1 Exercise 1 - Reciprocal lattice

a. Reciprocal lattice of FCC

Solution: Let's first define the primitive vectors for the FCC and BCC lattices. First the FCC structure

$$\hat{a}_1 = \frac{a}{2}\left(\hat{y}+\hat{z}\right), \tag{1}$$
$$\hat{a}_2 = \frac{a}{2}\left(\hat{z}+\hat{x}\right), \tag{2}$$
$$\hat{a}_3 = \frac{a}{2}\left(\hat{x}+\hat{y}\right). \tag{3}$$

Then, we define the primitive vectors for the BCC lattice

$$\hat{c}_1 = \frac{a}{2}\left(\hat{y}+\hat{z}-\hat{x}\right), \tag{4}$$
$$\hat{c}_2 = \frac{a}{2}\left(\hat{z}+\hat{x}-\hat{y}\right), \tag{5}$$
$$\hat{c}_3 = \frac{a}{2}\left(\hat{x}+\hat{y}-\hat{z}\right). \tag{6}$$

Here we used different names, $\hat{a}_i$, and $\hat{c}_i$ for convenience. Later we will need to be able to recognize vectors from one basis or another. Another important thing is to remember that $\hat{x}, \hat{y}, \hat{z}$ are orthonormal vectors.

First, we will obtain the reciprocal basis for the FCC structure. For this it will be helpful to calculate the box product separately.

$$\hat{a}_i \cdot (\hat{a}_2 \times \hat{a}_3),$$

using eqs. 1-3

$$\begin{aligned}
\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3) &= \frac{a^2}{4}\hat{a}_1 \cdot \left((\hat{z}+\hat{x}) \times (\hat{x}+\hat{y})\right), \\
&= \frac{a^2}{4}\hat{a}_1 \cdot \left(\hat{y}+\hat{z}-\hat{x}\right), \\
&= \frac{a^3}{8}\left(\hat{y}+\hat{z}\right) \cdot \left(\hat{y}+\hat{z}-\hat{x}\right), \\
&= \frac{a^3}{8}\left(\cancelto{1}{\hat{y}\cdot\hat{y}} + \cancelto{1}{\hat{z}\cdot\hat{z}}\right), \\
&= \frac{a^3}{4}.
\end{aligned} \tag{7}$$

We can proceed with out calculations of the reciprocal vectors,

$$\begin{aligned}
\hat{b}_1 &= \frac{2\pi \hat{a}_2 \times \hat{a}_3}{\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3)}, \\
&= \frac{2\pi a^2/4\left((\hat{z}+\hat{x}) \times (\hat{x}+\hat{y})\right)}{a^3/4}, \\
&= \boxed{\frac{2\pi}{a}\left(\hat{y}+\hat{z}-\hat{x}\right).}
\end{aligned} \tag{8}$$

Now the next one

$$\begin{aligned}\hat{b}_2 &= \frac{2\pi\hat{a}_3 \times \hat{a}_1}{\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3)},\\ &= \frac{2\pi a^2/4\left((\hat{x}+\hat{y}) \times (\hat{y}+\hat{z})\right)}{a^3/4},\\ &= \boxed{\frac{2\pi}{a}\left(\hat{z}+\hat{x}-\hat{y}\right),} \end{aligned} \tag{9}$$

And the last one,

$$\begin{aligned}\hat{b}_3 &= \frac{2\pi\hat{a}_1 \times \hat{a}_2}{\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3)},\\ &= \frac{2\pi a^2/4\left((\hat{y}+\hat{z}) \times (\hat{z}+\hat{x})\right)}{a^3/4},\\ &= \boxed{\frac{2\pi}{a}\left(\hat{x}+\hat{y}-\hat{z}\right).} \end{aligned} \tag{10}$$

And now we see, that the vectors defined in eqs. 8-10 are parallel to the primitive vectors of the BCC structure defined in eqs. 4-6. **Therefore, the reciprocal lattice of a FCC one is a BCC one.** ■

As we know, if we take now the $\hat{b}$ vectors of our resulting BCC structure and calculate the resulting reciprocal ones, we will go back to the original lattice, which was a FCC lattice (the reciprocal of the reciprocal lattice is the original). **Therefore, the reciprocal of a BCC lattice is an FCC one.** ■

b. Volumes

Solution: We now that the volume of the primitive cell is given by the box product. In eq. 7 we calculated the volume of the initial lattice. Let's now calculate the volume of the lattice formed by the $\hat{b}$ vectors.

$$\begin{aligned}\hat{b}_1 \cdot (\hat{b}_2 \times \hat{b}_3) &= \frac{(2\pi)^2}{a^2}\hat{b}_1 \cdot \left((\hat{z}+\hat{x}-\hat{y}) \times (\hat{x}+\hat{y}-\hat{z})\right),\\ &= \frac{(2\pi)^2}{a^2}\hat{b}_1 \cdot \left(\hat{y}-\hat{x}+\hat{z}+\hat{x}+\hat{y}+\hat{z}\right),\\ &= \frac{(2\pi)^2}{a^2}\hat{b}_1 \cdot \left(2\hat{y}+2\hat{z}\right),\\ &= \frac{(2\pi)^3}{a^3}2\left(\hat{y}+\hat{z}-\hat{x}\right) \cdot \left(\hat{y}+\hat{z}\right),\\ &= \frac{(2\pi)^3}{a^3}2\left(1+1\right),\\ &= \frac{(2\pi)^3}{a^3}4,\\ &= \frac{(2\pi)^3}{a^3/4}. \end{aligned} \tag{11}$$

If we remember, the volume of the direct lattice was $a^3/4$, hence, **the volume of the reciprocal cell is** $v_{rec} = (2\pi)^3/v_{dir}$. Where v_{rec} is the colume of the reciprocal cell, and v_{dir} the volume of the direct cell.

2 Exercise 2 - Reciprocal lattice 2

a. Reciprocal basis 2D

Solution: To tackle this problem it is useful to remember the following relation between the vectors of the direct and reciprocal basis

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}. \tag{12}$$

Now if we take vectors in two dimensions, this yields the following matrix equation

$$\begin{pmatrix} b_{1x} & b_{1y} \\ b_{2x} & b_{2y} \end{pmatrix} \begin{pmatrix} a_{1x} & a_{2x} \\ a_{1y} & a_{2y} \end{pmatrix} = 2\pi \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{13}$$

If we solve the equation for $\mathcal{B}$ then we have

$$\begin{pmatrix} b_{1x} & b_{1y} \\ b_{2x} & b_{2y} \end{pmatrix} = \frac{2\pi}{a_{1x}a_{2y} - a_{1y}a_{2x}} \begin{pmatrix} a_{2y} & -a_{2x} \\ -a_{1y} & a_{1x} \end{pmatrix}. \tag{14}$$

The vectors given in the assignment for the direct basis give us the matrix $\mathcal{A}$

$$\mathcal{A} = \begin{pmatrix} a & a/2 \\ 0 & a \end{pmatrix}, \tag{15}$$

therefore

$$\begin{pmatrix} b_{1x} & b_{1y} \\ b_{2x} & b_{2y} \end{pmatrix} = \frac{2\pi}{a^2} \begin{pmatrix} a & -a/2 \\ 0 & a \end{pmatrix} = \begin{pmatrix} 2\pi/a & -\pi/a \\ 0 & 2\pi/a \end{pmatrix}. \tag{16}$$

Hence, the primitive vectors of the reciprocal lattice are

$$\vec{b}_1 = \begin{pmatrix} 2\pi/a \\ 0 \end{pmatrix}, \quad \vec{b}_2 = \begin{pmatrix} -\pi/a \\ 2\pi/a \end{pmatrix}. \tag{17}$$

The respective drawings of the first and second Brillouin zones can be seen in fig. 1

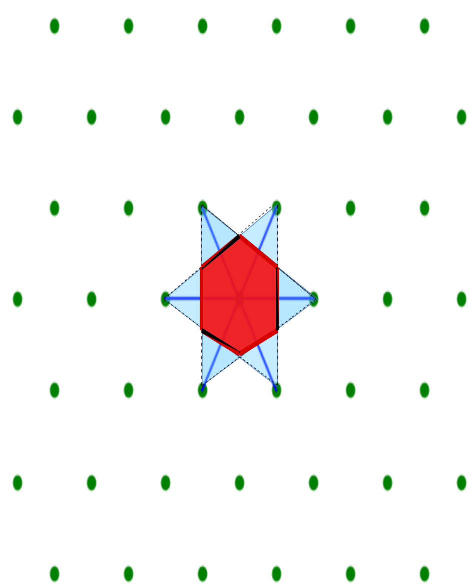

Figure 1: First (hexagon) and second (star) Brillouin zones.

b. Areas of the Brillouin zones

Solution: First we need to remember that all Brillouin zones have the same area. Then we only need to calculate the area of the first one. From fig. 1 we can see that the length apothem is half of the size of the vector $(2\pi/a, 0)$, that is $ap = \pi/a$. Now, by doing simple trigonometry and recalling that all the triangles inside the hexagon are equilateral, since it is a regular hexagon, we will have that the length of each side of the hexagon is equal to $b = 2ap/\sqrt{3}$. This result comes as a consequence of Pythagoras theorem. Finally, if we remember that the area of an hexagon is $6 * b * ap/2$ we find

$$A = \frac{6b(ap)}{2} = \frac{6(ap)^2}{\sqrt{3}} = \frac{2(\sqrt{3})^2\pi^2}{a^2\sqrt{3}} = \boxed{\frac{2\sqrt{3}\pi^2}{a^2}}. \tag{18}$$

3 Exercise 3 - Lattice planes

4 Exercise 4 - Periodic functions