2. The face-centered cubic (fcc) lattice = four times the fcc primitive unit cell. (Prove it ?!, see figures 10 & 11)

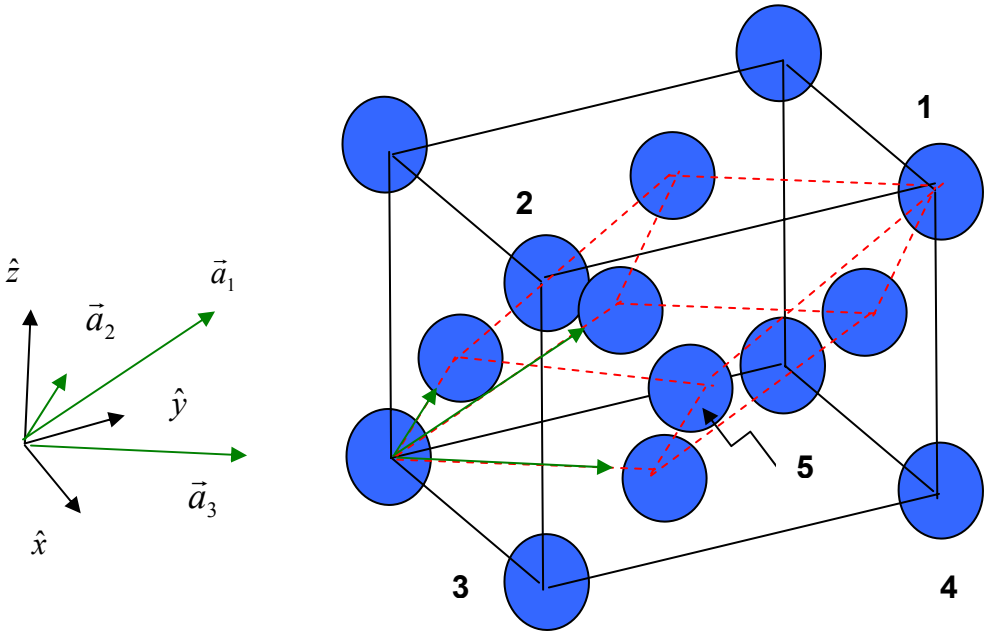

Figure 10: Conventional (solid line) and primitive (dash line) unit cells for the fcc Bravais lattice. The primitive cell has one quarter the volume of the conventional cell.

Question: Why do we need conventional cells to represent a Bravais lattice?

Answer:

A Bravais lattice is described as a lattice with basis by choosing a non-primitive unit cell because this cell has the full cubic symmetry of a Bravais lattice.

To emphasize the cubic symmetry of the bcc and fcc Bravais lattices, for example, we can show that they are descried as follows:

a) As a simple cubic (sc) lattice spanned by $a\hat{x}$, $a\hat{y}$ and $a\hat{z}$, the bcc Bravais lattice is described by the two-point basis (0, 0, 0) and $(\frac{a}{2}, \frac{a}{2}\frac{a}{2})$.

b) Also due to these lattice vectors, the fcc Bravais lattice is defined in terms of a four-point basis (0, 0, 0), $(\frac{a}{2}, \frac{a}{2}, 0)$, $(0, \frac{a}{2}, \frac{a}{2})$ and $(\frac{a}{2}, 0, \frac{a}{2})$.

Example:

When a set of primitive vectors for the Bcc lattice are given by $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$ and $\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$, as shown in figure 11,(where a is the side of each face of a conventional cubic unit cell) find the position of lattice point 1 as a linear combination of $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$.

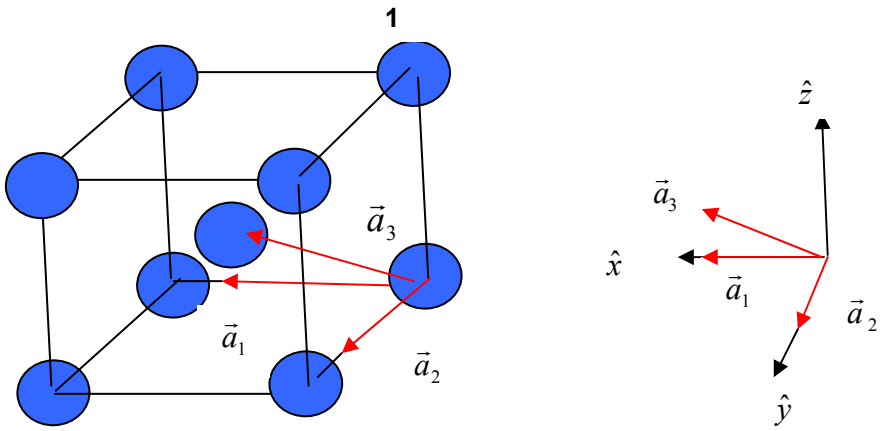

Figure 11: A set of symmetric primitive vectors for bcc Bravais lattice. The position vector of point 1 can be obtained in terms of the chosen primitive vectors.

Solution:

We need to find n_1, n_2, and n_3 in the position vector $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$. Point 1 is located at $\vec{R} = a\hat{z}$, thus;

$$n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 = a\hat{z}$$

By equating the coefficients of $\hat{x}$, $\hat{y}$ and $\hat{z}$ to get:

n_3 = 2, n_2 = -1 and n_1= -1.

$$\therefore \vec{R}_1 = -\vec{a}_1 - \vec{a}_2 + 2\vec{a}_3 .$$

Exercise: Show that the position vector of the point 1 in previous example can be written as $\vec{R}_1 = 2\vec{a}_1 + \vec{a}_2 + \vec{a}_3$ if another set of primitive vectors, shown in figure 8, is chosen instead, $\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$, $\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$ and $\vec{a}_3 = \frac{a}{2}(\hat{y} + \hat{x} - \hat{z})$.

Conclusion: Here you can deduce that there is more than one choice of set of primitive vectors not only to find the position of a single lattice point but also to generate the a whole bcc Bravais lattice.

Exercise: Find the positions of lattice points 1, 2, 3, 4 and 5, shown in figure 10, if a set of primitive vectors for fcc lattice is given by: $\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$ and $\vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{x})$.

Lattice constant and the volume of a unit cell:

The size of a unit cell may be specified by what is called the lattice constant a.

The volume of a unit cell can be determined by: $V = \left|\vec{a}_1 \bullet \vec{a}_2 \times \vec{a}_3\right|$.

[Note: For a sc unit cell $|\vec{a}_1|$ = $|\vec{a}_2|$ = $|\vec{a}_3|$ = a; but this is not the case for other cubic structures like bcc and fcc]

Question: What is the total number of lattice points in the unit cell of a sc?

Answer: 1.Why?

Why do we put all that emphasis on a unit cell?

We put emphasis on a unit cell because we need to investigate a representative volume (a unit cell) while analyzing the crystal. Also to find forces that hold the crystal lattice together, we can do that by calculating the forces between nearest atoms and next nearest atoms by finding the distances from a unit cell. Therefore, we relate the density of the solid to the atomic arrangement by looking at the fraction of the unit cell volume filled by atoms (i.e. packing fraction).

What is the importance of the periodic crystal lattice?

Knowing the properties of the periodic lattice allows us to determine the allowed energies of electrons that participate in the conduction process. Here it must be recalled that physical properties (like charge concentration, electron number density, or magnetic density) are invariant under translation of the form $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$.