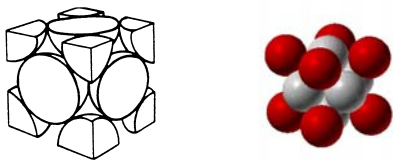


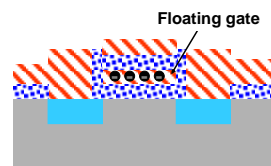
Class 1 & 2: Overview & Crystal Structure



PRIME Modules
Project-based Resources for Introduction to Materials Engineering

The two main non-volatile memory technologies are FLASH and hard drives

FLASH is an electronic memory that has "1" and "0" states by storing or not storing electrons



Magnetic hard drives have "1" and "0" states by having magnetic bits polarized in the N or S direction

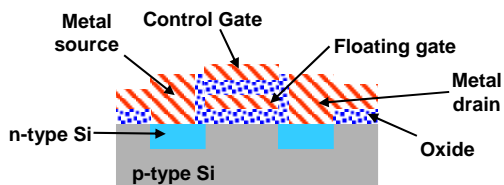


<http://researchweb.watson.ibm.com/research/gmr/basics.html>

FLASH technology relies on crystal structure and electrical properties

The 3-D crystal structure of the silicon controls the electrical properties of a FLASH device

Understanding the electrical properties of metals, semiconductors, and insulators is needed to understand how FLASH devices operate



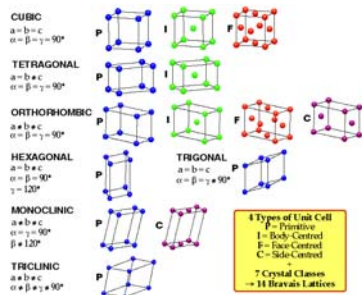
7 Crystal Systems Define axis in space by varying side lengths and angles

| | | |
|--------------|--|--|
| Cubic | $a = b = c, \alpha = \beta = \gamma = 90^\circ$ | |
| Tetragonal | $a = b \neq c, \alpha = \beta = \gamma = 90^\circ$ | |
| Orthorhombic | $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$ | |
| Rhombohedral | $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$ | |
| Hexagonal | $a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$ | |
| Monoclinic | $a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$ | |
| Triclinic | $a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$ | |

14 Bravais Lattices map out framework of identical points

A lattice site/point is an identical point on a lattice. It has the same atoms on it and surrounding it. Lattice sites can have more than one atom associated with them.

In this class, we are going to focus on the three cubic lattices (SC, BCC, and FCC)

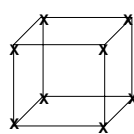


http://www.chem.ox.ac.uk/icl/heytes/structure_of_solids/Lecture1/Bravais.gif

A unit cell is a small, easy to draw subset of the crystal structure

The lattice type (SC, FCC, BCC) and the basis (the arrangement of atoms around each lattice point) define the crystal structure.

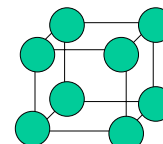
The unit cell is a small, easy to draw subset. The lattice extends into 3-D space.



SC Lattice



Basis: In this example, 1 green atom per lattice site



Unit Cell

A SC lattice with a atom per lattice site has 1 total atom in the unit cell

This figure shows the expanded view of a SC lattice with one atom per lattice site.

This differs from the ball and stick model in earlier slides. Here the actual space the atom takes up is drawn in.

In order not to double count atoms, you need to factor in how much of each atom is shared by neighboring unit cells.

$$8 \text{ Corner Atoms} \cdot \frac{1}{8} = 1 \text{ atom/unit cell}$$



Callister, Chapter 3

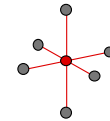
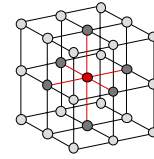
The SC lattice (with 1 atom/lattice site) has a coordination number of 6

The coordination number is the number of atoms an atom is bonded to.

It can be seen as the number of atoms that touch.

You need to count atoms in other unit cells.

For SC lattice with 1 atom per lattice site, the CN is 6



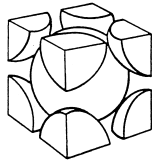
Callister, Chapter 3

BCC lattice with 1 atom per lattice site has 2 atoms per unit cell and a CN of 8

For a BCC lattice with 1 atom per lattice site, there are 2 atoms per unit cell

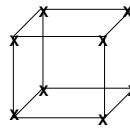
$$8 \text{ Corner Atoms} \cdot \frac{1}{8} + 1 \text{ inside} = 2 \text{ atom/unit cell}$$

For a BCC lattice with 1 atom per lattice site, the CN is 8

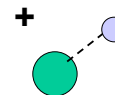


Callister, Chapter 3

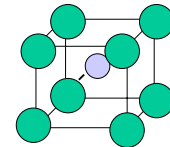
CsCl has a SC lattice with a basis of 2 atoms per lattice site



SC Lattice



Basis: 1 Cs (0,0,0) & 1 Cl (1/2,1/2,1/2)



CsCl Unit Cell

If you stamp that basis on every SC lattice site. You get the unit cell shown. Some of the atoms end up in other unit cells.

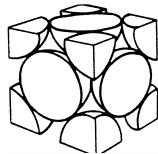
This is NOT a BCC lattice because the inside point is not identical to the others.

FCC lattice with 1 atom per lattice site has 4 atoms per unit cell and a CN of 12

For a FCC lattice with 1 atom per lattice site, there are 4 atoms per unit cell

$$8 \text{ Corner Atoms} \cdot \frac{1}{8} + 6 \text{ Corner Atoms} \cdot \frac{1}{2} = 4 \text{ atom/unit cell}$$

For an FCC lattice with 1 atom per lattice site, the CN is 12



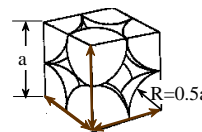
Callister, Chapter 3

Atomic Packing Factor is fraction of space in a unit cell taken up by an atom

$$APF = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

*assume hard spheres

APF for a simple cubic structure = 0.52

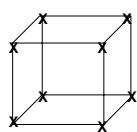


$$APF = \frac{1 \text{ atoms/unit cell} \cdot \frac{4}{3} \pi (0.5a)^3}{a^3}$$

close-packed directions contains $8 \times 1/8 = 1$ atom/unit cell

Adapted from Fig. 3.19, Callister 6e.

In summary, the combination of lattice and basis is a systematic way to catalog the 3 D arrangement of atoms in solids.

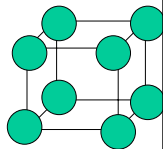


SC Lattice

+



=



Unit Cell

Basis: In this example, 1 green atom per lattice site