Day – 9

(Revision)

→ Reciprocal space:

Basis vectors from the real space basis

Restrict coeff. to integers → reciprocal lattice

plane – $(h\,k\,l)$

↓

normal: $h a_1^* + k a_2^* + k a_3^*$

Interplanar spacing: distance of plane from origin

1.) Lattice Parameters: $\{1, 1, 1, 90°, 45°, 90°\}$
Reciprocal space?

Ans.) $$g_{ij} = \begin{bmatrix} 1 & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1 \end{bmatrix}$$

$$\vec{p} = \frac{\vec{a_1}}{4} + \frac{\vec{a_3}}{2}$$

$$[p_1^* \; p_2^* \; p_3^*] = [1/4 \quad 0 \quad 1/2] \begin{bmatrix} 1 & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1 \end{bmatrix}$$

$$= \left[\frac{\sqrt{2}+1}{4} \quad 0 \quad \frac{4+\sqrt{2}}{8} \right]$$

→ cI (≡BCC):

$$\vec{b_1} = \frac{a}{2}[\hat{i} + \hat{j} + \hat{k}]$$

$$\vec{b_2} = \frac{a}{2}[-\hat{i} + \hat{j} - \hat{k}]$$

$$\vec{b_3} = \frac{a}{2}[\hat{i} - \hat{j} - \hat{k}]$$

$$g_{ij} = \begin{bmatrix} \frac{3a^2}{4} & -\frac{a^2}{4} & -\frac{a^2}{4} \\ -\frac{a^2}{4} & \frac{3a^2}{4} & -a^2/4 \\ -a^2/4 & -a^2/4 & \frac{3a^2}{4} \end{bmatrix}$$

$$= \frac{a^2}{4}\begin{bmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{bmatrix}$$

$$g_{ij}^{-1} = \frac{1}{a^2}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \qquad \begin{matrix} 1 \\ 1 \\ 1 \end{matrix}$$

$$\begin{bmatrix} b_1^* \\ b_2^* \\ b_3^* \end{bmatrix} = g_{ij}^{-1}\begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$= \frac{1}{2a}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}\begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \end{bmatrix}$$

$$= \frac{1}{2a}\begin{bmatrix} 2 & 2 & 0 \\ 0 & 2 & -2 \\ 2 & 0 & -2 \end{bmatrix}$$

$$= \frac{1}{a}\begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & -1 \\ 1 & 0 & -1 \end{bmatrix}$$