Day-8

→ Summary:

Directions	Planes
$[u\ v\ w]$	$(h\ k\ l)$
$\langle u\ v\ w \rangle$	$\{\bar{h}\ k\ l\}$

Symmetry related: One can be obtained from the other by a symmetry operation associated with the lattice.

→ computations related to planes:

$$Ax + By + Cz = D$$

$$\Rightarrow \frac{x}{D/A} + \frac{y}{D/B} + \frac{z}{D/C} = 1$$

$$S_1 = \frac{D}{A}, \quad S_2 = \frac{D}{B}, \quad S_3 = \frac{D}{C}$$

$$\Rightarrow \frac{x}{S_1} + \frac{y}{S_2} + \frac{z}{S_3} = 1$$

Intercept form of eq^n of plane

☆ Translate the plane along its normal such that it passes through origin.

$$\frac{x}{S_1} + \frac{y}{S_2} + \frac{z}{S_3} = 0$$

$$\frac{1}{S_1} = nh, \quad \frac{1}{S_2} = nk, \quad \frac{1}{S_3} = nl$$

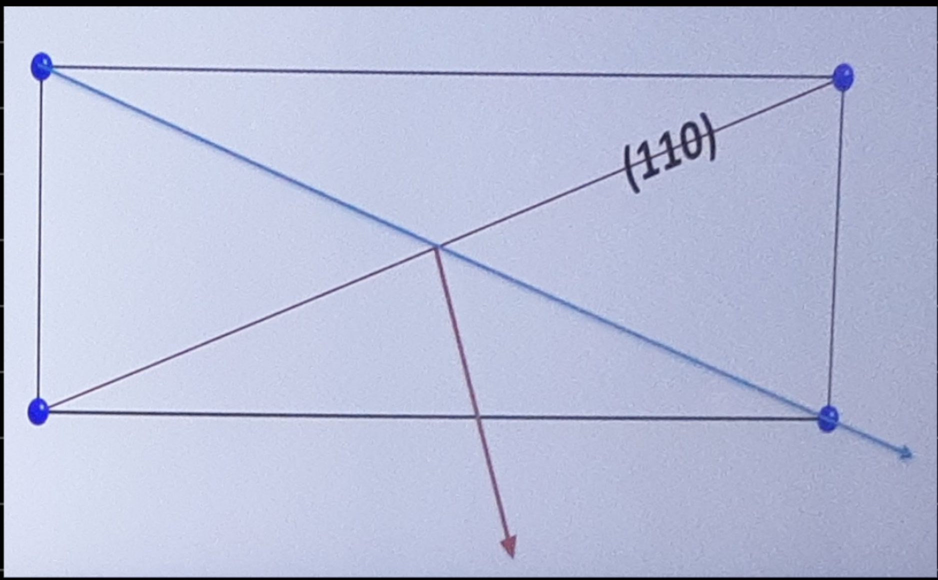
so $hx + ky + lz = 0$

$x\vec{a_1} + y\vec{a_2} + z\vec{a_3}$ is a vector on the plane.

(vector related to h, k, l)

$h\vec{a_1} + k\vec{a_2} + l\vec{a_3} = ?$

☆ consider of lattice. Projection viewed along [0 0 1]



(1 1 0) plane $\longrightarrow$ red trace

$[1 1 0] = [u\ v\ w]$ $\qquad$ $(h k l) \not\parallel [h k l]$ in general

$u = 1$ $\qquad$ $h = 1$

$v = 1$ $\qquad$ $k = 1$

$w = 0$ $\qquad$ $l = 0$

→ creation of another vector space (reciprocal space).

$\vec{a_1}, \vec{a_2}$ and $\vec{a_3} \longrightarrow u, v, w \in R$

serve as the basis for 3D space

dual space $\longrightarrow$ $\vec{a}_j^{\,*}$ (basis vectors of reciprocal)

$$\vec{a}_i \cdot \vec{a}_j^{\,*} = \cancel{2\pi}\,\delta_{ij}$$

δ_{ij} $\downarrow$ Kronecker Delta

can be anything, 2π there as k of wave vector given by $\frac{2\pi}{\lambda}$

$$\begin{bmatrix} \vec{a}_1 \\ \vec{a}_2 \\ \vec{a}_3 \end{bmatrix} \cdot \begin{bmatrix} \vec{a}_1^{\,*} & \vec{a}_2^{\,*} & \vec{a}_3^{\,*} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

As $\vec{a}_1^{\,*} \cdot \vec{a}_i = 0 \quad (i = 2, 3)$

so $\vec{a}_1^{\,*} \perp \vec{a}_2, \vec{a}_3$

$$\Rightarrow \vec{a}_1^{\,*} = k\,(\vec{a}_2 \times \vec{a}_3)$$

$$\vec{a}_1 \cdot \vec{a}_1^{\,*} = \vec{a}_1 \cdot k(\vec{a}_2 \times \vec{a}_3) = 1$$

$$\Rightarrow k\,[\vec{a}_1 \;\; \vec{a}_2 \;\; \vec{a}_3] = 1$$

$\downarrow$

For unit cell, volume (V)

so $k = \dfrac{1}{V}$ $(= l = m)$

$$\therefore \vec{a}_1^{\,*} = \frac{1}{V}(\vec{a}_2 \times \vec{a}_3)$$

☆ Reciprocal space metric tensor:

$$g_{ij}^* = \vec{a}_i^* \cdot \vec{a}_j^*$$

☆ $\boxed{\text{Shorcuts!}}$

Real $\longleftrightarrow$ Reciprocal space

$$\vec{a}_m^* = g_{mi}^{-1}\,\vec{a}_i$$

$$\vec{p}_m^* = p_i\, g_{im}$$

$$g_{mk}^* = g_{im}^{-1}$$

For eg: $p = p_i \vec{a}_i = p_j^* \vec{a}_j^*$

Take $\vec{p} \cdot \vec{a}_k = p_i \vec{a}_i \cdot \vec{a}_k = p_j^* a_j^* a_k$

$$= p_i g_{ik} = p_k^*$$