Determine the lattice points per cell in the cubic system

Simple cubic:
Lattice points are located only at the corners of the cube

8 corners \( \times \frac{1}{8} = 1 \)

In BCC unit cells, lattice points are located at the corners and the center of the cube:

8 corner \( \times \frac{1}{8} + 1 \text{ center} \times 1 = 2 \)

In FCC unit cells, lattice points are located at the corners and faces of the cube:

8 corners \( \times \frac{1}{8} + 6 \text{ faces} \times \frac{1}{2} = 4 \)
Calculate the radius of an atom that will just fit into a cubic site

\[ 2R + 2r = 2R \sqrt{3} \]

\[ \frac{r}{R} = 0.732 \]
Problem

• Calculate the change in volume that occurs when BCC iron is heated and changes to FCC iron. The lattice parameter of BCC iron is 2.863 Å and of FCC iron is 3.591 Å.

Volume of BCC cell = $a^3 = 2.863 = 23.467$
Volume of FCC cell = $a^3 = 3.591 = 46.307$

But the FCC unit cell contains four atoms and the BCC unit cell contains only two atoms. Two BCC unit cells with a total volume of 46.934 will contain 4 atoms.

Volume change/atom = $(46.307 - 46.934)/46.934 = -1.34\%$

Steel contracts on heating!!
If a steel with a composition $x\%$ carbon is cooled from the Austenite region at about 770 °C ferrite begins to form. This is called proeutectoid (or pre-eutectoid) ferrite since it forms before the eutectoid temperature.
Problem

- A hypoeutectoid steel contains 22.5% eutectoid ferrite. What is the average carbon content?

\[ \text{Total ferrite} = \text{proeutectoid ferrite} + \text{eutectoid ferrite} \]

\[
\frac{6.67-x}{6.67-0.02} = \frac{0.80-x}{0.80-0.02} + 0.225
\]

\[ X = 0.2 \]
Problem

A 0.90 percent C hypereutectoid plain-carbon steel is slowly cooled from about 900°C to a temperature just slightly above 723°C. Calculate the weight percent proeutectoid cementite and the weight percent austenite present in this steel.

\[
\text{Wt } \% \text{ austenite} = \frac{6.67 - 0.90}{6.67 - 0.80} \times 100\% = 98.3\%
\]

\[
\text{Wt } \% \text{ cementite} = \frac{0.90 - 0.80}{6.67 - 0.80} \times 100\% = 1.7\%
\]
A 1.10 percent C hypereutectoid plain-carbon steel is slowly cooled from about 900°C to a temperature just slightly below 723°C.

(a) Calculate the weight percent proeutectoid cementite present in the steel.

(b) Calculate the weight percent eutectoid cementite and the weight percent eutectoid ferrite present in the steel.

(a) The weight percent proeutectoid cementite will be:

\[
\text{Wt \% proeutectoid cementite} = \frac{1.10 - 0.80}{6.67 - 0.80} \times 100\% = \frac{0.3}{5.87} \times 100\% = 5.1\%
\]
\[
\text{Wt} \% \text{ eutectoid ferrite} = \frac{6.67 - 1.10}{6.67 - 0.02} \times 100\% = \frac{5.57}{6.65} = 83.8\% 
\]

\[
\text{Wt} \% \text{ eutectoid cementite} = \text{Wt} \% \text{ total cementite} - \text{Wt} \% \text{ proeutectoid cementite} \\
= \left[ \frac{1.10 - 0.02}{6.67 - 0.02} \times 100\% \right] - 5.1\% \\
= 11.1\%
\]
An Example  
(Assume a Eutectoid Low Carbon Steel)

(a) Water-quench to room Temperature.
(b) Hot-quench at 690°C & hold 2 hr; water-quench
(c) Hot-quench at 610°C & hold 3 min; water-quench
(d) Hot-quench at 580°C & hold 2 sec; water-quench
(e) Hot-quench at 450°C & hold 1 hr; water-quench

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Types of Atomic & Molecular Bonds

- Primary Atomic Bonds
  - Ionic Bonds
  - Covalent Bonds
  - Metallic Bonds
- Secondary Atomic & Molecular Bonds
  - Permanent Dipole Bonds
  - Fluctuating Dipole Bonds
Ionic Bonding

- Large interatomic forces are created by the “coulombic” effect produced by positively and negatively charged ions.
- Ionic bonds are “nondirectional”.
- The “cation” has a + charge & the “anion” has the - charge.
- The cation is much smaller than the anion.
Energy vs. Separation Distance

\[ E = - \frac{\partial F}{\partial a} \]
Covalent Bonding in Carbon

- A carbon atom can form $sp^3$ orbitals directed symmetrically toward the corners of a tetrahedron. [Note the examples below.]

Methane, CH$_4$
Metallic Bonding

• Large interatomic forces are created by the sharing of electrons in a delocalized manner to form strong **nondirectional** bonding.

  [Note the schematic representation of copper atoms arranged in a FCC crystal at the left, and the representation of the cloud of electrons surrounding the positively charged cores.]

  *Positive ion cores*

  *Valence electrons in the form of electron charge clouds*
Secondary Atomic & Molecular Bonds
[Van der Waals Bonds]

• Permanent Dipole Bonds
  – Weak intermolecular bonds are formed between molecules which possess permanent dipoles.
  – A dipole exists in a molecule if there is asymmetry in its electron density distribution.
14 Bravais Lattices
There are three principle crystal structures for metals:

- (a) Body-centered cubic (BCC)
- (b) Face-centered cubic (FCC)
Face-centered cubic (FCC)
Body-centered cubic (BCC)
Hexagonal close-packed (HCP)
Alloys & Their Phase Diagrams
Cu-Ni: Binary Isomorphous Alloy Example

![Diagram of Cu-Ni phase diagram with annotations for Liquidus line, Solidus line, and Tie line.]

- Liquidus line
- Solidus line
- Tie line
- $w_0 = 53$ wt% Ni
- $w_L = 45$ wt% Ni
- $w_s = 58$ wt% Ni
- 1084°C
- 1300°C
- 1455°C

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The Lever Rule

To compute the amount of solid phase:

Fraction of the solid phase = \( \frac{(W_0 - W_l)}{(W_s - W_l)} \)

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The Iron-Iron Carbide Phase Diagram

- **α ferrite**: BCC iron crystal lattice
- **Austenite**: FCC crystal
- **Cementite**: Hard and brittle
The Iron-Iron Carbide Eutectoid System

Note: pearlite is not a phase, but a combination of ferrite and cementite.
Diffusive Transformation of FCC to BCC in Pure Fe

- Above 914° C pure Fe is face centered cubic (FCC).
- Below 914° C the thermodynamically stable phase of pure Fe is body centered cubic (BCC).
- Note that the speed of the “interface” in this transformation is zero at 914° C.

Why this shape?

- Increasing driving force
- Less thermal energy
The standard practice to display diffusive transformations is with the “Time-Temperature-Transformation” (TTT) diagram. It is also known as the “Isothermal-Transformation” diagram or “C-curve”.

The TTT diagram for the diffusive f.c.c.->b.c.c. transformation of pure Fe is shown at the right.
The two curves are related

Consider the 1% transformation line (1% of the fcc to transform to bcc)

1) The transformation rate is zero both at 910 and −273 C so the time required for the transformation is infinite at these temperatures

2) The transformation rate is a maximum at 700 C so the time for the 1% transformation must be a minimum at 700 C
Fe-C Interstitial Solid Solution in Ferrite & Martensite

The Carbon atoms cannot fit into interstitial spaces in the BCC ferrite structure like they can in the FCC Austinite and produce a BCT (schematically shown below).

Note in the BCT the Carbon atoms force the unit cell to be elongated in the c-direction. The largest interstitial void in BCC iron has a diameter of 0.072-nm.