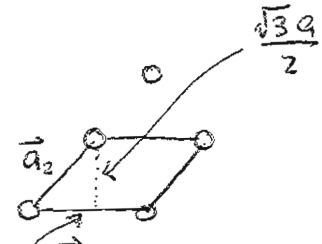
Reciprocal Lattice Cont.

hexagonal



$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$$

$$a_3 = c\hat{z}$$

$$\vec{b}_1 = 2\pi \frac{a_2 \times \vec{a}_3}{\vec{a}_1 \cdot (a_2 \times a_3)}$$

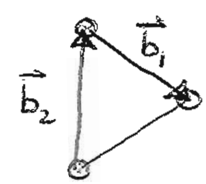
$$\vec{a}_2 \times \vec{a}_3 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{a}{2} & \frac{\sqrt{3}a}{2} & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{\sqrt{3}ac}{2}\hat{x} - \frac{ac}{2}\hat{y}$$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{\sqrt{3}\,a^2 c}{2}$$

$$\boxed{\vec{b}_1 =} \frac{2\pi\left(\frac{\sqrt{3}ac}{2}\hat{x} - \frac{ac}{2}\hat{y}\right)}{\frac{\sqrt{3}\,a^2 c}{2}} = \boxed{\frac{2\pi}{a}\hat{x} - \frac{2\pi}{\sqrt{3}a}\hat{y}}$$

$$\vec{a}_3 \times \vec{a}_1 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ a & 0 & 0 \end{vmatrix} = ac\hat{y}$$

$$\boxed{\vec{b}_2 =} \frac{2\pi(ac\hat{y})}{\frac{\sqrt{3}a^2c}{2}} = \boxed{\frac{2\pi}{\left(\frac{\sqrt{3}a}{2}\right)}\hat{y}}$$

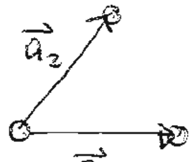


$$\vec{a}_1 \times \vec{a}_2 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a & 0 & 0 \\ \frac{a}{2} & \frac{\sqrt{3}a}{2} & 0 \end{vmatrix} = \frac{\sqrt{3}a^2}{2}\hat{z}$$

$$\boxed{\vec{b}_3 =} \frac{2\pi(\sqrt{3}a^2/2)\hat{z}}{\sqrt{3}a^2c/2} = \boxed{\frac{2\pi}{c}\hat{z}}$$

__hexagonal__ __Direct__

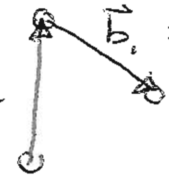
$\frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y} = \vec{a}_2$



$\vec{a}_1 = a\hat{x}$

__Reciprocal__

$\frac{2\pi}{\left(\frac{\sqrt{3}a}{2}\right)}\hat{y} = \vec{b}_2$



$\vec{b}_1 = \frac{2\pi}{a}\hat{x} - \frac{2\pi}{\sqrt{3}a}\hat{y}$

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verify: $\vec{a}_1 \perp \vec{b}_2 \Rightarrow \vec{a}_1 \cdot \vec{b}_2 \stackrel{\checkmark}{=} 0$

also $\vec{a}_2 \perp \vec{b}_1 \Rightarrow \vec{a}_2 \cdot \vec{b}_1 \stackrel{\checkmark}{=} 0$

$$\& \quad \vec{a}_1 \cdot \vec{b}_1 = (a\hat{x}) \cdot \left(\frac{2\pi}{a}\hat{x} - \frac{2\pi}{\sqrt{3}a}\hat{y}\right) \stackrel{\checkmark}{=} 2\pi$$

$$\& \quad \vec{a}_2 \cdot \vec{b}_2 = \left(\frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}\right) \cdot \left(\frac{2\pi}{\frac{\sqrt{3}a}{2}}\hat{y}\right) \stackrel{\checkmark}{=} 2\pi$$

First Brillouin Zone

$\equiv$ Wigner-Seitz primitive cell of the reciprocal lattice

__for fcc__ $\Rightarrow$ first B.Z. = W.-S. primitive cell of bcc

__for bcc__ $\Rightarrow$ 1^{st} B.Z = W.S. primitive cell of fcc

Miller Indices

correspondence between reciprocal lattice vectors and families of lattice planes

conveniently, for any set of lattice planes in a Bravais lattice, the shortest possible reciprocal lattice vector $\perp$ to the planes defines the Miller indices $h\ k\ \ell$

- Miller indices depend on the specified primitive reciprocal lattice vectors

given $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$,

the shortest $\vec{k}$ $\perp$ the lattice planes is

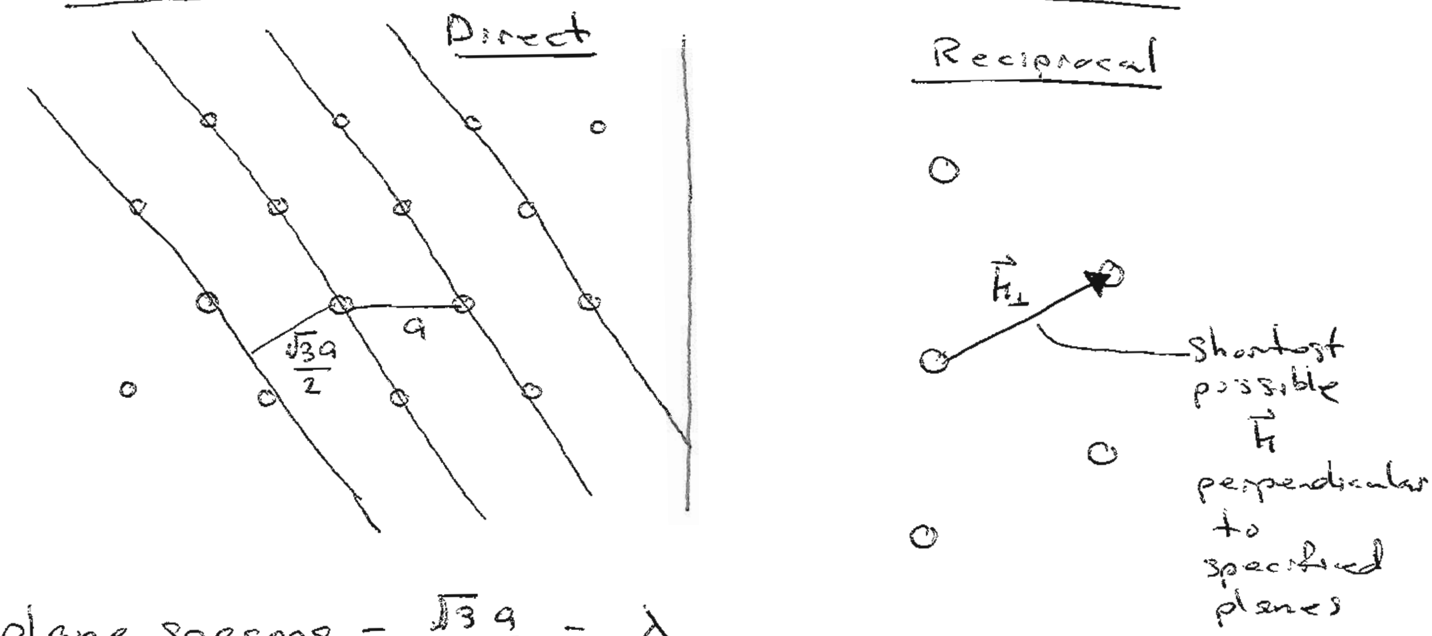
$$\vec{k}_\perp = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$$

$\Rightarrow$ Miller indices of family of planes will be

h, k, ℓ

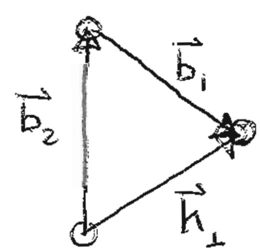
using parentheses symbolically to mean the Miller indices of the given plane

Go back to hexagonal as example



$$\text{plane spacing} = \frac{\sqrt{3}\,a}{2} = \lambda$$

What Miller indices specify these planes?



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

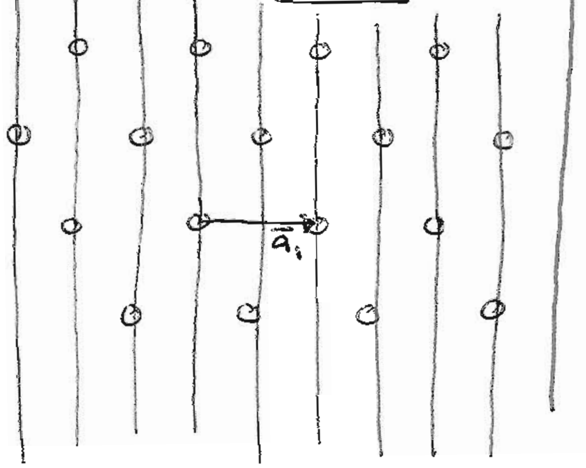
$\Rightarrow$ $\boxed{\text{Miller indices are } 1,1,0}$

$\Rightarrow$ (110) planes

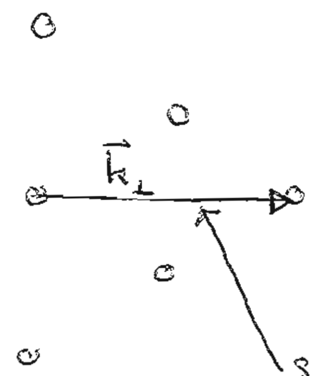
Note
$$\frac{2\pi}{\lambda} = \frac{2\pi}{\left(\frac{\sqrt{3}a}{2}\right)} = |\vec{h}_\perp| = |\vec{b}_2| = \left|\frac{2\pi}{\left(\frac{\sqrt{3}a}{2}\right)}\hat{y}\right|$$

more hexagonal

Direct



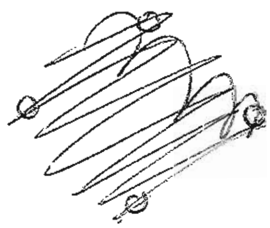
Reciprocal

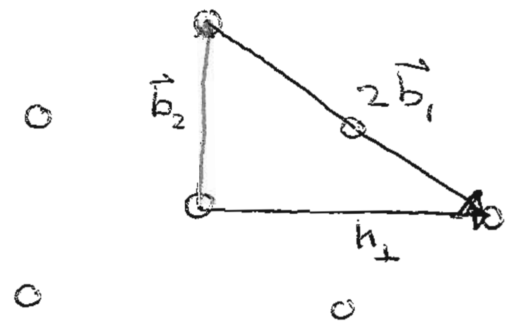


shortest $\vec{h}$ which is perpendicular to set of planes

plane spacing $= \frac{a}{2} = \lambda$

what are the Miller indices?





$$\vec{h}_\perp = 2\,\vec{b}_1 + 1\,\vec{b}_2 + 0\,\vec{b}_3$$

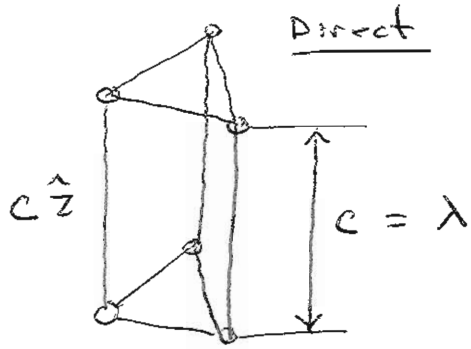
$\Rightarrow$ Miller indices 2, 1, 0

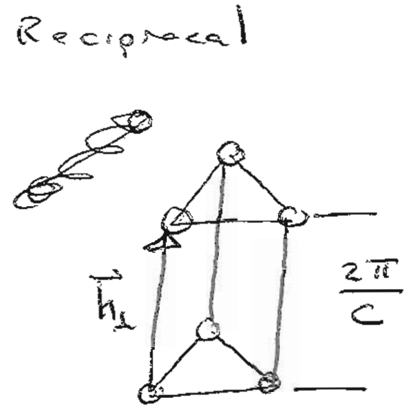
$\Rightarrow$ planes are (210) planes

Note $\frac{2\pi}{\lambda} = \frac{2\pi}{(a/2)} = |\vec{h}_\perp| = \left| 2\,\frac{2\pi}{a}\,\hat{x} \right|$

hexagonal case

consider the planes $\perp$ $\hat{z}$ - direction





Miller indices?

$$\vec{h}_\perp = \vec{b}_3 = \frac{2\pi}{c}\hat{z} = 0\,\vec{b}_1 + 0\,\vec{b}_2 + 1\,\vec{b}_3$$

$\Rightarrow$ 0,0,1 are Miller indices

(0 0 1) planes