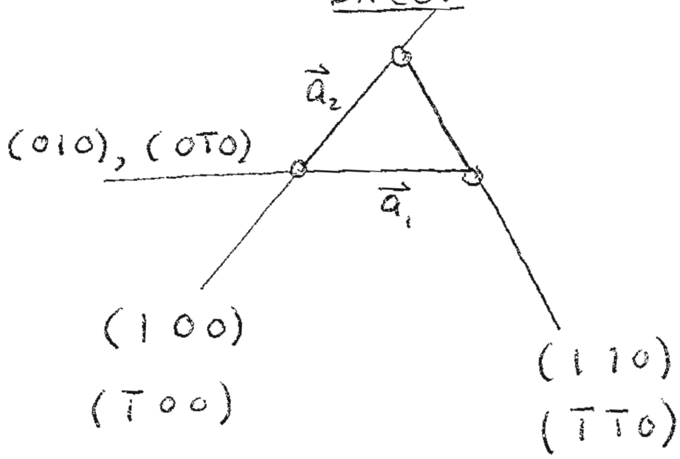
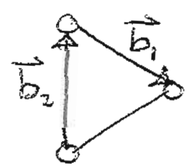
- Miller indices for <u>hexagonal</u> case using 3-index (h k l) notation turned out rather "strange and unexpected"

- This, however is a natural consequence of the 3-fold symmetry

<u>Direct</u>



<u>Reciprocal</u>



therefore it seems odd that planes having the same symmetry should have plane notation which looks non-symmetrical. i.e. how can a (100) plane be similar to a (110) plane?

equivalent planes ?? $\left(\begin{matrix}(1\ 0\ 0) \\ (1\ 1\ 0)\end{matrix}\right.$

As one may guess, since hexagonal has 3 different in-plane directions which are equivalent, it is therefore reasonable to use 3 different indices for the in-plane direction.

∴ hexagonal is best described using

<u>4-index notation</u>

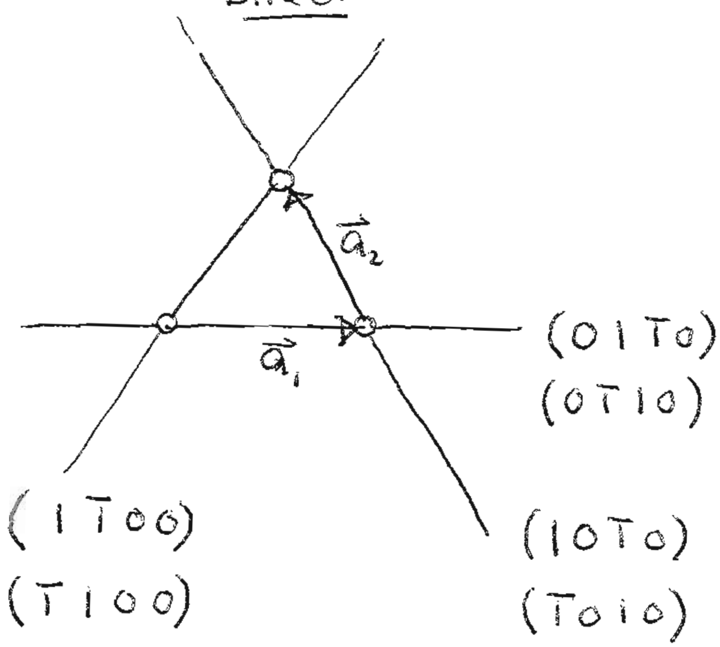
3 in-plane indices
(1 is a "dummy" index)

1 out-of-plane index.

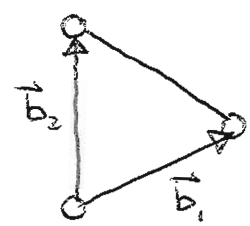
they are:

$$(h \quad k \quad \underbrace{-(h+k)}_{\text{dummy index}} \quad l)$$

<u>Direct</u>



<u>Reciprocal</u>



~~Similarly for other planes as well~~

$\perp$ vector to these planes denoted using square braces i.e. vector $\perp$ to $(1\bar{1}00)$ is $[1\bar{1}00]$ <u>etc</u> 88

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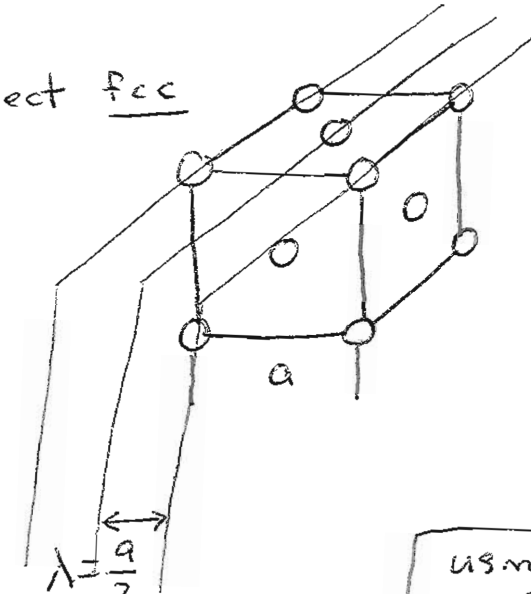
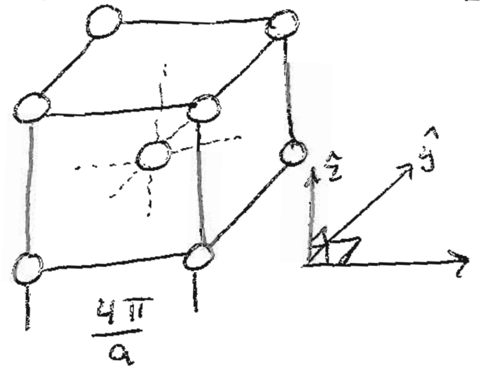
direct fcc



reciprocal of fcc = bcc



$\boxed{\text{using symmetrical primitive vectors}}$

$$\left\{\begin{aligned} \vec{b}_1 &= \frac{4\pi}{a}\frac{1}{2}\left(\hat{y} + \hat{z} - \hat{x}\right) \\ \vec{b}_2 &= \frac{4\pi}{a}\frac{1}{2}\left(\hat{z} + \hat{x} - \hat{y}\right) \\ \vec{b}_3 &= \frac{4\pi}{a}\frac{1}{2}\left(x + \hat{y} - \hat{z}\right) \end{aligned}\right.$$

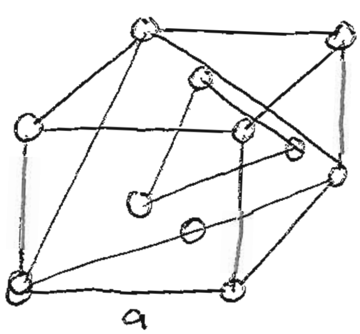
using symmetric set,

$$\vec{k}_{\perp, min} = \frac{4\pi}{a}\hat{x} = \vec{b}_2 + \vec{b}_3 + 0\vec{b}_1$$

$$= 0\vec{b}_1 + 1\vec{b}_2 + 1\vec{b}_3$$

$\Rightarrow$ $\boxed{\text{planes are } (0\ 1\ 1) \text{ in this system}}$

$$\frac{2\pi}{a/2} = \frac{2\pi}{\lambda} = |\vec{k}_\perp| \stackrel{\checkmark}{=} \frac{4\pi}{a}$$



$\perp$ to body diagonal planes

$$\lambda = \frac{\sqrt{3}\,a}{3} = \frac{a}{\sqrt{3}} \qquad \vec{h}_\perp = \frac{4\pi}{a}\frac{1}{2}\left(\hat{x} + \hat{y} + \hat{z}\right)$$

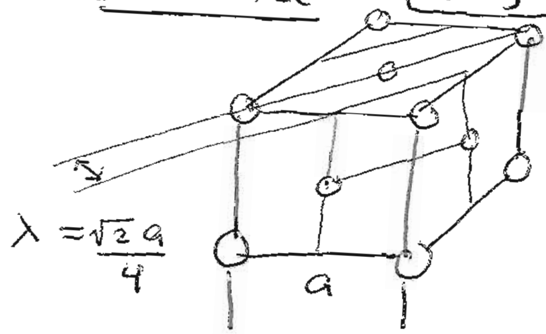
in symmetric P.V. set,

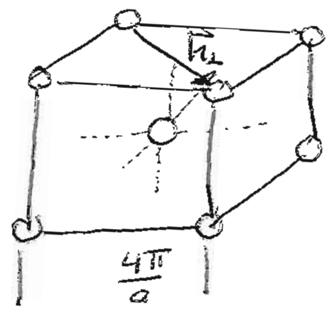
$$\vec{h}_\perp = 1\vec{b}_1 + 1\vec{b}_2 + 1\vec{b}_3$$

$\Rightarrow$ $\boxed{(1\ 1\ 1) \text{ planes}}$

$$\frac{2\pi}{a/\sqrt{3}} = \frac{2\pi}{\lambda} = |\vec{h}_\perp| \stackrel{\checkmark}{=} \frac{4\pi}{a}\frac{\sqrt{3}}{2}$$

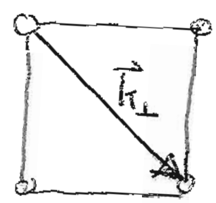
direct fcc $\quad$ using symmetrical vector set $\quad$ reciprocal bcc





$$\frac{2\pi}{(\sqrt{2}a/4)} = \frac{2\pi}{\lambda} = |\vec{h}_\perp| \overset{\checkmark}{=} \frac{4\pi\sqrt{2}}{a}$$

top view



$$|\vec{k}_\perp| = \frac{4\pi}{a}\sqrt{2}$$

$$\boxed{1}\vec{b}_1 + \boxed{1}\vec{b}_2 + \boxed{2}\vec{b}_3 = \vec{h}_\perp = \frac{4\pi}{a}(\hat{x} + \hat{y})$$

$\Rightarrow$ $\boxed{(112) \text{ planes}}$

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

$$\frac{4\pi}{a}(\hat{x} + \hat{y}) = \frac{4\pi}{a}\frac{1}{2}\left[(-h+k+l)\hat{x} + (h-k+l)\hat{y} + (h+k-l)\hat{z}\right]$$

$$2\hat{x} + 2\hat{y} = [\;]$$

$\Rightarrow$

$2 = -h+k+l \qquad 2 = h-k+l \qquad 0 = h+k-l$

$2 = 2h \Rightarrow \boxed{h=1}$

& $2 = 2k \Rightarrow \boxed{k=1}$

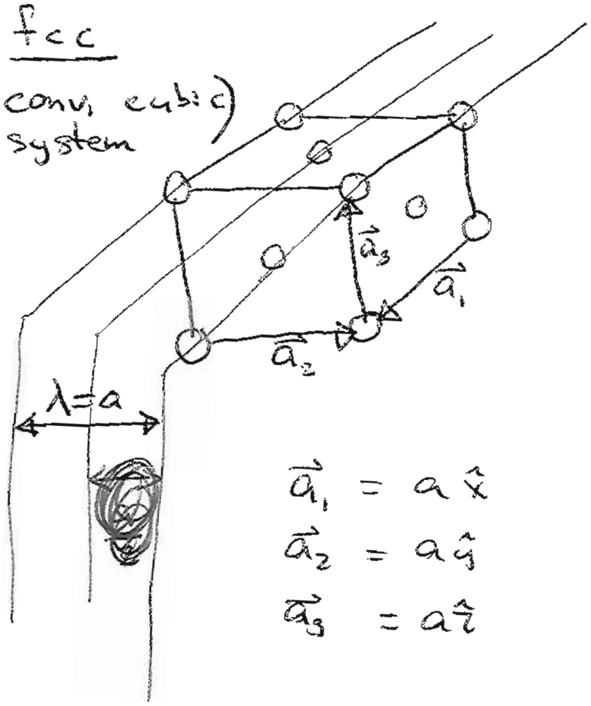
$\Rightarrow \boxed{l=2}$

These results using symmetrical set are not very intuitive

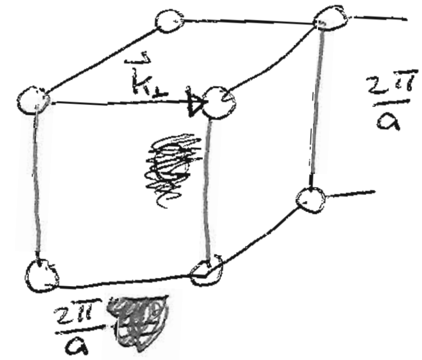
$\Rightarrow$ use a different approach

fcc

(in conv. cubic system)



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



$$\vec{b}_1 = \frac{2\pi\, a^2\, \hat{x}}{a^3}$$

$$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$$

$$\& \quad \vec{b}_2 = \frac{2\pi}{a}\hat{y}$$

$$\vec{b}_3 = \frac{2\pi}{a}\hat{z}$$

using conventional cube (sc) + 4-atom basis (4-pt.)

cube face planes

$$\lambda = a$$

$$\frac{2\pi}{a} = \frac{2\pi}{\lambda} = |\vec{h}_\perp| \stackrel{\checkmark}{=} \frac{2\pi}{a}$$

$$\vec{k}_\perp = \frac{2\pi}{a}\hat{x}$$

$$\vec{h}_\perp = 1\vec{b}_1 + 0\vec{b}_2 + 0\vec{b}_3$$

$\Rightarrow$ (1 0 0) planes

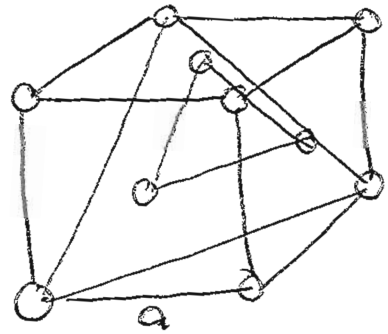
including basis

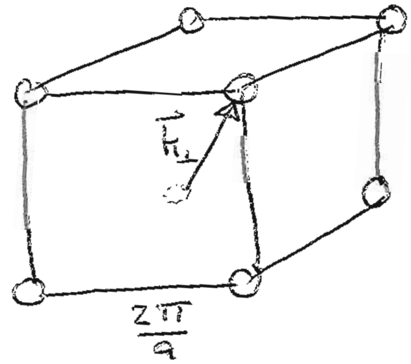
$$s = \overset{\text{planar}}{\text{spacing}} = \frac{\lambda}{2} \Rightarrow \vec{k}_{\perp,s} = 2\vec{k}_\perp = 2\left(\frac{2\pi}{a}\right)\hat{x}$$

$$= 2\vec{b}_1 + 0\vec{b}_2 + 0\vec{b}_3$$

$\Rightarrow$ $\boxed{\text{(2 0 0) planes}}$

fcc





In conventional cube system,
planes $\perp$ to body diagonal

$\Rightarrow$ all planes include <u>both</u> face-center <u>and</u> corner atoms

$$\lambda = \frac{\sqrt{3}\,a}{3} = \frac{a}{\sqrt{3}} \qquad \vec{K}_{\perp, min} = \frac{2\pi}{a}(\hat{x}+\hat{y}+\hat{z})$$

$$= \vec{b}_1 + \vec{b}_2 + \vec{b}_3$$

$$\Rightarrow \boxed{(1\,1\,1) \text{ planes}}$$

$$\frac{2\pi}{a/\sqrt{3}} = \frac{2\pi}{\lambda} = |\vec{K}_\perp| \overset{\checkmark}{=} \frac{2\pi}{a}\sqrt{3}$$

Therefore, you can see that it is convenient to use the conventional (simple cubic) cell for fcc and bcc lattices, to describe families of planes.

But, you have to remember that you are dealing with a <u>SC Bravais lattice</u> + <u>basis</u> of 4 pts. The basis atoms <u>must</u> be considered in order to describe diffraction.

Also, simplicity of SC direction vectors is "paid for" by the addition of certain complexity, i.e. cube face-type planes with closest interplanar spacing are (200) planes,

(100) planes are ...