The Unit Cell

There are 7 types of unit cells (figure 12.1.a), defined by edge lengths (a,b,c) and angles \(\alpha\), \(\beta\), and \(\gamma\). In this class we will only focus on the cubic unit cell, and there are three types of cubic cells that you need to be familiar with, and these are represented in figure 12.1.b.

- \(\alpha\) = angle in the x,y plane
- \(\beta\) = angle in the y,z plane
- \(\gamma\) = angle in the x,y plane

Figure\(^\text{PageIndex{1}}\): The 7 types of unit cells. In this class we will only look at cubic systems, and will identify 3 types of cubic unit cells (figure. 12.b)

Cubic Unit Cell

The cubic unit cell is the smallest repeating unit when all angles are 90\(^\circ\)C and all lengths are equal (figure 12.1.b). As such, each axis is defined by a Cartesian coordinate. Each cubic cell has 8 atoms in each corner of the cube, and that atom is shared with 8 neighboring cells. In the Body Centered Cubic Cell (BCC) there is an additional atom in the center of the cube, and in the face centered cubic cell, an atom is shared between two unit cells along the face. Please watch the YouTube video as this can help a lot.
Figure\(\PageIndex{2}\): Three type of cubic unit cells, each is described in detail below.

Video\(\PageIndex{1}\): “Lattice Structure Part 1”, created by Mark McClure, narrated by Sally Vallabha of UN-Pembroke, https://youtu.be/Rm-i1c7zr6Q
Simple (Primative) Cubic Unit Cell

![Diagram of Simple (Primative) Cubic Unit Cell]

- 1 particle per unit cell
- Coordination number = 6
- 52% of space occupied by particles
- Simple Cubic Stacking
  - Along Cartesian coordinates
  - Very inefficient and rarely seen in nature

**Figure\(\PageIndex{3}\):** Unit cell for primitive cubic cell and stacking diagram for Simple Cubic Stacking which this results in.

Body centered cubic unit cell

![Diagram of Body centered cubic unit cell]
**Figure 4:** Unit cell for body centered cubic cell and stacking hexagonal close packed structure it results in. This has a repeating alignment of ABABABAB where every other layer lines up.

- 2 particles per unit cell
- coordination number = 8
- 68% of space occupied by particles
- Hexagonal Close Packing (HCP)
  - second layer sits in grove of first with third in grove of second and in line with first (ABA structure)
  - Common with metals, including all alkali, Cr, V, Ba and Fe

**Face Centered Cubic**

**Figure 5:** Unit cell for face centered unit cell, and diagram of Cubic Close Packed structure that it results in. Note each row has neighbors shifted from the Cartesian coordinate of their plan, and as you move up the lattice there is an ABCABCABC stacking, where every third layer aligns. This is the form oranges would stack in a grocery store.

- 4 particles per unit cell
- coordination number = 12
- 74% of space occupied by particles
- Cubic Closest Packing Structure
  - explained in video 12.1.a at 5' 26".
  - along Cartesian coordinates
Determining Atomic Radii from Density, Molar Mass and Crystal Structure

The strategy is to use the following to calculate the volume of the unit cell, and then the length of each side. Once this is done, you can use the packing and the geometry of the structure to calculate the radii. The information you need are:

- density
- Molar Mass
- Avogadro's number
- number atoms per unit cell
- pythagorean theorem

So these all have a similar strategy

1. Calculate Volume of Unit Cell (number of atoms in unit cell depends on type of cell)
2. Calculate length of the sides of the unit cell (same for all)
3. Use packing to figure radii (different for each type)

A. Simple Cubic Cell

Exercise \(\PageIndex{1}\)

A. Given the density of Polonium = 9.32 g/ml, calculate radii of a Polonium atom if it forms a Simple Cubic Cell.

**Problem:** Polonium is the only element that is simple cubic (has 1 atom/unit cell). Note the length of unit cell is 2 radii, and thus if we can calculate the length of the unit cell, we can calculate the radius. When we say there is one atom per unit cell, we are not saying the volume of the atom is the volume of the unit cell. It is 52% the volume (see above).
Video\PageIndex{2}): Solution to the radii of Po from its density.

**Answer:**

1. Find the volume of the unit cell

\[
\frac{1 \text{ atom Po}}{\text{unit cell}} \left( \frac{1 \text{ mol Po}}{6.02 \times 10^{23} \text{ atoms}} \right) \left( \frac{208.9 \text{ g Po}}{1 \text{ mol}} \right) \left( \frac{1 \text{ ml}}{9.32 \text{ g}} \right) = 3.72 \times 10^{-23} \frac{\text{ml}}{\text{unit cell}}
\]

2. Find the length of the unit cell

\[l = \sqrt[3]{V} = \sqrt[3]{3.72 \times 10^{-23} \text{cm}^3} = 3.34 \times 10^{-8} \text{cm} = 334 \text{pm}\]

3. Find radii

Since each side is 2r, r is 1/2 half the length, or 167pm

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**B. Body Centered Cubic**

Exercise \PageIndex{2})

**Problem:** Molybdenum forms body centered cubic cells, if the density of Mo is 10.28 g/ml, what would its radius be?
This is the toughest, as the diagonal through the cell from vertices X to Y with length "c" equals 4 radii. It makes a right triangle with side a and b, the diagonal of a face, we note that $a^2 + a^2 = b^2$ and $a^2 + b^2 = c^2$

Answer:

1. Find Volume of unit cell:

$$\frac{2 \text{ atom Mo}}{\text{unit cell}} \left( \frac{1 \text{ mol Mo}}{6.02 \times 10^{23} \text{ atoms}} \right) \left( \frac{95.95 \text{ g Mo}}{1 \text{ mol}} \right) \left( \frac{1 \text{ ml Mo}}{10.26 \text{ g}} \right) = 3.11 \times 10^{-23} \text{ ml/unit cell}$$
2. Find length of unit cell

\[a=\sqrt[3]{V}=\sqrt[3]{3.11\times10^{-23}\text{cm}^3}=3.15\times10^{-8}\text{cm}=314\text{pm}\]

3. Find radii

a. Find diagonal of face "b"

\[b=\sqrt{2a^2}=\sqrt{2(314)^2}=444\text{pm}\]

b. Find diagonal through cube "c"

\[c=\sqrt{a^2+b^2}=\sqrt{314^2+444^2}=544\text{pm}\]

c. "c" = 4r, so \(r=136\text{pm}\)

C. Face Centered Cubic

Exercise \(\PageIndex{3}\))

**Problem:** Calcium forms a face centered cubic cell with a density of 1.54 g/ml, what would its radius be?
Answer:

1. Find Volume of unit cell:

\[ \frac{4 \text{ atom Ca}}{\text{unit cell}} \times \frac{1 \text{ mol CA}}{6.02 \times 10^{23} \text{ atoms}} \times \frac{40.08 \text{ g Ca}}{\text{mol}} \times \frac{1 \text{ ml Mo}}{1.54 \text{ g}} = 1.73 \times 10^{-22} \text{ ml/unit cell} \]

2. Find length of unit cell

\[ a = \sqrt[3]{V} = \sqrt[3]{1.72 \times 10^{-22} \text{ cm}^3} = 5.57 \times 10^{-8} \text{ cm} = 557 \text{ pm} \]

3. Find radii

   a. Find diagonal of face "c"

   \[ c = \sqrt{2a^2} = \sqrt{2(557)^2} = 787 \text{ pm} \]

   b. since the diagonal of the surface is 4r, r = 197 pm

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**Crystal Defects**

Defects in a crystal can give it unique properties. Defects occur when another entity becomes part of the crystal, and there are many types of defects, two that are worth noting are substitutional and interstitial.
Substitutional Defects

These occur when a different substance substitutes for one of the components of the crystal. For example Ruby is $\text{Al}_2\text{O}_3$ with a few $\text{Cr}^{3+}$ replacing $\text{Al}^{3+}$ ions.

![Figure 6: Substitutional defect](image)

Interstitial Defects

These occur when a substance which is not part of the crystal fits into the interstitial regions, and does not displace a component of the crystal. Carbide steel is a form of interstitial defect where carbon enters the holes of the iron structure, and this affects its properties like hardness and ductility.

![Figure 7: Example of an interstitial defect](image)

- **Contributors**
  - Bob Belford
  - some images from anonymous
  - some images from anonymous were modified
• some images from Chris P Schaller