

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

$$\hat{a}_1 = \frac{a}{2} (\hat{y} + \hat{z}), \quad (1)$$

$$\hat{a}_2 = \frac{a}{2} (\hat{z} + \hat{x}), \quad (2)$$

$$\hat{a}_3 = \frac{a}{2} (\hat{x} + \hat{y}). \quad (3)$$

Then, we define the primitive vectors for the BCC lattice

$$\hat{c}_1 = \frac{a}{2} (\hat{y} + \hat{z} - \hat{x}), \quad (4)$$

$$\hat{c}_2 = \frac{a}{2} (\hat{z} + \hat{x} - \hat{y}), \quad (5)$$

$$\hat{c}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z}). \quad (6)$$

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

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

We can proceed with our calculations of the reciprocal vectors,

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

Now the next one

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

And the last one,

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

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.

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

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 volume 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

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

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

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

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

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

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

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

therefore

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

Hence, the primitive vectors of the reciprocal lattice are

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

3 Exercise 3 - Lattice planes

4 Exercise 4 - Periodic functions