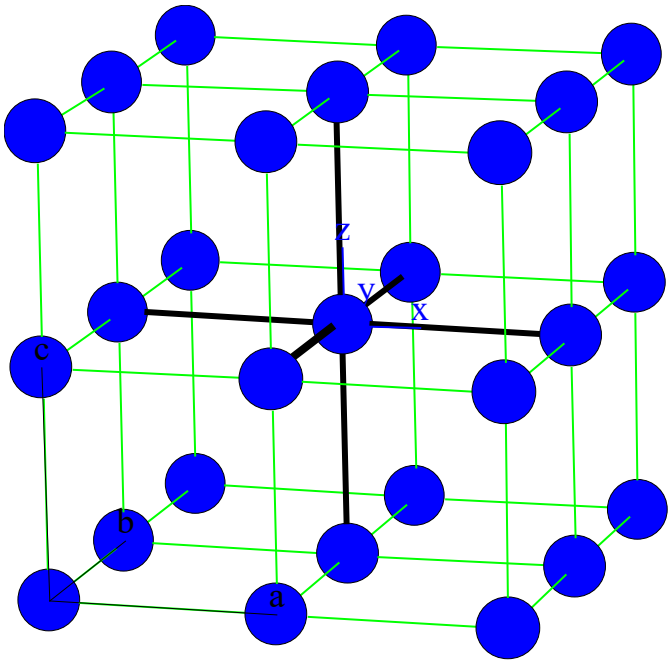
Lecture 8: Important Crystal Structures

1. Simple Cubic (SC) Structure

The simple cubic structure contains one lattice point located at the corners of the cube. Each atom located at a corner is shared equally among eight neighboring cubes. Therefore, the total number of atoms per unit cell is:



Number of atoms = 8 × (1/8) = 1 atom per unit cell.

Primitive lattice vectors:

$a_1 = (a, 0, 0)$
$a_2 = (0, a, 0)$
$a_3 = (0, 0, a)$

i.e,

$\vec{a}_1 = a\hat{x}$
$\vec{a}_2 = a\hat{y}$
$\vec{a}_3 = a\hat{z}$

Basis:

One atom is located at the lattice point.

As discussed before: 1/8 * 8=1

Coordination number:
The coordination number represents the number of 1st nearest neighboring atoms. For the simple cubic structure, the coordination number is 6. The distance to the nearest neighbor is a.

Exercise:
Try to determine the positions of these nearest neighboring atoms.

Solution:

$$\begin{aligned} &2\ atoms\ at && \pm a\hat{x} \\ &2\ atoms\ at && \pm a\hat{y} \\ &2\ atoms\ at && \pm a\hat{z} \end{aligned}$$

2. Body-Centered Cubic (BCC) Structure

The body-centered cubic structure contains **one lattice point at the center of the unit cell in addition to eight lattice points at the corners.** Thus, the total number of lattice points per unit cell is ***two***.

Number of atoms = 8 × (1/8) + 1 = 2 atoms per unit cell.

Primitive lattice vectors:

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

Basis:

Two atoms per unit cell.

Coordination number:
For the body-centered cubic structure, the coordination number is 8. The distance to the nearest neighbor is (√3/2)a.

Exercise:
Try to determine the positions of these nearest neighboring atoms.

Solution:

$$at\ \frac{a}{2}(\pm a\hat{x} \pm a\hat{y} \pm a\hat{z})$$

The fractional coordinates of the nearest neighbors relative to the atom at the origin are:

- (1/2, 1/2, 1/2)
- (1/2, 1/2, −1/2)
- (1/2, −1/2, 1/2)
- (−1/2, 1/2, 1/2)
- (−1/2, −1/2, 1/2)
- (−1/2, 1/2, −1/2)
- (1/2, −1/2, −1/2)
- (−1/2, −1/2, −1/2)

The nearest-neighbor distance is calculated using one of the vectors, for example:

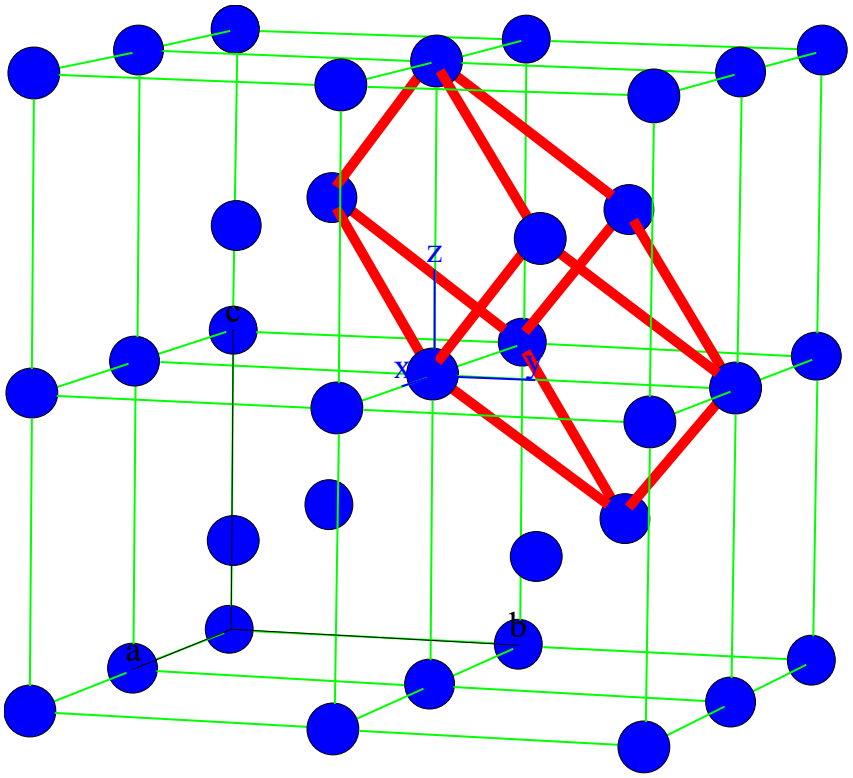
R = (a/2)(1, 1, 1).

The magnitude of this vector is:

$|R| = (a/2)\sqrt{(1^2 + 1^2 + 1^2)} = (\sqrt{3}/2)a.$

3. Conventional and Primitive Cells (BCC)

The conventional unit cell of the body-centered cubic structure is a simple cube, as shown in the figure. The primitive unit cell is highlighted in red and is called a rhombohedral cell.

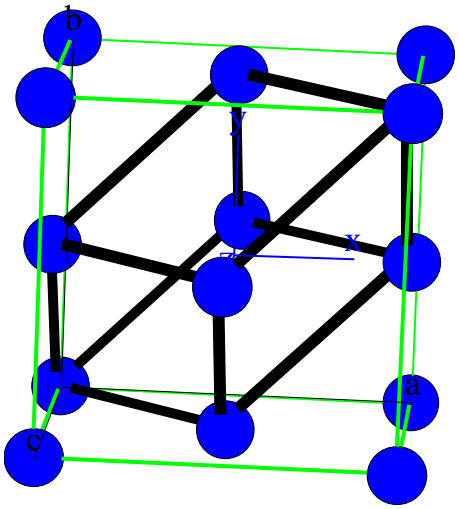


Exercise:

Prove that the volume of the primitive cell is equal to half the volume of the conventional unit cell.

4. Face-Centered Cubic (FCC) Structure

The face-centered cubic structure contains lattice points at the centers of the cube faces in addition to the corner lattice points. The total number of lattice points per unit cell is four.



Number of atoms = 8 × (1/8) + 6 × (1/2) = 4 atoms per unit cell.

Primitive lattice vectors:

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{z})$$

Basis:

Four atoms per unit cell.

At the corner :1/8 * 8 + at the faces center: 1/2*6= 4

located at: $\vec{d}_1 = a(0,0,0)$ $\vec{d}_2 = \frac{a}{2}(1,1,0)$ $\vec{d}_3 = \frac{a}{2}(0,1,1)$ $\vec{d}_4 = \frac{a}{2}(1,0,1)$

Coordination number:

For the face-centered cubic structure, the coordination number is 12.

Exercise:

Try to determine the positions of these nearest neighboring atoms.

Solution:

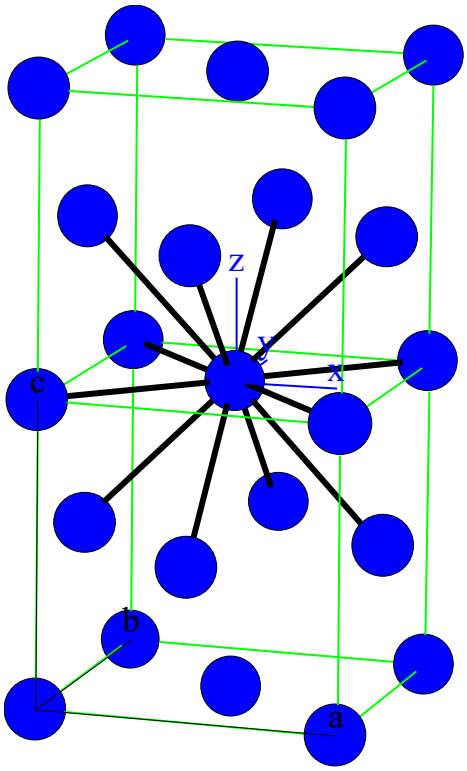
4 *atoms at* $a(\pm\hat{x} \pm \hat{y})$

4 *atoms at* $a(\pm\hat{y} \pm \hat{z})$

4 *atoms at* $a(\pm\hat{x} \pm \hat{z})$

Note:

The coordination number is defined as the number of closest neighboring atoms to which a given atom is bonded. For the FCC structure, = 12.



Visualization:

https://demonstrations.wolfram.com/CubicCrystalLattices/

Summarization:

Property	Simple Cubic (SC)	Body-Centered Cubic (BCC)	Face-Centered Cubic (FCC)
Volume of a conventional cell	a^3	a^3	a^3
Lattice points per conventional cell	1	2	4
Volume of a primitive cell	a^3	$\frac{1}{2} a^3$	$\frac{1}{4} a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors	6	8	12
Nearest-neighbor distance	a	$\sqrt{3}\, a / 2 = 0.866\, a$	$a / \sqrt{2} = 0.707\, a$
Number of second neighbors	12	6	6
Second-neighbor distance	$\sqrt{2}\, a$	a	a
Packing fraction	$\pi/6 \approx 0.524$	$\sqrt{3}\, \pi / 8 \approx 0.680$	$\pi / (3\sqrt{2}) \approx 0.740$