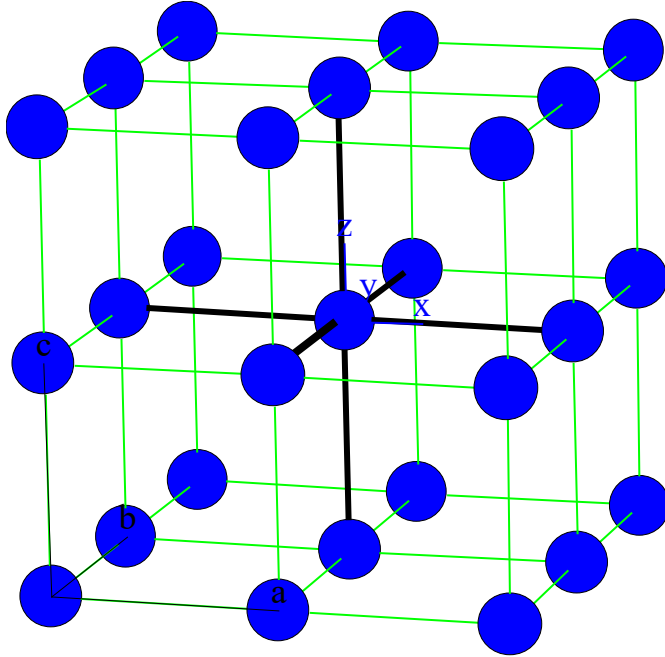


# Lecture 8: Important Crystal Structures

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## 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.



The total number of lattice points per unit cell is  $= 8 \times (1/8) = 1$  lattice point per unit cell.

Primitive lattice vectors:

$$\mathbf{a}_1 = (a, 0, 0)$$

$$\mathbf{a}_2 = (0, a, 0)$$

$$\mathbf{a}_3 = (0, 0, a)$$

i.e.,

$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

$$\vec{a}_3 = a\hat{z}$$

- For the SC Bravais lattice, the conventional cubic unit cell is also a primitive unit cell.

**Basis:**

One atom located at each lattice point.

As discussed before:  $1/8 \times 8 = 1$

**Coordination number:**

The coordination number represents the number of 1<sup>st</sup> nearest neighboring atoms surrounding a given atom. 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:**

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

## 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 =  $8 \times (1/8) + 1 = 2$  lattice points 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  $(\sqrt{3}/2)a$ .

**Exercise:**

Try to determine the positions of these nearest neighboring atoms.

**Solution:**

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

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:

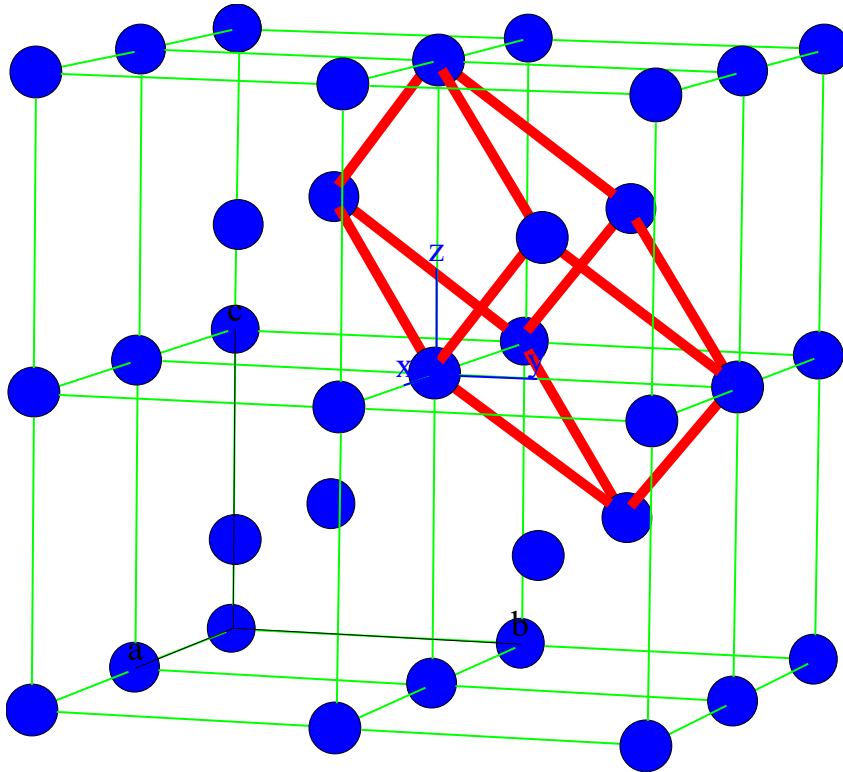
$$\mathbf{R} = (a/2)(1, 1, 1).$$

The magnitude of this vector is:

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

### 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.

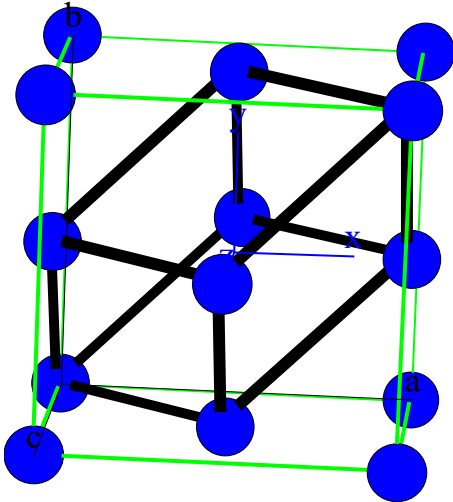


**Exercise:**

**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 =  $8 \times (1/8) + 6 \times (1/2) = 4$  lattice points 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:**

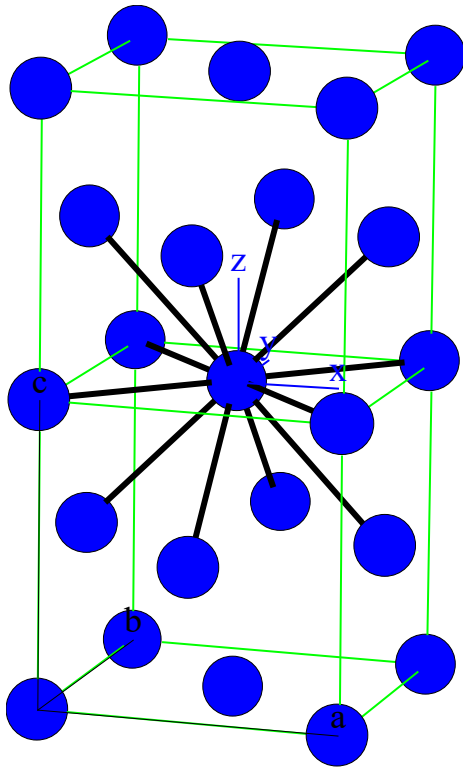
4 atoms at  $a(\pm\hat{x} \pm \hat{y})$

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                     | $\pi/6 \approx 0.524$ | $\sqrt{3} \pi / 8 \approx 0.680$ | $\pi / (3\sqrt{2}) \approx 0.740$ |