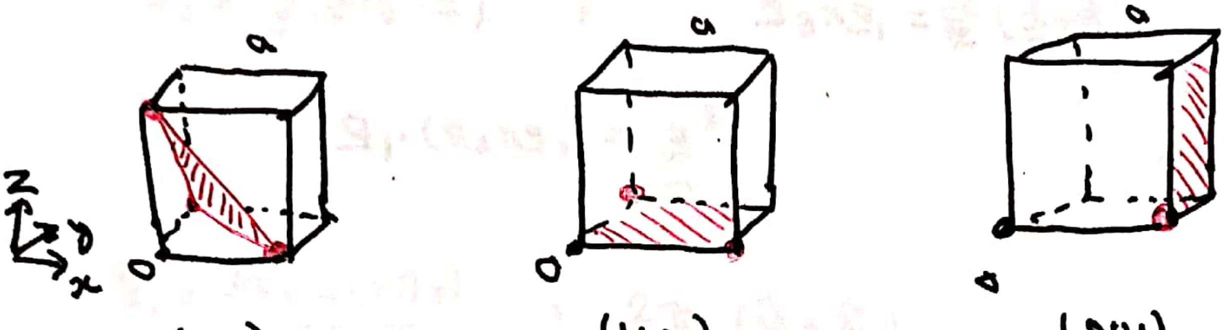
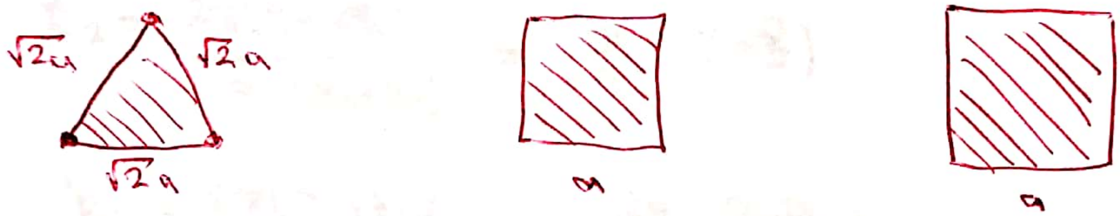
13) Choosing the bottom front left vertex of a primitive cell of a simple cubic lattice as an origin the three planes (111), (110) and (100) are:

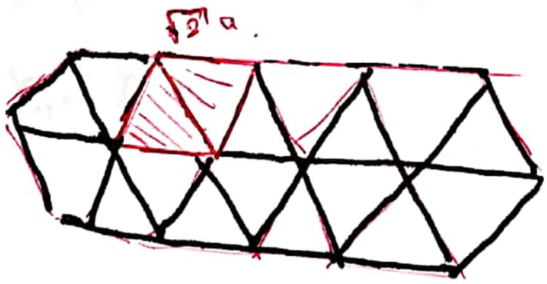


(111) (110) (001)



(110) and (001) are both square lattices.

(111) gives a hexagonal lattice with the equilateral triangle being one half of a primitive cell



(14) BCC has primitive lattice vectors

$$\left.\begin{aligned} \underline{a}_1 &= \frac{a}{2}(-\hat{\underline{x}}+\hat{\underline{y}}+\hat{\underline{z}}) \\ \underline{a}_2 &= \frac{a}{2}(\hat{\underline{x}}-\hat{\underline{y}}+\hat{\underline{z}}) \\ \underline{a}_3 &= \frac{a}{3}(\hat{\underline{x}}+\hat{\underline{y}}-\hat{\underline{z}}) \end{aligned}\right\} \Rightarrow \begin{aligned} \underline{a}_1\times\underline{a}_2 &= \frac{a^2}{2}(\hat{\underline{x}}+\hat{\underline{y}}) \\ \underline{a}_2\times\underline{a}_3 &= \frac{a^2}{2}(\hat{\underline{y}}+\hat{\underline{z}}) \\ \underline{a}_3\times\underline{a}_1 &= \frac{a^2}{2}(\hat{\underline{x}}+\hat{\underline{z}}) \end{aligned}$$

$$\underline{a}_1\cdot(\underline{a}_2\times\underline{a}_3) = \frac{a^3}{2}$$

$$\underline{b}_1 = \frac{2\pi(\underline{a}_2\times\underline{a}_3)}{\underline{a}_1\cdot(\underline{a}_2\times\underline{a}_3)} = \frac{2\pi}{a}(\hat{\underline{y}}+\hat{\underline{z}})$$

$$\underline{b}_2 = \frac{2\pi(\underline{a}_3\times\underline{a}_1)}{\underline{a}_1\cdot(\underline{a}_2\times\underline{a}_3)} = \frac{2\pi}{a}(\hat{\underline{x}}+\hat{\underline{z}})$$

$$\underline{b}_3 = \frac{2\pi(\underline{a}_1\times\underline{a}_2)}{\underline{a}_1\cdot(\underline{a}_2\times\underline{a}_3)} = \frac{2\pi}{a}(\hat{\underline{x}}+\hat{\underline{y}})$$

These are primitive lattice vectors of a FCC lattice with conventional lattice spacing $\frac{4\pi}{a}$.

Volume of primitive cell of the reciprocal lattice is

$$\underline{b}_1\cdot(\underline{b}_2\times\underline{b}_3) = \frac{8\pi^3}{a^3}(\hat{\underline{y}}+\hat{\underline{z}})\cdot\{\hat{\underline{z}}+\hat{\underline{y}}\} = \frac{16\pi^3}{a^3}$$

For any lattice with reciprocal lattice vectors

$$\underline{b}_1 = 2\pi \frac{\underline{a}_2 \times \underline{a}_3}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}, \quad \underline{b}_2 = 2\pi \frac{\underline{a}_3 \times \underline{a}_1}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}$$

$$\underline{b}_3 = 2\pi \frac{\underline{a}_1 \times \underline{a}_2}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)} . \quad V_c = \underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)$$

the reciprocal lattice of the reciprocal lattice has primitive lattice vectors

$$\underline{b}_1' = \frac{2\pi (\underline{b}_2 \times \underline{b}_3)}{\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)}, \quad \underline{b}_2' = 2\pi \frac{(\underline{b}_3 \times \underline{b}_1)}{\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)}$$

$$\underline{b}_3' = \frac{2\pi (\underline{b}_1 \times \underline{b}_2)}{\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)}$$

$$\underline{b}_1 \times \underline{b}_2 = \frac{4\pi^2 (\underline{a}_2 \times \underline{a}_3) \times (\underline{a}_3 \times \underline{a}_1)}{\{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)\}^2}$$

$$= \frac{4\pi^2 \{\{(\underline{a}_2 \times \underline{a}_3) \cdot \underline{a}_3\} \underline{a}_1 - \{(\underline{a}_2 \times \underline{a}_3) \cdot \underline{a}_1\} \underline{a}_3\}}{\{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)\}^2}$$

$$= -\frac{4\pi^2 \underline{a}_3}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}$$

Similarly $\quad \underline{b}_2 \times \underline{b}_3 = \dfrac{-4\pi^2 \underline{a}_1}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}$

$$\underline{b}_3 \times \underline{b}_1 = -\frac{4\pi^2 \underline{a}_2}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}$$

$$\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3) = \frac{2\pi(\underline{a}_2 \times \underline{a}_3)}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)} \cdot \left\{ \frac{-4\pi^2 \underline{a}_1}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)} \right\}$$

$$= \frac{-8\pi^3}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}$$

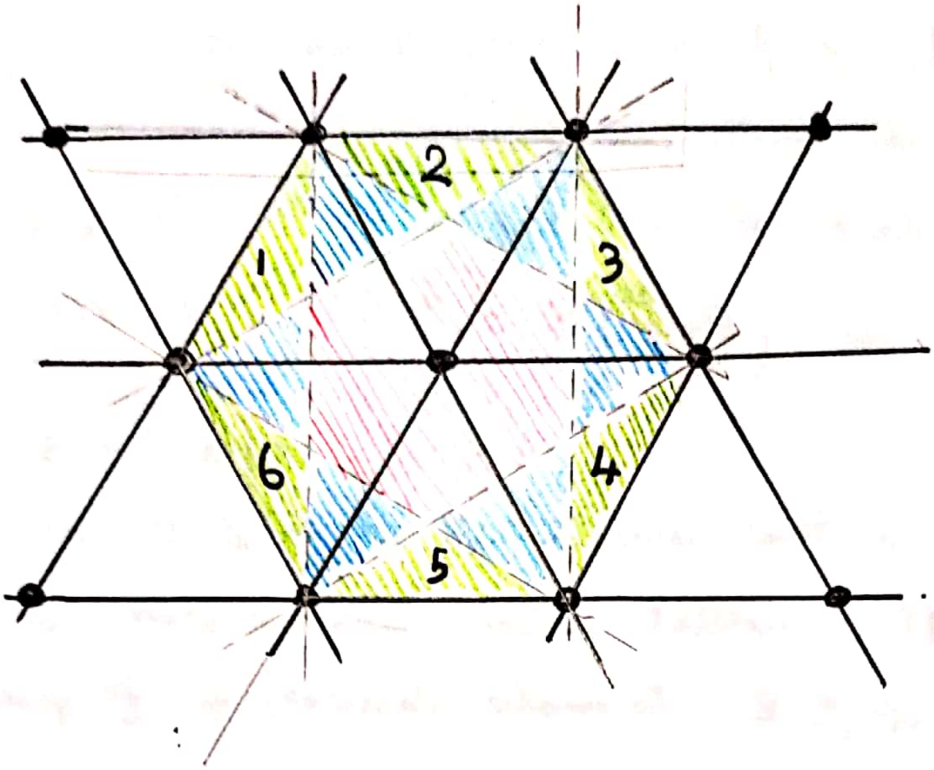
$$\underline{b}_3' = \frac{2\pi(\underline{b}_1 \times \underline{b}_2)}{\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)} = \frac{(-8\pi^3 \underline{a}_3)}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)} \cdot \left\{ \frac{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}{(-8\pi^3)} \right\} = \underline{a}_3$$

$$\underline{b}_2' = \frac{2\pi(\underline{b}_3 \times \underline{b}_1)}{\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)} = \frac{-8\pi^2 \underline{a}_2}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)} \cdot \left\{ \frac{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}{-8\pi^3} \right\} = \underline{a}_2$$

$$\underline{b}_1' = \frac{2\pi(\underline{b}_2 \times \underline{b}_3)}{\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)} = \frac{-8\pi^2 \underline{a}_1}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)} \cdot \left\{ \frac{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)}{-8\pi 3} \right\} = \underline{a}_1$$

$$\Rightarrow \quad \underline{b}_1' = \underline{a}_1, \quad \underline{b}_2' = \underline{a}_2, \quad \underline{b}_3' = \underline{a}_3$$

The reciprocal lattice of a reciprocal lattice is the original direct lattice.



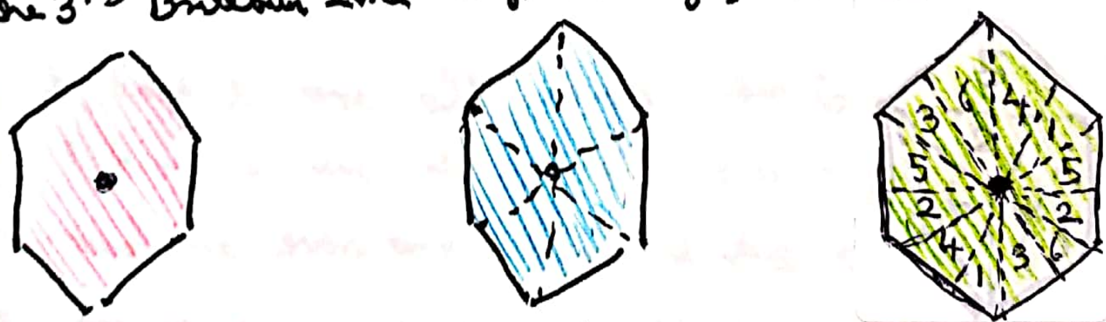
1^{ST} Brillouin zone is red

2^{ND} Brillouin zone is blue

3^{RD} Brillouin zone is green.

Perpendicular bi-sectors of lattice vectors between neighbouring points are dashed lines.

The triangles can all be assembled into primitive cells by translating them by a lattice vector (for the 3^{RD} Brillouin zone the green triangles must also be cut in two).



1^{ST} Brillouin zone

2^{ND} Brillouin zone

3^{RD} Brillouin zone.

(16) A conventional cell of a FCC lattice contains 4 primitive cells and so contains 4 complete lattice points, which we can take to be at the origin, $\underline{0}$, and $\underline{a}_1 = \frac{a}{2}(\hat{\underline{y}}+\hat{\underline{z}})$, $\underline{a}_2 = \frac{a}{2}(\hat{\underline{z}}+\hat{\underline{x}})$ $\underline{a}_3 = \frac{a}{2}(\hat{\underline{x}}+\hat{\underline{y}})$.

We can think of a FCC lattice with a monatomic basis as being a simple cubic lattice with a basis consisting of 4 identical atoms at $\underline{0}$, $\underline{a}_1$, $\underline{a}_2$ and $\underline{a}_3$.

Reciprocal lattice vectors of a simple cubic lattice with lattice spacing a are.

$$\underline{G}_{hkl} = \frac{2\pi}{a}(h\hat{\underline{x}} + k\hat{\underline{y}} + l\hat{\underline{z}})$$

Structure factors are

$$S_{hkl} = 1 + e^{i\underline{a}_1 \cdot \underline{G}} + e^{i\underline{a}_2 \cdot \underline{G}} + e^{i\underline{a}_3 \cdot \underline{G}}$$

$$= 1 + e^{\pi i(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k)}$$

If h, k and l are all even, this is 4.
If h, k and l are all odd it is again 4.
If two are even and one is odd it is 0.
If one is even and two are odd it is again 0.

(17) The reciprocal lattice vectors of a simple cubic lattice, with a primitive cell of side a, and a BCC lattice with primitive lattice vectors are not the same. The former has reciprocal lattice vectors

$$\underline{b}_1 = \frac{2\pi}{a}\hat{\underline{x}}, \quad \underline{b}_2 = \frac{2\pi}{a}\hat{\underline{y}}, \quad \underline{b}_3 = \frac{2\pi}{a}\hat{\underline{z}}$$

The latter has

$$\underline{b}_1' = \frac{2\pi}{a}(\hat{\underline{y}}+\hat{\underline{z}}), \quad \underline{b}_2' = \frac{2\pi}{a}(\hat{\underline{x}}+\hat{\underline{z}}), \quad \underline{b}_3' = \frac{2\pi}{a}(\hat{\underline{x}}+\hat{\underline{y}})$$

There are reciprocal lattice vectors of the former which are not reciprocal lattice vectors of the latter.

e.g. $\underline{b}_1 \neq h'\underline{b}_1' + k'\underline{b}_2' + l'\underline{b}_3'$ for any integers h', k' and l'. All reciprocal lattice vectors of the latter are reciprocal lattice vectors of the former.

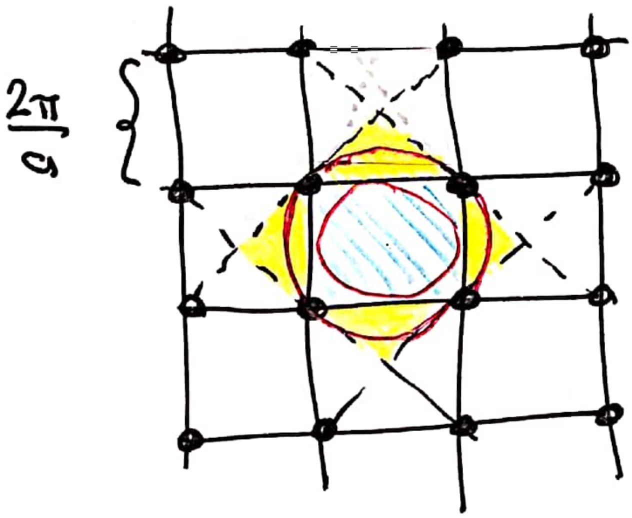
$$\underline{G}' = h'\underline{b}_1' + k'\underline{b}_2' + l'\underline{b}_3', \quad \text{with } h', k', l' \in \mathbb{Z},$$

$$= \frac{2\pi}{a}\left\{(h'+l')\hat{\underline{y}} + (k'+h')\hat{\underline{z}} + (k'+l')\hat{\underline{x}}\right\}$$

$$= \frac{2\pi}{a}(h\hat{\underline{x}} + k\hat{\underline{y}} + l\hat{\underline{z}})$$

with $h = k'+l'$, $k = h'+l'$, $l = (k'+h')$ all integers.

(18) The reciprocal lattice of a square lattice with square primitive cells of side a is another square lattice with primitive cells of side $\frac{2\pi}{a}$. The first 2 Brioullin zone are shown in blue and yellow below



wavelength $\lambda = \sqrt{2}\, a \Rightarrow K = \frac{2\pi}{\lambda} = \frac{\sqrt{2}\,\pi}{a}$

wavelength $\lambda = 2a \Rightarrow K = \frac{2\pi}{\lambda} = \frac{\pi}{a}$

Two circles of radius $\frac{2\pi}{a}$ and $\frac{\sqrt{2}\,\pi}{a}$ in K-space are drawn in red. Any circle with a radius between these two values intersects the edges of the blue square in 8 places – these are points where the tip of a wave-vector lies on a Brioullin zone. There will be 8 peaks in the diffraction pattern.