**L5. The Iron - Carbon System**

1. ***Calculate the theoretical volume change accompanying a polymorphic transformation in a pure metal from the FCC to BCC crystal structure.***

***Assume the hard-sphere atomic model and that there is no change in atomic volume before and after the transformation.***

**FCC has 4 atoms/unit cell:**

**a\_FCC = 2√2\*R**

**V\_FCC = (2√2\*R)^3 = 16√2\*R^3 = 45.25 \* R^3**

**BCC has 2 atoms/unit cell:**

**a\_BCC = 4\*R / √3**

**V\_BCC = (4\*R/√3)^3 = 64\*R^3 / 3√3 = 41.57 \* R^3**

**Volume change :**

**[(V\_BCC - V\_FCC) / V\_FCC ]\* 100 = [(41.57 - 45.25) / 45.25] \* 100 = -8.14 %**

**The theoretical volume change is = -8.14% => the volume decreases when trandforming from FCC to BCC.**

1. *Calculate the number of octahedral sites that uniquely belong to one FCC unit cell.*

Octahedral sites have a coordination number of 6. These are interstitial “holes” betweeen atoms where smaller atoms can fit

In an FCC unit cell octahedral sites are located - at the center of the unit cell - 1 full site

-at the centers of each edge - each edge site is shared between 4 adjacent unit cells

There are :

* 12 edges (each with 1 octahedral site shared among 4 cells) => 12\* 1/4 = 3
* 1 center site inside the unit cell => fully belongs to it

Total octahedral sites/FCC unit cell :

3(edges) + 1(center) = 4 (octahedral sites that uniquely belong to 1 FCC unit cell)

1. *A 0.77% C eutectoid plain-carbon steel is slowly cooled from 750°C to a temperature just below 727°C. Assuming complete transformation to ferrite and cementite:*
2. ***Calculate the weight percent eutectoid ferrite formed.*** *b.* ***Calculate the weight percent eutectoid cementite formed.***

**So at 727 C, the eutectoid reaction is:**

γ (austenite, FCC) -> **α (ferrite, BCC) + Fe3C (cementite)**

**This occurs at :**

* **Autectoid composition C\_0 = 0.77%**
* **Ferrite composition C\_α = 0.022%**
* **Cementite composition C\_Fe3C = 6.7%**

**Use lever rule in order to find the weight fraction of each phase:**

**Formula for ferrite:**

**W\_α = (C\_Fe3C - C\_0) / (C\_Fe3C - Cα)**

**Formula for cementite:**

**W\_Fe3C = (C\_0 - C\_α) / (C\_Fe3C - Cα)**

**=> W\_α = (6.7 - 0.77) / (6.7 - 0.022) = 5.93 / 6.678 = 0.888 = 88.8 %**

**=> W\_Fe3C = (0.77 - 0.022) / (6.7 - 0.022) = 0.748 / 6.678 = 0.112 = 11.2 %**