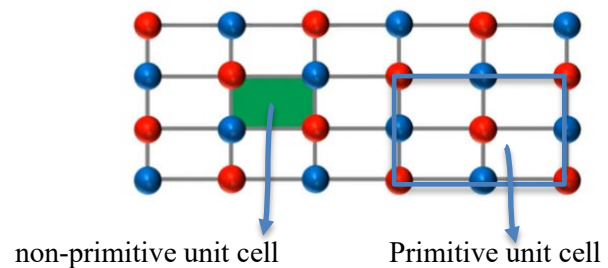
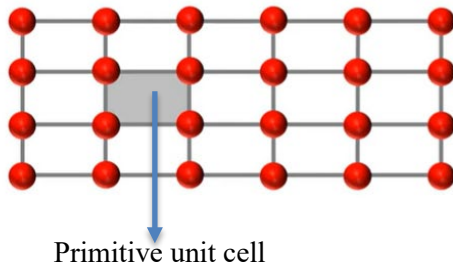
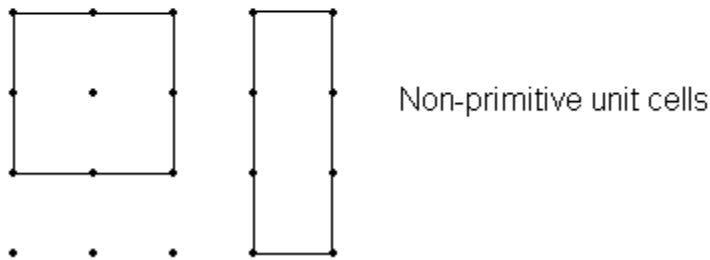
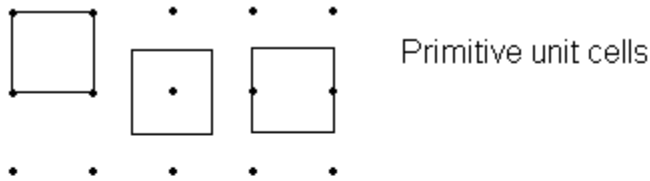


Lecture 3: Primitive Lattice Cell

As discussed in the last lecture, a primitive lattice cell is a minimum-volume cell that, when translated by the lattice vectors, reproduces the entire lattice without gaps or overlaps.

There are several methods to determine the primitive lattice cell and its primitive vectors.



Number of lattice points and atoms in the Cell

The number of lattice points in a cell is calculated by summing the fractional contributions of all lattice points associated with that cell:

$$n = \sum_i N_i f_i$$

Explanation of the Symbols

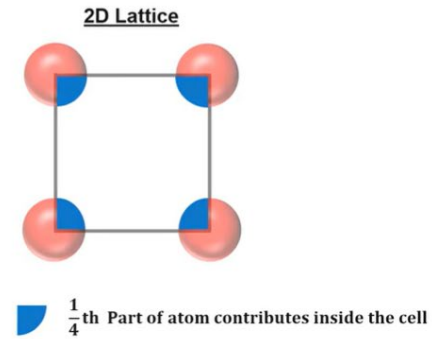
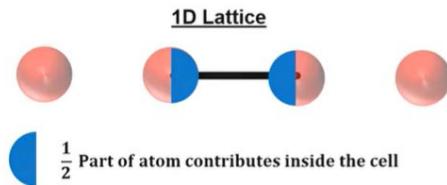
n: Total number of lattice points per unit cell.

i: Index that labels the different atomic positions in the unit cell (corners, edges, faces, body

center, or inside the cell).

N_i : Number of lattice points located at position i .

f_i : Fraction of each atom (associated with a lattice point) at position i that belongs to one unit cell, since atoms on boundaries are shared with neighboring unit cells.



Typical Fractional Contributions

Corner atom: $f = 1/8$

Edge-centered atom: $f = 1/4$

Face-centered atom: $f = 1/2$

Body-centered atom: $f = 1$

Example 1: Simple Cubic (SC) Structure

Given:

A simple cubic unit cell has atoms only at the corners.

Solution:

Corner atoms: 8

Each corner atom contributes $1/8$

$$n = 8 \times 1/8 = 1$$

Answer:

$n = 1$ lattice point per unit cell.

Example 2: Body-Centered Cubic (BCC) Structure

Given:

Atoms at 8 corners and 1 body center.

Solution:

Corner atoms: $8 \times 1/8 = 1$

Body-centered atom: $1 \times 1 = 1$

$$n = 1 + 1 = 2$$

Answer:

$n = 2$ lattice points per unit cell.

Example 3: Face-Centered Cubic (FCC) Structure

Given:

Atoms at 8 corners and 6 face centers.

Solution:

Corner atoms: $8 \times 1/8 = 1$

Face-centered atoms: $6 \times 1/2 = 3$

$$n = 1 + 3 = 4$$

Answer:

$n = 4$ lattice points per unit cell.

Example 4: FCC Unit Cell

For a face-centered cubic (FCC) unit cell:

8 corner atoms contribute: $8 \times 1/8 = 1$

6 face-centered atoms contribute: $6 \times 1/2 = 3$

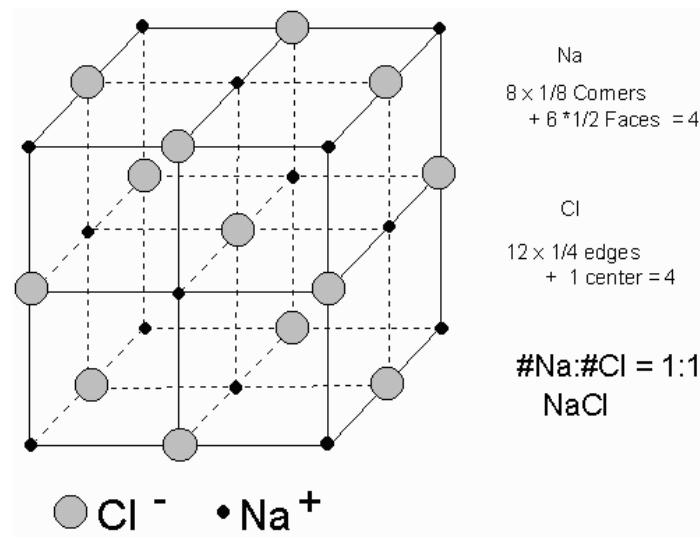
Total number of lattice points per unit cell:

$$n = 1 + 3 = 4$$

The summation over i means that we add the contributions from all distinct atomic positions in the unit cell.

How do we calculate the number of atoms in a primitive cell (or unit cell)? This can be explained using the following rules:

- Atoms located at the corners are counted as $1/8$ each (total = 1 atom).
- Atoms located at the body center are counted as 1 atom.
- Atoms located at the centers of faces are counted as $1/2$ each (total = 3 atoms).
- Atoms located at the centers of edges are counted as $1/4$ each (total = 3 atoms).

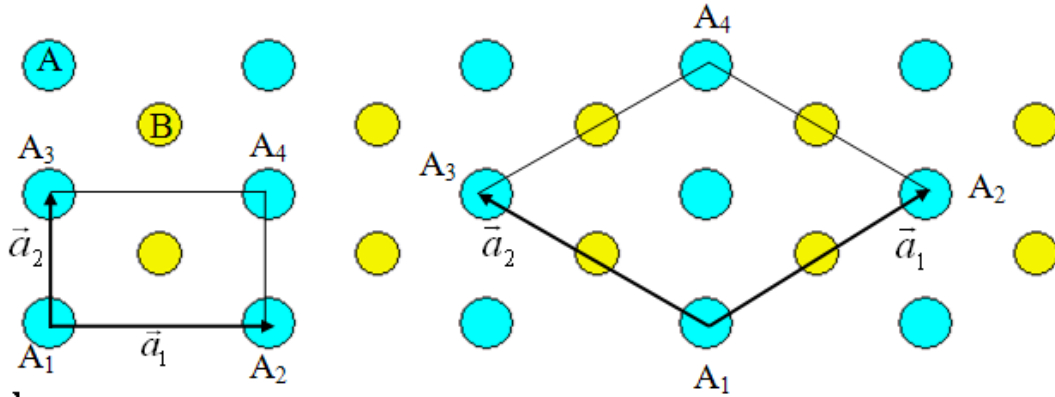


How to Construct a Primitive Cell

Method 1

Assume we have a two-dimensional lattice containing two different types of atoms, **A** and **B**.

Question: How do we determine the primitive cell of this lattice?



Steps:

1. Choose any atom or lattice point and label it A₁.
2. Move from A₁ in any direction until reaching another atom of the same type A; label it A₂ with vector $\vec{a}_1$.
3. From A₁, move in another direction until reaching a third atom of the same type A; label it A₃ with vector $\vec{a}_2$.

Note that $\mathbf{a}_1$ and $\mathbf{a}_2$ are not necessarily lattice vectors.

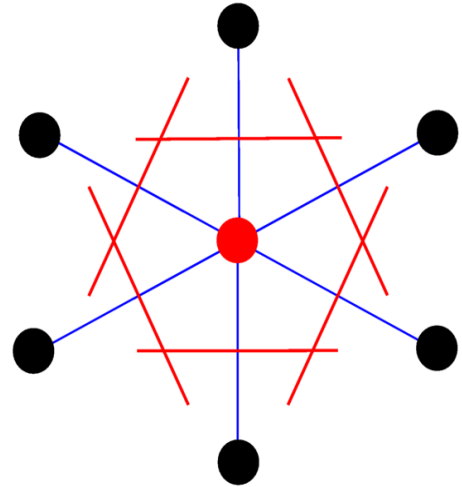
Using $\mathbf{a}_1$ and $\mathbf{a}_2$, a cell (A₁A₂A₃A₄) can be constructed. If this cell contains no additional atoms of type A inside it, then it is a primitive cell.

The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are primitive translation vectors if their translations reproduce the lattice.

Method 2: Wigner–Seitz Cell

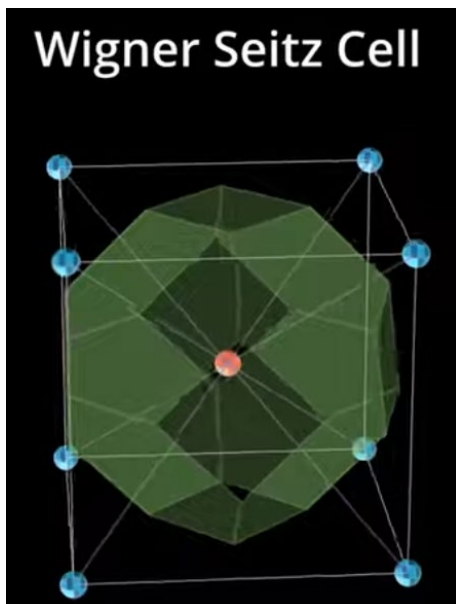
Steps:

1. Choose a lattice point.
2. Draw lines connecting this point to its nearest neighboring lattice points.
3. At the midpoint of each connecting line, draw a perpendicular bisector.
4. The smallest region enclosed by these bisectors is called the Wigner–Seitz cell.

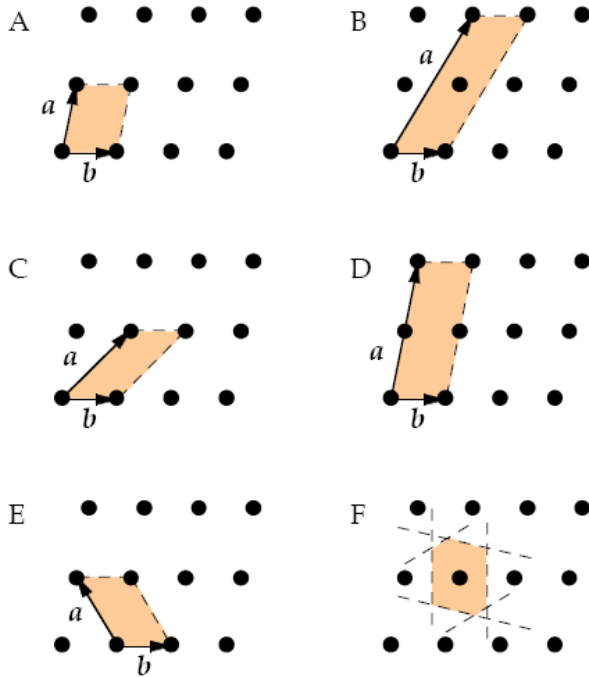


Example 5: Wigner–Seitz Cell in 3D for Body-centered cubic

<https://www.youtube.com/shorts/VajxpcKqxhM>



Exercise: Which of the shaded cells in Figures A–F are primitive unit cells? Explain briefly.



Calculation of Area and Volume of the Primitive Cell

In two dimensions (2D), the area of the primitive cell is given by:

$$A = |\mathbf{a}_1 \times \mathbf{a}_2|$$

In three dimensions (3D), the volume of the primitive cell is given by:

$$V = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$$

Crystal Density

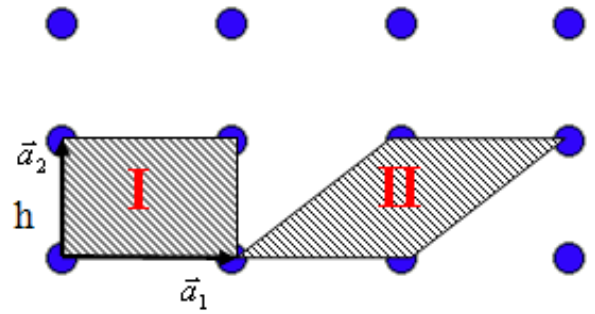
The density of a crystal (ρ) can be calculated using:

$$\rho = m / V$$

where m is the mass of one unit cell and V is the volume of the unit cell.

Exercise -1

Compare the areas of Cell I and Cell II and comment on whether both cells are primitive unit cells of the lattice.



Exercise -2

Given a three-dimensional lattice with primitive vectors:

$$\mathbf{a}_1 = (1, 0, 0)\mathbf{a}$$

$$\mathbf{a}_2 = (1, -1, 0)\mathbf{a}$$

$$\mathbf{a}_3 = (0, 0, 2)\mathbf{a}$$

where $\mathbf{a}$ is a constant. Determine the volume of the primitive cell.

Answer:

$$V = 4\mathbf{a}^3$$

Example 6: A cell with Edge-Centered Points

Given:

Atoms at 8 corners and 12 edge centers.

Solution:

$$\text{Corner atoms: } 8 \times 1/8 = 1$$

$$\text{Edge-centered atoms: } 12 \times 1/4 = 3$$

$$n = 1 + 3 = 4$$

Answer:

$n = 4$ atoms per unit cell.

Example 7: Mixed Atomic Positions

Given:

Atoms at 8 corners, 6 face centers, and 1 atom fully inside the cell.

Solution:

$$\text{Corner atoms: } 8 \times 1/8 = 1$$

$$\text{Face-centered atoms: } 6 \times 1/2 = 3$$

$$\text{Interior atom: } 1 \times 1 = 1$$

$$n = 1 + 3 + 1 = 5$$

Answer:

$n = 5$ atoms per unit cell.