

Kittel (7th Edition). Chapter 2. Problem 1.
 © Kwok-Wai Ng, 2005.

(a)

Let the planes intercept the base vectors \bar{a}_1 , \bar{a}_2 , and \bar{a}_3 at $p\bar{a}_1$, $q\bar{a}_2$, and $r\bar{a}_3$.

If we have to multiply the reciprocals of p , q , and r with a common factor s to form the Miller indices, i.e.

$$s \begin{pmatrix} 1 & 1 & 1 \\ p & q & r \end{pmatrix} = (h \ k \ l) \Rightarrow p = \frac{s}{h}, \quad q = \frac{s}{k}, \quad r = \frac{s}{l}$$

Note : 1. There is always a lattice plane passing through the origin

2. s used to multiply $1/p$, $1/q$, and $1/r$ is an integer

3. The reason why $s \neq 1$ is because the p , q , r chosen is not the plane closest to the origin. $s = \dots, -3, -2, -1, 0, 1, 2, 3, \dots$ correspond to consecutive lattice planes (all have the same Miller indices hkl). $s = 0$ is the plane passing through the origin, $s = \pm 1$ are the nearest planes at either side of the $s = 0$ plane and so on.

In the derivation below we can simply choose $s = 1$, but we keep it there until the end.

The plane is generated by vectors $(p\bar{a}_1 - q\bar{a}_2)$ and $(p\bar{a}_1 - r\bar{a}_3)$, hence we need only to show these two vectors are perpendicular to \vec{G} :

$$\begin{aligned} \vec{G} \cdot (p\bar{a}_1 - q\bar{a}_2) &= (h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3) \cdot (p\bar{a}_1 - q\bar{a}_2) \\ &= (h\bar{b}_1 + k\bar{b}_2) \cdot \left(\frac{s}{h}\bar{a}_1 - \frac{s}{k}\bar{a}_2 \right) \quad (\bar{b}_3 \perp \bar{a}_1 \text{ and } \bar{a}_2) \\ &= h\bar{b}_1 \cdot \frac{s}{h}\bar{a}_1 - k\bar{b}_2 \cdot \frac{s}{k}\bar{a}_2 \quad (\bar{b}_1 \perp \bar{a}_2 \text{ and } \bar{b}_2 \perp \bar{a}_1) \\ &= \frac{2\pi s}{V} [(\bar{a}_2 \times \bar{a}_3) \cdot \bar{a}_1 - (\bar{a}_3 \times \bar{a}_1) \cdot \bar{a}_2] \\ &= \frac{2\pi s}{V} [(\bar{a}_3 \times \bar{a}_1) \cdot \bar{a}_2 - (\bar{a}_3 \times \bar{a}_1) \cdot \bar{a}_2] = 0 \end{aligned}$$

$$\begin{aligned} \vec{G} \cdot (p\bar{a}_1 - r\bar{a}_3) &= (h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3) \cdot (p\bar{a}_1 - r\bar{a}_3) \\ &= (h\bar{b}_1 + l\bar{b}_3) \cdot \left(\frac{s}{h}\bar{a}_1 - \frac{s}{l}\bar{a}_3 \right) \quad (\bar{b}_2 \perp \bar{a}_1 \text{ and } \bar{a}_3) \\ &= h\bar{b}_1 \cdot \frac{s}{h}\bar{a}_1 - l\bar{b}_3 \cdot \frac{s}{l}\bar{a}_3 \quad (\bar{b}_1 \perp \bar{a}_3 \text{ and } \bar{b}_3 \perp \bar{a}_1) \\ &= \frac{2\pi s}{V} [(\bar{a}_2 \times \bar{a}_3) \cdot \bar{a}_1 - (\bar{a}_1 \times \bar{a}_2) \cdot \bar{a}_3] \\ &= \frac{2\pi s}{V} [(\bar{a}_1 \times \bar{a}_2) \cdot \bar{a}_3 - (\bar{a}_1 \times \bar{a}_2) \cdot \bar{a}_3] = 0 \end{aligned}$$

(b)

Suppose we have to multiply \vec{G} with a factor t so that the tip $t\vec{G}$ is on the plane :

$$(p\vec{a}_1 - t\vec{G}) \cdot \vec{G} = 0 \quad (\text{we have already proved that } \vec{G} \perp \text{ plane})$$

$$\Rightarrow p\vec{a}_1 \cdot \vec{G} = tG^2$$

$$\Rightarrow p\vec{a}_1 \cdot h\vec{b}_1 = tG^2$$

$$\Rightarrow s\vec{a}_1 \cdot \left[\frac{2\pi\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \right] = tG^2$$

$$\Rightarrow t = \frac{2\pi s}{G^2}$$

$$\therefore |t\vec{G}| = \frac{2\pi s}{G^2} G = \frac{2\pi s}{G}$$

Distance between planes = Distance between the ($s = 1$) plane and the origin

$$= \frac{2\pi}{G}$$

Note : 1. There is always a lattice plane passing through the origin

2. s used to multiply p , q , and r is an integer

3. The reason why $s \neq 1$ is because the p , q , r chosen is not the plane closest to the origin. $s = \dots, -3, -2, -1, 0, 1, 2, 3, \dots$ correspond to consecutive lattice planes (all have the same Miller indices hkl). $s = 0$ is the plane passing through the origin, $s = \pm 1$ are the nearest planes at either side of the $s = 0$ plane and so on.

(c)

Reciprocal lattice of a simple cubic of lattice parameter a is again a simple cubic of lattice parameter

$\frac{2\pi}{a}$. $\therefore \vec{b}_1, \vec{b}_2,$ and \vec{b}_3 are perpendicular to each other and each has a magnitude of $\frac{2\pi}{a}$.

$$\therefore G = \sqrt{\left(\frac{2\pi h}{a}\right)^2 + \left(\frac{2\pi k}{a}\right)^2 + \left(\frac{2\pi l}{a}\right)^2} = \frac{2\pi}{a} \sqrt{h^2 + k^2 + l^2}$$

$$d(hkl) = \frac{2\pi}{G} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \text{or} \quad d^2 = \frac{a^2}{h^2 + k^2 + l^2}$$