

University of Wales Trinity Saint David

Structure and Properties – Calculations Assignment

BEng Material Science – M5X01185

Question 1

a) Evaluate the statement “pressure affects the allotropy of pure iron”

A species can have more than one crystal structure, this is known as polymorphism. When this occurs in elemental solids it's called allotropy.

Iron is an allotropic material; it's crystalline structure changes dependant on pressure and external temperature during solidification.

Le Chatelier's Principle states 'when a system experiences a disturbance, it will respond to restore a new equilibrium state'. Crystalline structures have a different number of atoms per unit cell meaning that the atomic packing factor differs for each arrangement.

Iron Type	Structure Type	Atomic Packing Factor	Atoms/Unit Cell
Alpha	Body Centred Cubic (BCC)	0.68	2
Gamma and Delta	Face Centred Cubic (FCC)	0.74	4
Epsilon	Hexagonal Close Packed (HCP)	0.74	6

In low pressure environments, BCC iron forms. With increasing pressure, the system's equilibrium shifts in order to oppose the change; HCP iron forms at higher pressures in order to fit a larger number of atoms in each unit cell.

(Note, changing temperature also affects the formation of iron crystal structures).

b) A hypothetical metal has a FCC structure with a density of 8.94g/cm^3 and an atomic weight of 63.5g/mol . Calculate the radius of one of its atoms.

Using the theoretical density calculation,

$$\rho = \frac{nA}{V_c N_A}$$

Given,

$$\rho = 8.94\text{g/cm}^3$$

$$A = 63.5\text{g/mol}$$

$$(\text{Avogadro's constant } N_A = 6.022 \times 10^{23})$$

FCC has four atoms per unit cell so $n = 4$

$$8.94 = \frac{(4)(63.5)}{V_c(6.022 \times 10^{23})}$$

$$V_c(6.022 \times 10^{23}) = \frac{(4)(63.5)}{8.94}$$

$$V_c(6.022 \times 10^{23}) = 28.41$$

$$V_c = \frac{28.41}{(6.022 \times 10^{23})}$$

$$V_c = 4.72 \times 10^{-23}$$

Given that,

$$V_c = a^3$$

Therefore,

$$a^3 = 4.72 \times 10^{-23}$$

$$a = \sqrt[3]{4.72 \times 10^{-23}}$$

$$a = 3.61 \times 10^{-8}$$

For FCC $4r = (\sqrt{2})(a)$

$$r = \frac{(\sqrt{2})(a)}{4}$$

Substituting a value for a,

$$r = \frac{(\sqrt{2})(3.61 \times 10^{-8})}{4}$$

$$r = 1.28 \times 10^{-8} \text{ cm}$$

c) *Analyse the difference between crystal structure and atomic structure.*

Crystal Structures	Atomic Structures
The crystal structure describes the arrangement of atoms (or molecules) within a crystalline compound.	The atomic structure is the arrangement of subatomic species within an atom.
This structure is an organised repetitive lattice structure.	This structure is complex.
Made up of cations, anions, metal ions and free roaming electrons.	Made up of electrons, neutrons and protons.
Crystalline structure varies dependent on components within the crystal.	The general structure is the same in all atoms.

d) *In a cubic unit cell one corner atom is located at the origin of a coordinate system (0,0,0). What are the direction indices for a vector that passes from point ($\frac{1}{2}$, 1, $\frac{1}{2}$) to point (1, $\frac{1}{2}$, $\frac{1}{2}$)?*

Head - Tail

$[1 \frac{1}{2} \frac{1}{2}]$ - $[\frac{1}{2} 1 \frac{1}{2}]$

$$(1 - \frac{1}{2}) = \frac{1}{2}$$

$$(\frac{1}{2} - 1) = -\frac{1}{2}$$

$$(\frac{1}{2} - \frac{1}{2}) = 0$$

Therefore, direction indices = $[\frac{1}{2} -\frac{1}{2} 0]$

Simplified, $[\bar{2}20]$

e) Sketch the following planes in a cubic unit cell:

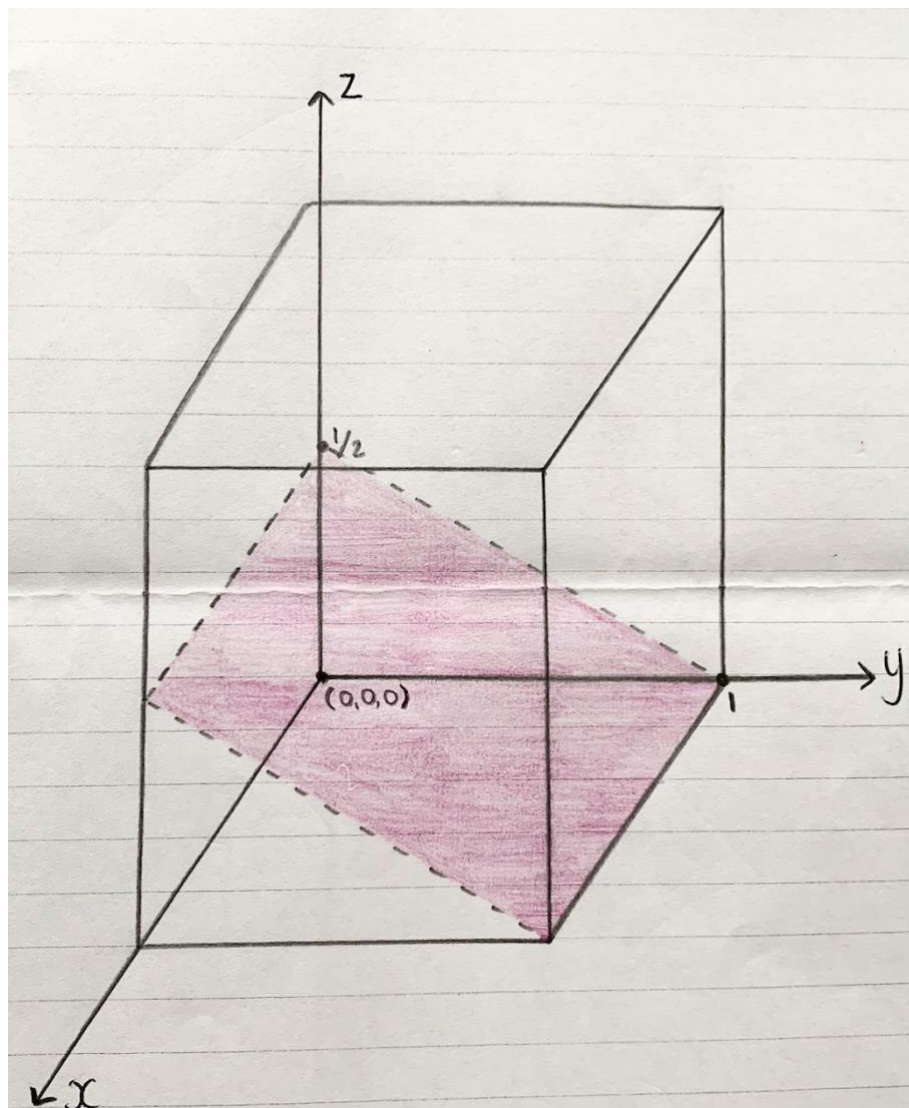
i) $[012]$

xyz $[012]$

Reciprocal value $[\infty 1 \frac{1}{2}]$

Therefore, the y axis is intercepted at 1 and the z axis is intercepted at a $\frac{1}{2}$

Note, the number of values for the x intercept are infinite.

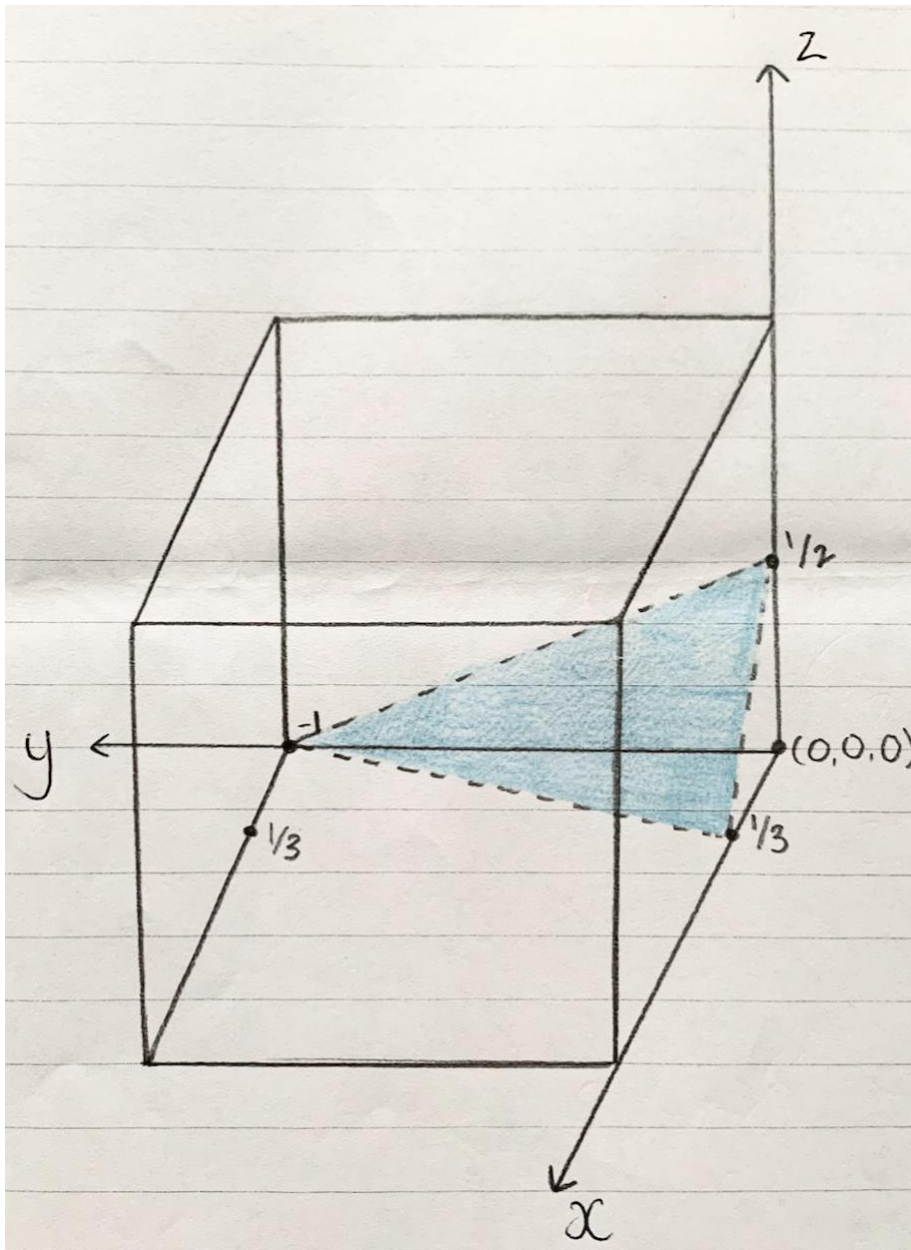


ii) $[3\bar{1}2]$

xyz $[3\bar{1}2]$

Reciprocal value $[\frac{1}{3} \bar{1} \frac{1}{2}]$

Therefore, the x axis is intercepted at $\frac{1}{3}$, the y axis is intercepted at -1 and the z axis is intercepted at a $\frac{1}{2}$

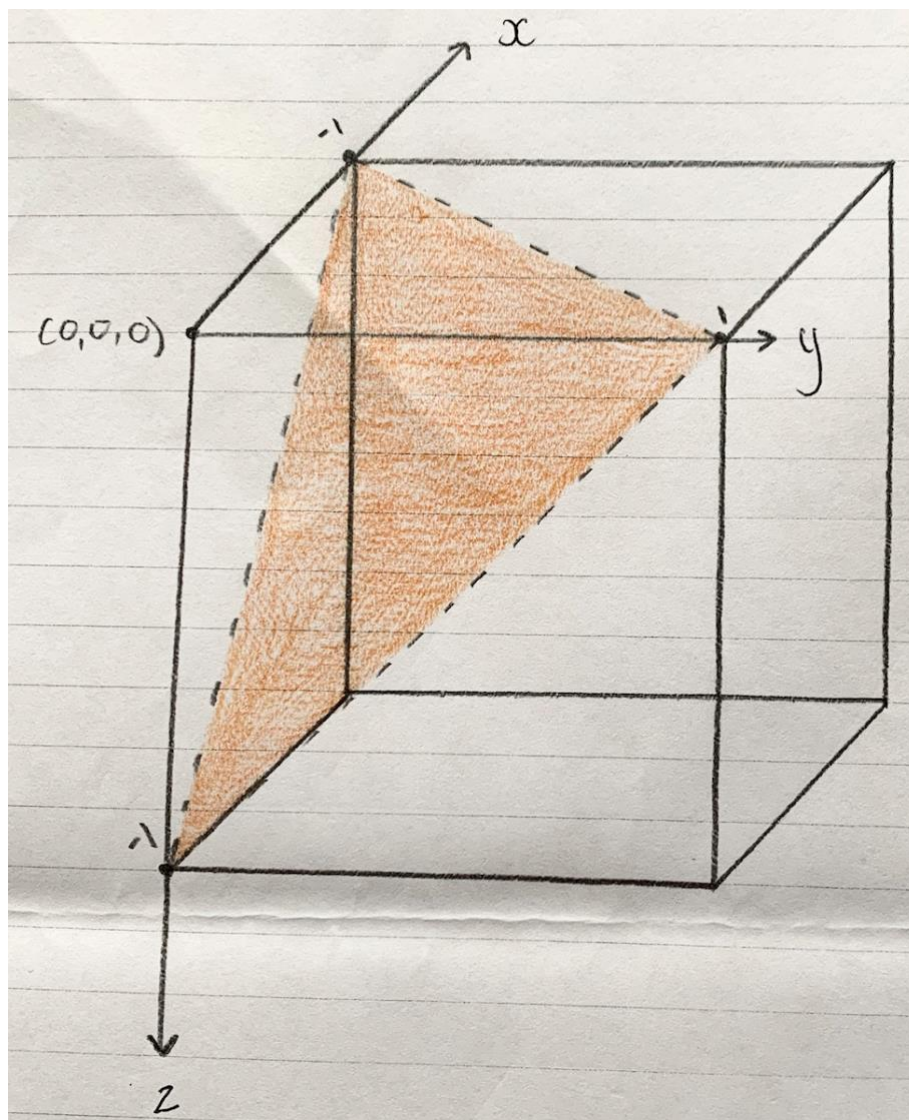


iii) $[\bar{1}\bar{1}\bar{1}]$

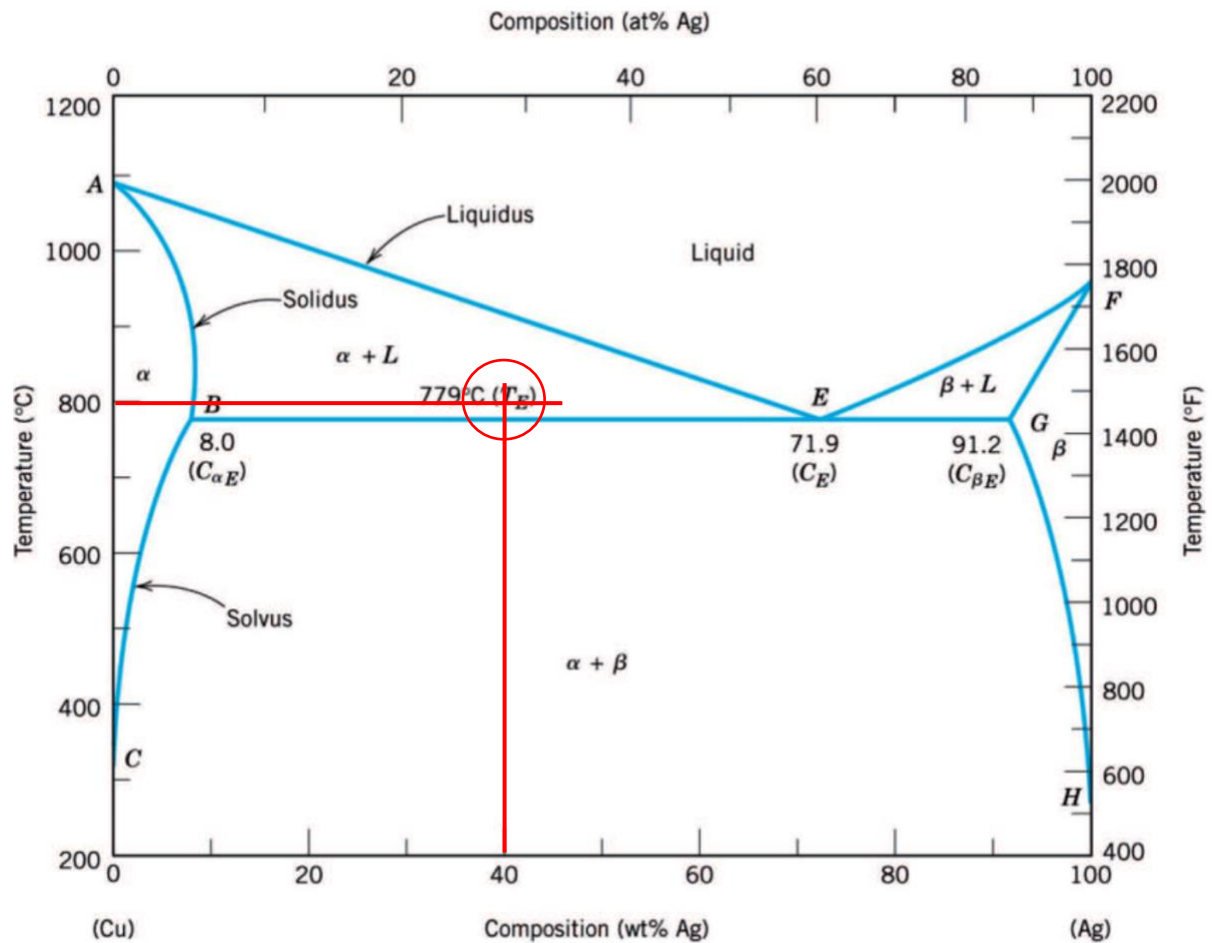
xyz $[\bar{1}\bar{1}\bar{1}]$

Reciprocal value $[\bar{1}\ \bar{1}\ \bar{1}]$

Therefore, the x axis is intercepted at -1, the y axis is intercepted at 1 and the z axis is intercepted at a -1.



Question 2

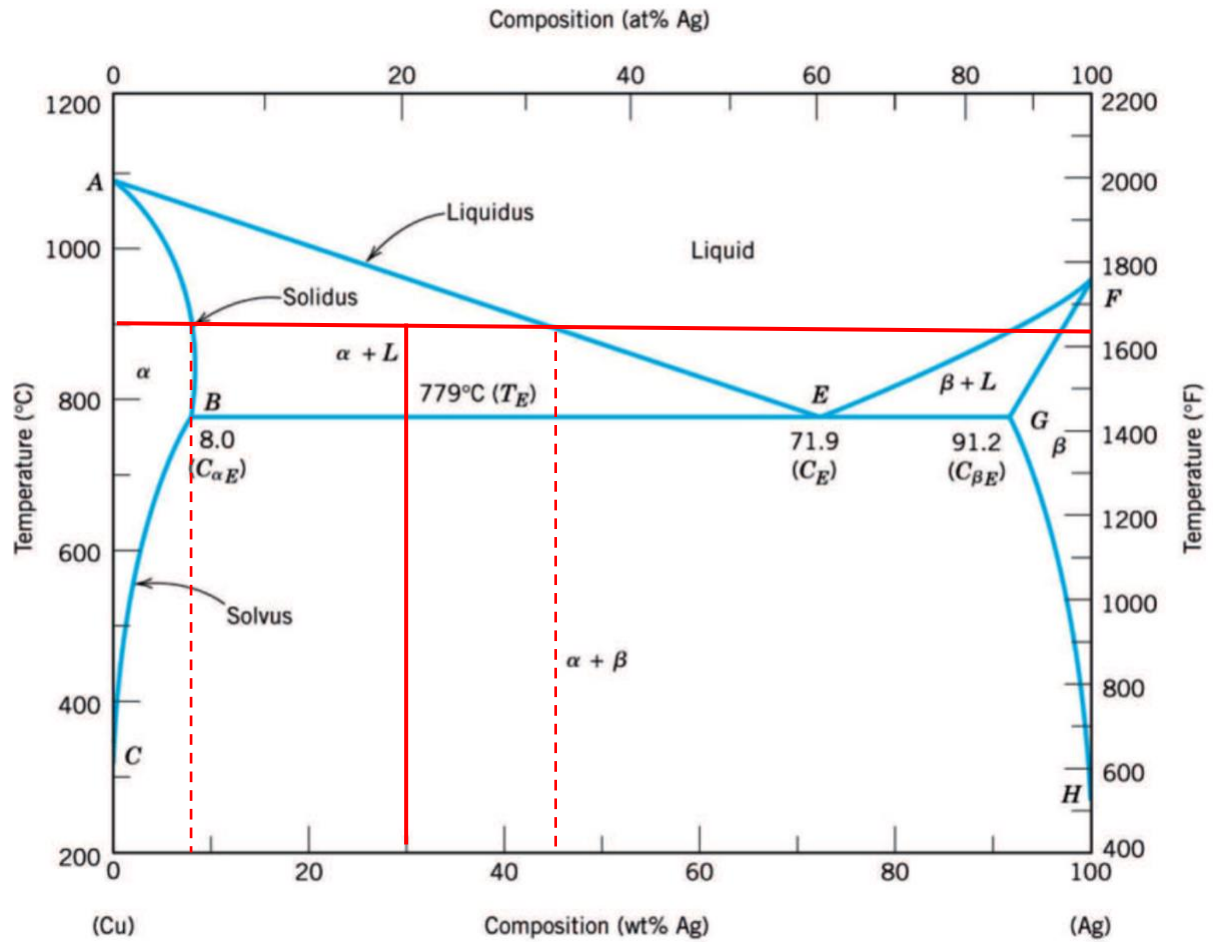


In the copper silver phase diagram shown above:

- a) What phases are present in an alloy of composition 40wt% Ag 60wt% Cu at a temperature of 800°C?

Alpha and Liquidus phase ($\alpha + L$ phase shown in diagram).

- b) Calculate the compositions in wt% Ag and Cu for both the α and liquid phases at a temperature of 900°C and a composition of 30wt%Ag 70wt%Cu.



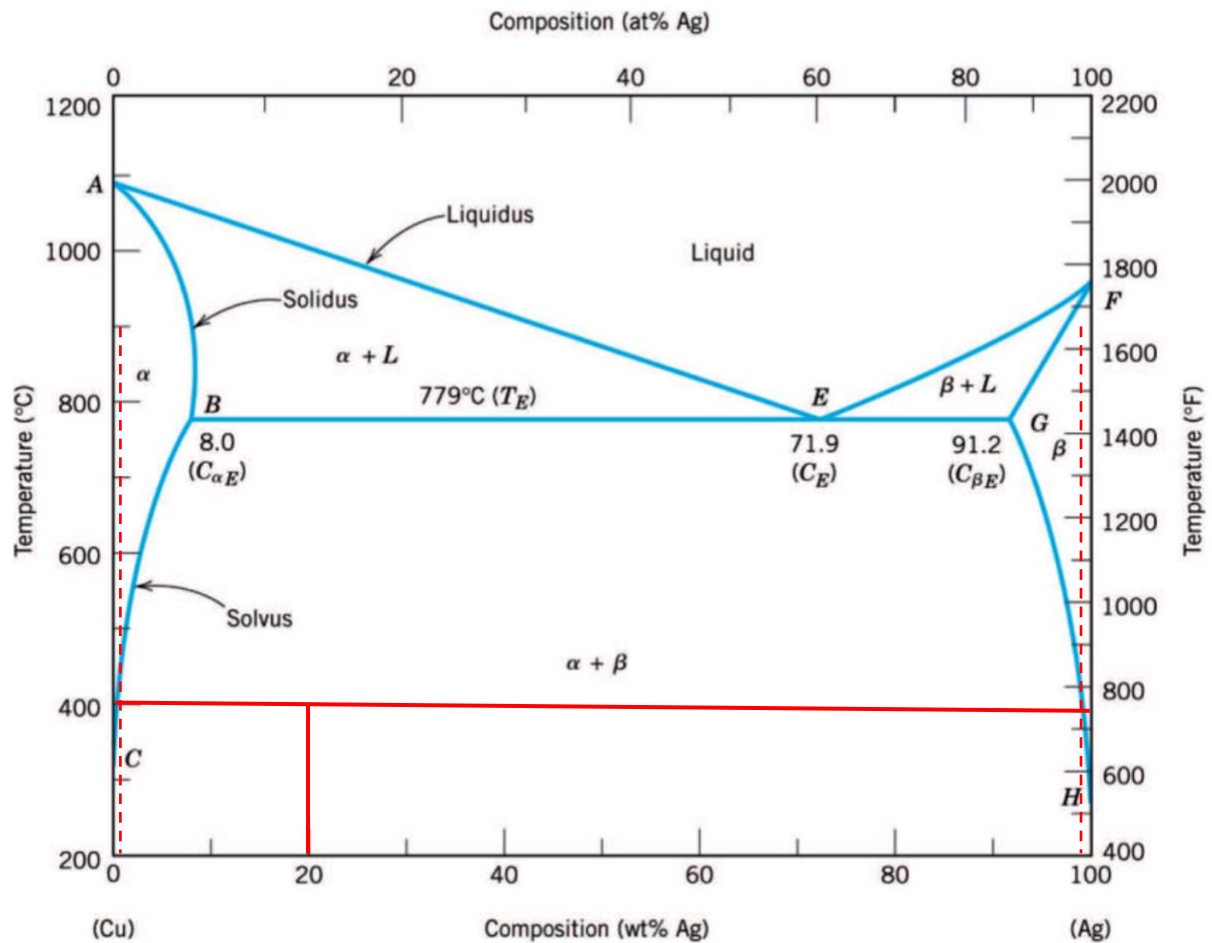
C=30
C1=8
C2=45

$$\frac{C2 - C}{C2 - C1}$$

$$\frac{45 - 30}{45 - 8} = 0.41$$

Composition = 41%

- c) Calculate the fraction phase amount of both α and β for an alloy of composition 20wt% Ag80wt% Cu at a temperature of 400°C?



C=20
C1=1
C2=98

Phase fraction for α is

$$\frac{C_2 - C}{C_2 - C_1} \frac{98 - 20}{98 - 1} = 0.804$$

Phase fraction for β is

$$\frac{C - C_1}{C_2 - C_1} \frac{20 - 1}{98 - 1} = 0.196$$

(Note, there is less than 1% of other phases present at this temperature).

Question 3

a) Explain the differences between Schottky and Frenkel defects in ceramics.

A Schottky defect is where one cation and one anion are removed from the crystalline structure, the ratio of cation vacancies and anion vacancies must remain the same to ensure charge neutrality within the crystal.

Alternatively, a Frankel defect is where an ion from another sub lattice moves to a different location within the lattice, leaving behind a vacancy. The number of ions will remain the same.

Schottky Defects	Frankel Defects
Decreases the density of the crystal.	The density of the crystal does not change.
Ions are removed from the lattice structure.	Ions are relocated within the lattice structure (at the interstitial site).
Usually occurs when ions are similar sizes.	Usually occurs when cations and anions are very different in size.
Cations and anions are removed in pairs.	Single ions can move from their initial occupancy.
Electrical charge remains the same.	Overall electrical neutrality remains the same however the dielectric constant somewhat alters.

b) For Schottky defects, calculate the number of cation-vacancy/cation interstitial defect pairs given that the Boltzmann's constant, $k = 8.62 \times 10^{-5} \text{ eV/K}$.
 The temperature, $T = 500^\circ\text{C}$.
 The energy required for the formation of each Schottky defect, $Q_u = 2.6 \text{ eV}$.
 The number of lattice sites, $N = 1.58 \times 10^{28} \text{ lattice sites/m}^3$.

$$Nv = N \exp\left(\frac{-Q_u}{kT}\right)$$

$$Q_u = 2.6 \text{ eV}$$

$$k = 8.62 \times 10^{-5} \text{ eV/K}$$

$$T = 500^\circ\text{C}, \text{ also } 773 \text{ K}$$

$$N = 1.58 \times 10^{28} \text{ lattice sites/m}^3$$

$$Nv = (1.58 \times 10^{28}) \exp\left(\frac{-2.6}{(8.62 \times 10^{-5})(773)}\right)$$

$$Nv = 5.32 \times 10^{19} \text{ vacancies/m}^3$$

Question 4

Car bodies are usually made of steel.

i) Using your knowledge of material properties, analyse the properties of steel and give 5 bullet points on why you think steel is a suitable material for this use.

- Steel has a high strength to weight ratio, meaning it is robust and safe with crash resistant structures without compromising on fuel economy and keeping emissions to a minimum.
- Steel is extremely malleable, so is easily made into specific intricate shapes dependant on the customers' needs. This property is also advantageous to the car manufacturers as steels are easily formed into desirable parts making further processing easy and cost effective.
- Steel is relatively cheap to produce and to purchase making it far more cost effective than other potential metals. The raw materials are abundant and easily obtainable, this not only keeps cost down but also means steel can be made in very large quantities.
- Steel can be endlessly recycled; scrap steel can be remanufactured into high quality steels for use over and over again.
- As long as steel is properly rolled, then coatings or paint can be added to allow variations in the final product, this is desirable in automotive products for aesthetic purposes.

ii) If you had to redesign a car body to make it lighter, predict 5 factors you would need to consider?

- The safety of the vehicle would need to be considered as priority, a lighter car body cannot compromise the integrity and durability of the material. The material must be strong and safe when in a collision, meaning the strength to weight ratio would need to be higher.
- Lightweight materials introduce more noise and vibration, and although these can be countered through additional materials added, said additions will counter any weight loss and increase the weight of the body. It must be considered whether issues introduced by weight loss of the body compromise vehicle functionality.
- Lighter materials that are as strong, safe and useable are often a lot more expensive and complex to manufacture, it must be considered whether the material can be produced in large quantities and is it cost efficient?
- It would need to be considered how increasing strength affects ductility; the material must be formable for manufacturing purposes.

- The life expectancy of the vehicle needs to be considered, corrosion is a risk for any car body part and lighter metals can corrode quicker and weaken over time. A potential coating may be added to lighter weight material to avoid this.