr} = e^{ikna} = 1$

$k = \frac{2\pi}{a}$

We have discussed lattices of atoms which have property that if you move to a new location $\vec{r} \to \vec{r} + \vec{R}$ your environment looks the same.

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

It turns out to be very useful to ask which $\vec{k}$ vectors generate plane waves which obey this same periodicity

$$e^{i\vec{k}\cdot\vec{r}} = e^{i\vec{k}\cdot(\vec{r}+\vec{R})} \implies e^{i\vec{k}\cdot\vec{R}} = 1$$

The answer is $\vec{G}$ $\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$ (k_i integers)

where $$\vec{b}_1 = \frac{2\pi}{V_c}\,\vec{a}_2 \times \vec{a}_3$$

$$\vec{b}_2 = \frac{2\pi}{V_c}\,\vec{a}_3 \times \vec{a}_1$$

$V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

volume of unit cell

$$\vec{b}_3 = \frac{2\pi}{V_c}\,\vec{a}_1 \times \vec{a}_2$$

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

eg $\vec{b}_1 \cdot \vec{a}_1 = 2\pi$ obviously

likewise $\vec{b}_1 \cdot \vec{a}_2 = 0$ also obvious $\vec{a}_2 \perp \vec{a}_2 \times \vec{a}_3$

So $$\vec{k}\cdot\vec{R} = \underbrace{(k_1 n_1 + k_2 n_2 + k_3 n_3)}_{\text{integer}}2\pi \implies e^{i\vec{k}\cdot\vec{R}} = 1$$

project:

R-2

The reciprocal of the reciprocal lattice is the original lattice.

Almost obvious interchange roles of $\vec{k}$ and $\vec{R}$.

But calc also prove

$$\vec{c}_1 = \frac{2\pi}{V_c'} \vec{b}_2 \times \vec{b}_3 = \frac{2\pi}{V_c'}\left(\frac{2\pi}{V_c}\right)^2 (\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)$$

$$\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A}\cdot\vec{C}) - \vec{C}(\vec{A}\cdot\vec{B}) \qquad \text{"BAC-CAB"}$$

$$\sim \quad \vec{a}_1 \underbrace{[(\vec{a}_3 \times \vec{a}_1)\cdot a_2]}_{V_c} - \vec{a}_2 \underbrace{[(\vec{a}_3 \times \vec{a}_1)\cdot \vec{a}_1]}_{0}$$

$$= \frac{2\pi}{V_c'}\left(\frac{2\pi}{V_c}\right)^2 V_c \vec{a}_1$$

$$V_c' = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$$

$$= \left(\frac{2\pi}{V_c}\right)^3 (\vec{a}_2 \times \vec{a}_3) \cdot \underbrace{[(\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)]}_{V_c \vec{a}_1}$$

from above

$$= \left(\frac{2\pi}{V_c}\right)^3 V_c^2 = \frac{(2\pi)^3}{V_c}$$

Finally $\quad \vec{c}_1 = 2\pi \underbrace{\frac{V_c}{(2\pi)^3}}_{1/V_c'} \left(\frac{2\pi}{V_c}\right)^2 V_c \vec{a}_1 = \vec{a}_1$

whew!

project:

R-3

SC $\vec{a}_1 = a\hat{x}$ $\vec{a}_2 = a\hat{y}$ $\vec{a}_3 = a\hat{z}$

$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$ $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$ $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$ $\rightarrow$ also SC

Can easily show

FCC reciprocal lattice is BCC

BCC " " " FCC

follows also from page R-2

Wigner Seitz cell of Reciprocal lattice $\leftrightarrow$ "First Brillouin Zone"

Units of $\hat{a}_i$ $\rightarrow$ length

G $\rightarrow$ 1/length (wavenumber k)

HW1

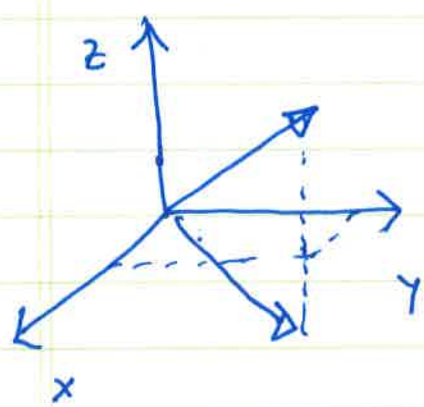
(1) Delay problem 8 to HW2

(2) Matrix associated with operation which transforms a vector.

A) Change length by 2; same direction

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} 2x \\ 2y \\ 2z \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

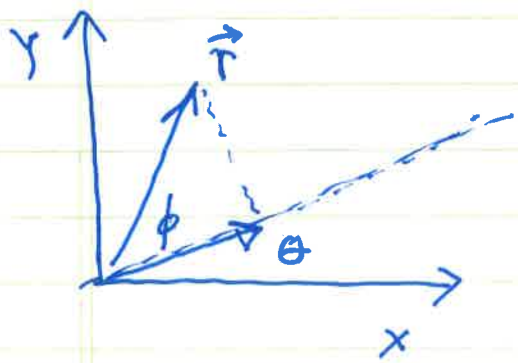
B) Reflect in xy plane



$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x \\ y \\ -z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

State general approach
$\hat{O}$(unit vectors) $\to$ columns

c) Project $\begin{pmatrix} x \\ y \end{pmatrix}$ onto line making angle θ wrt $\hat{x}$ axis



??

Miller Indices

REVIEW

Lattice points $\vec{G}$ in reciprocal space have the property that $e^{i\vec{G}\cdot\vec{r}}$ is periodic in real space when $\vec{r} \to \vec{r} + \vec{R}$

(in fact, this $e^{i\vec{G}\cdot\vec{R}} = 1$ was the definition of $\{\vec{G}\}$)

This relates real space $\longleftrightarrow$ reciprocal space

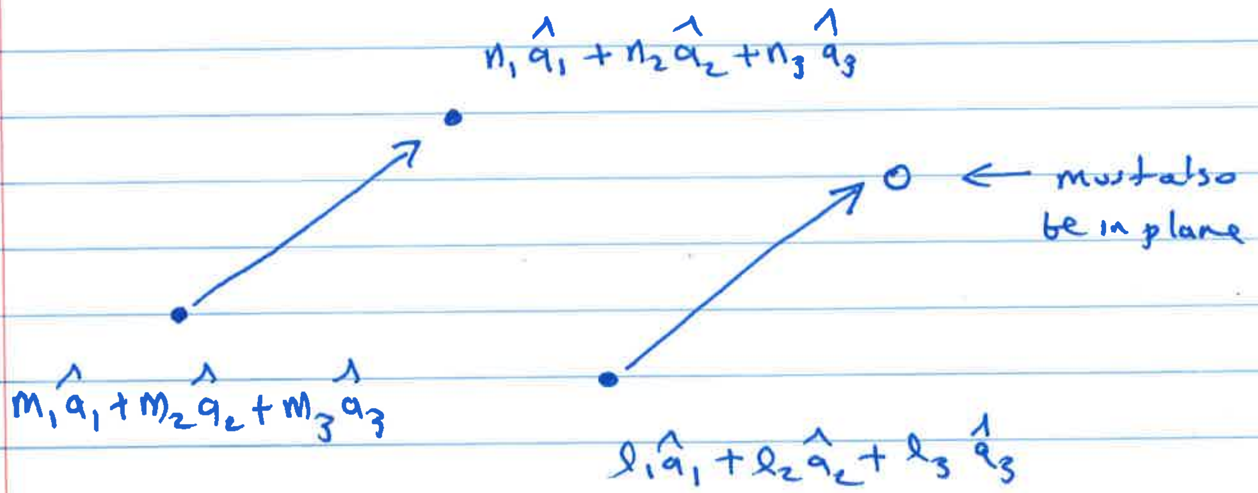
Another link between the two is provided by considering the collection of planes which contain atoms in the crystal.

Both these links will underlie our discussion of diffraction.

A lattice plane is a plane containing at least 3 non-collinear lattice points. Because of translational symmetry, such a plane must contain an infinite number of lattice points.

MIA

• 3 points in plane



o must also be in plane because

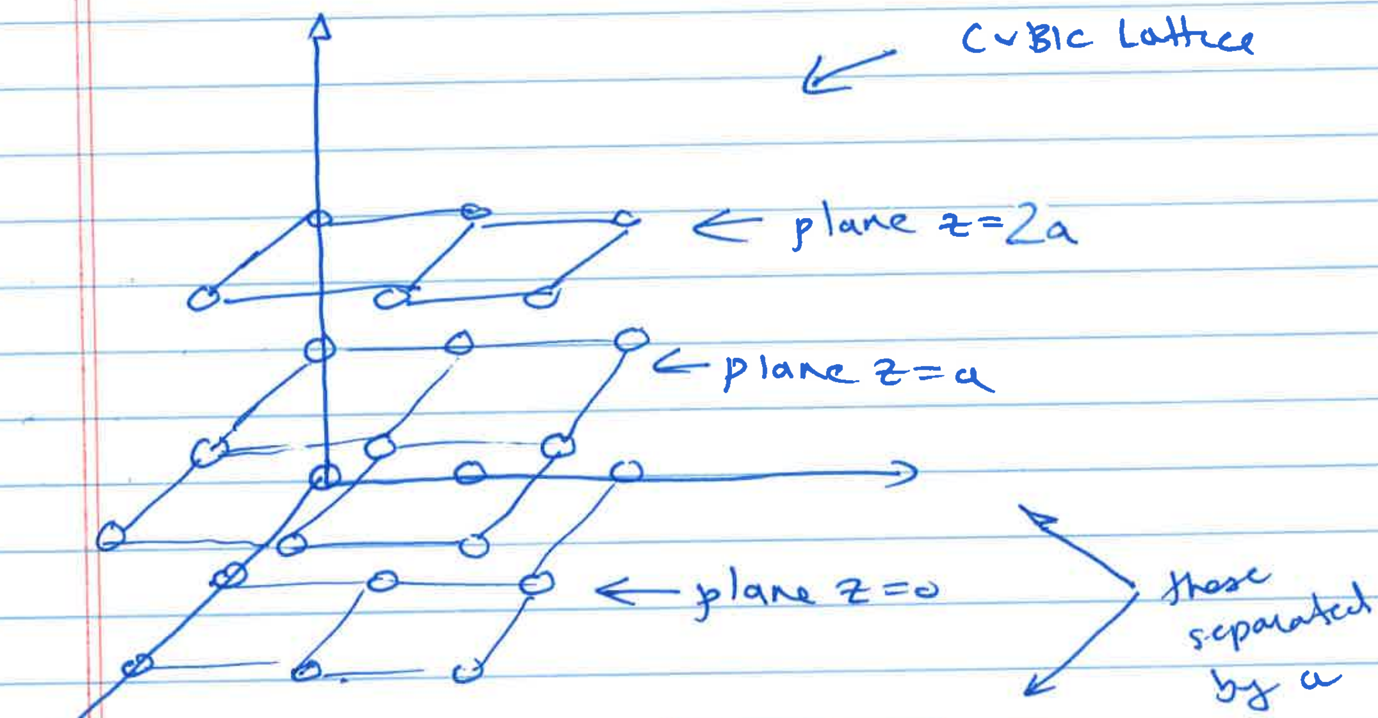
$$\vec{r}_o = l_1\hat{a}_1 + l_2\hat{a}_2 + l_3\hat{a}_3$$

$$+ (n_1 - m_1)\hat{a}_1 + (n_2 - m_2)\hat{a}_2 + (n_3 - m_3)\hat{a}_3$$

$$= \underbrace{(l_1 + n_1 - m_1)}_{\text{an integer} \dots}\hat{a}_1 + \dots$$

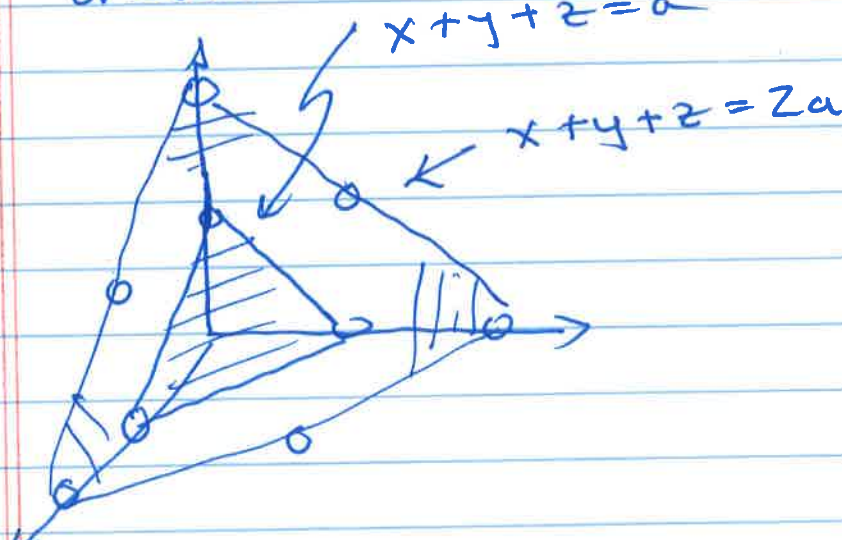
M2

A "family" of lattice planes is a parallel set of equally spaced lattice planes containing all points of the 3D Bravais lattice.



$\boxed{\text{or } x, y}$

or even



What is separation? Consider points

$\frac{1}{3}(a,a,a)$ on $x+y+z=a$

$\frac{2}{3}(a,a,a)$ $x+y+z=2a$

distance between them is $\sqrt{(a/3)^2+(a/3)^2+(a/3)^2}$

$= a/\sqrt{3}$

$\boxed{\text{Eqn of Plane}}$

WLOG normalize eqn so $a^2+b^2+c^2=1$

3D space − (1 constraint) → 2D surface

$$ax + by + cz = d$$

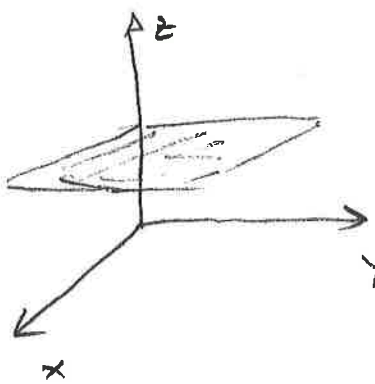
$$(a,b,c)\cdot(x,y,z) = d$$

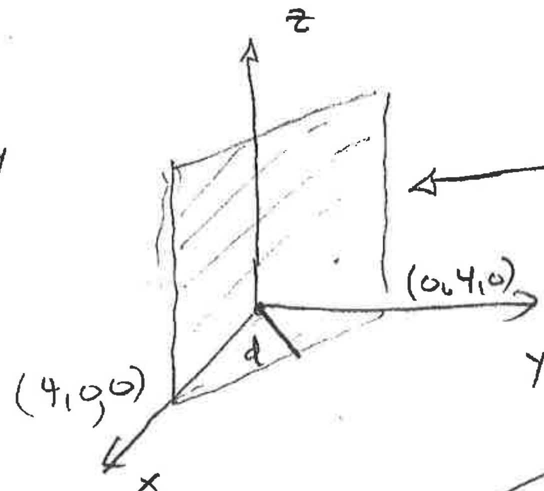
geometrical significance

shortest distance of plane to origin

$(a,b,c) \Rightarrow$ normal to plane

Examples $\quad z = 3 \quad (a,b,c) = (0,0,1) \Rightarrow \hat{z}$





$x + y = 4$

$(a,b,c) = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$

$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)\cdot(x\ y\ z)$

$= \frac{4}{\sqrt{2}}$

clearly this is $\hat{n}$ to plane

clearly this is distance d to origin

P2

We are often interested in the surfaces upon which a function is constant, eg equipotential surfaces in E+M, or isotherms in stat mech, (or the lines of constant height on a contour map while you are hiking!)

Why do we call $f(\vec{r}) = f_0 e^{i\vec{k}\cdot\vec{r}}$ a "plane wave"?

Answer: The surfaces $f(\vec{r}) = \text{constant}$ are planes

This is almost obvious. For $f(\vec{r}) = \text{const}$ we need

$$\vec{k}\cdot\vec{r} = c$$

But we have just reminded ourselves this is the equation of a plane!

M3

<u>Theorem</u>: Given a family of lattice planes separated by distance d there are reciprocal lattice vectors $\vec{G}$ $\perp$ to those planes and the shortest length of $\{\vec{G}\}$ is $2\pi/d$.

$*$ Before proving emphasize impt point: Another interpretation of reciprocal lattice vectors is that they are the vectors $\perp$ to lattice planes.

$\boxed{\text{NOTES P1 and P2 HERE}}$

<u>Proof of theorem</u>

We have seen <u>any</u> plane is defined by $\hat{n}\cdot\vec{r} = d$

If we consider the vector $\frac{2\pi}{d}\hat{n}$ we see $\frac{2\pi}{d}\hat{n}\cdot\vec{r} = 2\pi$

Therefore $e^{i\frac{2\pi}{d}\hat{n}\cdot\vec{r}} = 1$ so $\frac{2\pi}{d}\hat{n}$ is a reciprocal lattice vector. This is also clearly true of $4\pi/d\;\hat{n}$, $6\pi/d\;\hat{n}$ ... but $2\pi/d\;\hat{n}$ is shortest.

Examples for cubic lattice

Planes $\{ \ldots z = -2a;\ z = -a;\ z = 0;\ z = +a;\ z = +2a \ldots \}$

normal is $\hat{n} = \hat{z}$ Thm says $\vec{G} = \frac{2\pi}{a}\hat{z}$

separation is a is shortest RLV

check: $\hat{a}_1 = \hat{x}$ $\vec{b}_1 = 2\pi/a\ \hat{x}$

$\hat{a}_2 = \hat{y}$ $\vec{b}_2 = 2\pi/a\ \hat{y}$

$\hat{a}_3 = \hat{z}$ $b_3 = 2\pi/a\ \hat{z}$

Eg $\hat{b}_1 = \frac{2\pi}{V_c}(\hat{a}_2 \times \hat{a}_3) = \frac{2\pi}{a^3}a^2\hat{x} = 2\pi/a\ \hat{x}$

$\vec{G} = 2\pi/a\left(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}\right)$

$2\pi/a\ \hat{z}$ is indeed a RLV

and also clearly is shortest

planes $\{ \ldots x+y+z = a;\ x+y+z = 2a;\ x+y+z = 3a \ldots \}$

Normal is $(1,1,1)\,1/\sqrt{3}$

distance between planes is $a/\sqrt{3}$ (see page M2) or M4A

Thm says $\frac{2\pi}{a/\sqrt{3}}\underbrace{1/\sqrt{3}(\hat{x}+\hat{y}+\hat{z})}_{\hat{n}} = \frac{2\pi}{a}(\hat{x}+\hat{y}+\hat{z})$

This is indeed one of the RLV $\frac{2\pi}{a}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$

and is the shortest possible one in the class $n_1 = n_2 = n_3$

M4A

$x+y+z=a$ $\qquad$ $x+y+z=2a$

$(1\ 1\ 1)\cdot(x\ y\ z)=a$ $\qquad$ $(1\ 1\ 1)\cdot(x\ y\ z)=2a$

$\underbrace{\frac{1}{\sqrt{3}}(1\ 1\ 1)}_{\hat{n}}\cdot(x\ y\ z)=\frac{1}{\sqrt{3}}a$ $\qquad$ $\frac{1}{\sqrt{3}}(1\ 1\ 1)\cdot(x\ y\ z)=\frac{2a}{\sqrt{3}}$

distance to origin $\qquad$ distance to origin

$\frac{2a}{\sqrt{3}}-\frac{a}{\sqrt{3}}=\frac{a}{\sqrt{3}}$

= distance between planes

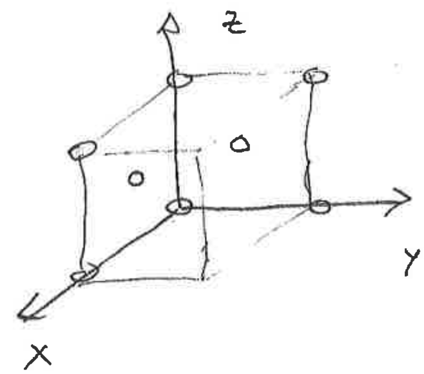
M-5

Another Example (fcc)

$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$$
$$\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$$
$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y})$$

Note: bcc!

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}-\hat{x})$$
$$\vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{z}-\hat{y})$$
$$\vec{b}_3 = \frac{2\pi}{a}(\hat{y}+\hat{x}-\hat{z})$$



One set of planes is $z = -a, -\frac{a}{2}, 0, \frac{a}{2}, a, \ldots$

separation $d = a/2$

Theorem says there are $\vec{G}$ normal to planes, ie $\vec{G} = \#\hat{z}$

the shortest of which is length $\frac{2\pi}{(a/2)} = \frac{4\pi}{a}$

use $n_1 n_2 n_3$ instead of $k_1 k_2 k_3$ in lecture

$$k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3 = \#\hat{z}$$

$$\frac{2\pi}{a}(-k_1+k_3+k_2)\hat{x} + \frac{2\pi}{a}(k_1+k_3-k_2)\hat{y} + \frac{2\pi}{a}(k_1+k_2-k_3)\hat{z} = \#\hat{z}$$

$$-k+k_3+k_2 = 0$$
$$k_1+k_3-k_2 = 0$$
$$\Rightarrow k_3 = 0, \quad k_1 = k_2$$

$$\downarrow$$
$$\frac{2\pi}{a}2k_1\hat{z}$$
$$\frac{4\pi}{a}k_1\hat{z}$$

integer

shortest length $\frac{4\pi}{a}$ ✓

M6

Crystallographers often describe lattice structures via the "Miller indices". These are just the integers which give the shortest $\vec{g}$ normal to a set of lattice planes. That is if

$$\vec{g}_{min} = n_1 \hat{b}_1 + n_2 \hat{b}_2 + n_3 \hat{b}_3$$

Then Miller indices are $(n_1\ n_2\ n_3)$

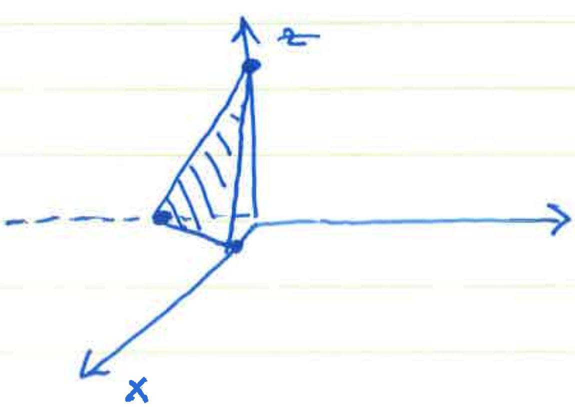
Usual notation is $\bar{3}$ for -3.

Example Miller indices $(4\bar{2}1)$

mean lattice plane has normal $\hat{n} \sim 4\hat{x} - 2\hat{y} + \hat{z}$

$\hat{n} \cdot \vec{r} = d/2\pi$ ← you need to be told d as well as Miller indices to know everything...

$$4x - 2y + z = d/2\pi$$



$\left(\frac{d}{8\pi}, 0, 0\right)$

$\left(0, \frac{-d}{4\pi}, 0\right)$

$\left(0, 0, d/2\pi\right)$

intercepts are inversely proportional to Miller indices...