

Chemmat 121

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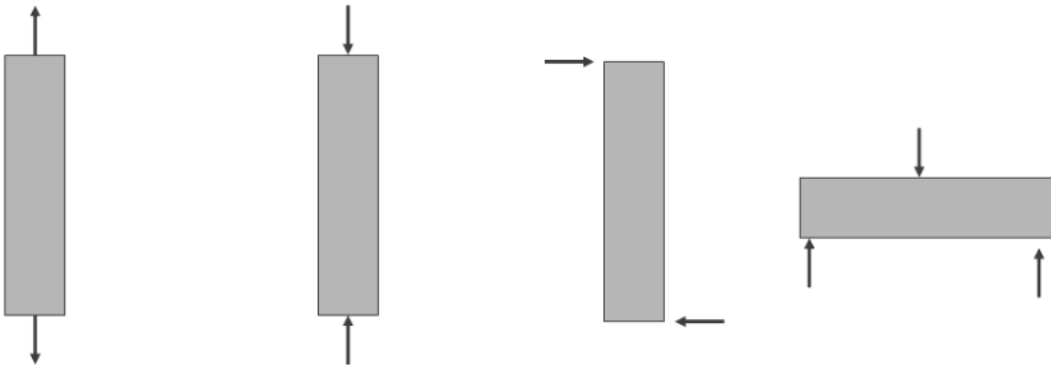
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1 Deformation and structure of solids

1.1 Strength

How much force can a material withstand before it fails? That's a materials strength. A material can fail in several ways but the two most common are fracturing and permanent deformation.



Some types of force that a material/object can undergo
From left: Tension, Compression, Shear and a Combination.

1.2 Stress

Engineers typically talk about stress instead of forces because stress is just a force proportional to its area. Stress is represented by the greek letter sigma (σ) and is given by the force (F) divided by the cross-sectional area (A).

$$\sigma = \frac{F}{A}$$

Cross-sectional area is the area that is perpendicular to the applied force

Example

Given: $m = 25 \text{ kg}$, $d = 10 \text{ mm}$

$$A = \pi r^2$$

$$A = \pi \times \frac{(0.01)^2}{2}$$

$$F = 25 \times 9.81$$

$$\sigma = \frac{F}{A}$$

$$\sigma = 3,120,000 \text{ Pa}$$

$$\sigma = 3.12 \text{ MPa}$$



1.3 Strain

Strain is how long something gets compared to its original size. Stress and strain are related very closely and the stress against strain graph is a very important thing to materials engineering. Strain is given by the change in length over the original length.

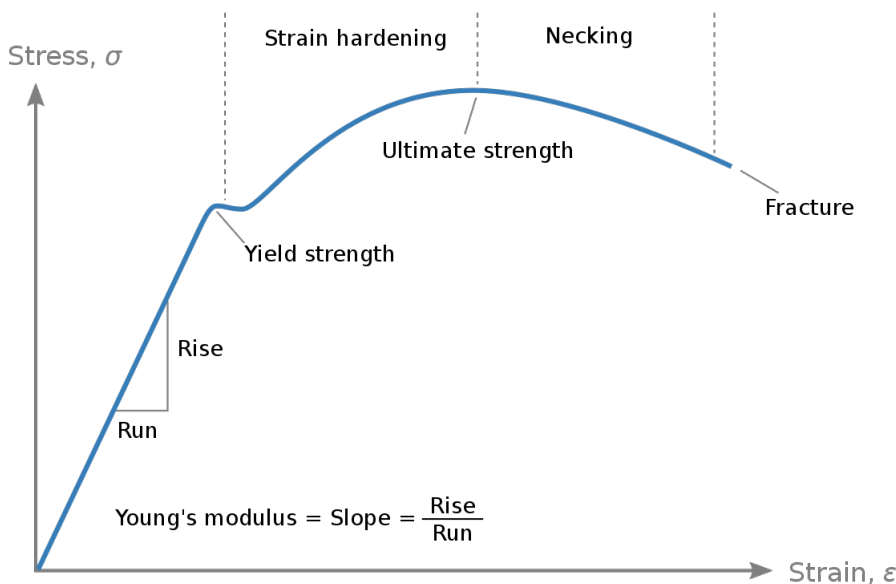
$$\epsilon = \frac{\Delta L}{L_o}$$

Strain is unitless but is commonly expressed as a percentage (%).

Example

$$\begin{aligned}\epsilon &= \frac{\Delta L}{L_o} \\ &= \frac{100.32 \text{ mm} - 100 \text{ mm}}{100 \text{ mm}} \\ &= \frac{0.32 \text{ mm}}{100 \text{ mm}} \\ &= 0.0032 \\ &= 0.32\%\end{aligned}$$

1.4 Stress-Strain Curve



The area under the curve is $F \times d$ and gives the 'toughness' which is approximately the energy required.

Necking is a localised reduction in thickness, which reduces diameter, which reduces area, increasing stress. This causes it to fail.

1.5 Poisson's Ratio

Poisson's ratio is the relationship between deformation for a given material. It is a measure of the Poisson effect, that describes the expansion or contraction of a material in directions perpendicular to the direction of loading. It has no units and is represented by the greek character 'nu' (ν). For most materials $\nu \approx 0.3$.

$$\nu = \frac{-\epsilon_x}{\epsilon_z}$$

1.6 Young's Modulus

The Young's Modulus of a material is a measure of the 'stiffness'. It is the gradient of the elastic part of the stress-strain curve for a given material. It has units of Pascals (Pa) and is represented by the capital letter E.

$$E = \frac{\Delta\sigma}{\Delta\epsilon}$$

1.7 Steel

Steel has what is called a 'discontinuous yield'. This means at the yield strength there is a bit of 'noise' and it moves a little randomly before becoming nonlinear.

1.8 0.2% Proof Stress

The 0.2% Proof Stress of a material is a geometrical construct that is used when the yield stress of a material cannot be properly determined. It is a very slight overestimate (generally) that can be calculated by drawing a line parallel to the actual curve at a strain of 0.002 and finding the intersection with the original curve. This stress value is the approximation.

1.9 Safety Factor

The safety factor is a scalar value that demonstrates how much more stress a material can hold relative to the requirement. I.e. if, for example, $F \approx 1000\text{ N}$ the engineers might pretend $F = 2000\text{ N}$. This would give a safety factor of 2. When the conditions of the material are more uncertain, you would want a higher safety factor.

1.10 Engineering Stress vs Real Stress

In engineering, we draw a stress-strain graph as going 'down' after the ultimate tensile strength. In reality, because of the effect of necking, it goes up after this. As engineers, we use the model because it is easier to handle theoretically.

1.11 Ductility

Ductility is a measure of how much something can deform elastically (with 100% recovery / without permanent deformation). The stress-strain graph of a ductile material will have a longer elastic section while a more brittle material (less ductile) will have a shorter one. It is generally described by one of two equations:

Percentage Elongation

$$= \frac{\Delta L}{L_o} \times 100\%$$

Percentage Reduction in Area

$$= \frac{\Delta A}{A_o} \times 100\%$$

2 Microstructure and mechanical properties

2.1 Crystal Structure

If a material is crystalline, the atoms of a material have **LONG RANGE ORDER**. This means the material is made up of a crystal lattice made of repeating units called 'unit cells'.

There are 14 possible crystal arrangements but this course will only look at three. We describe arrangements by looking at the unit cell. The unit cell is a tessellating shape that has all the information to describe the entire lattice.

The unit cell has 4 important properties:

- Number of atoms
- Co-ordination Number (The number of neighbours for the unit cell)
- Unit Cell Dimension (The length of each side of the cell written 'a')
- Atomic Packing Factor (Amount of space taken up by the atoms)

$$a = \text{Atomic Packing Factor} = \frac{\text{volume of atoms}}{\text{volume of unit cell}}$$

2.1.1 Body Centered Cubic

Body Centered Cubic (BCC) has one atom at each corner of a cube and one right in the middle.



- Number of Atoms = $2 = 1 + 8 \times \frac{1}{8}$
- Co-ordination Number = 8
- Unit cell dimension = $\frac{4R}{\sqrt{3}}$
- APF = 0.68 = 68%

2.1.2 Face Centered Cubic

Face Centered Cubic (FCC) has one atom at each corner of a cube and one in the middle of each face of the cube.

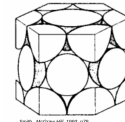


Callister, CP Edition, Wiley & Sons, 2002, p.87

- Number of Atoms = 4
- Co-ordination Number = 12
- unit cell dimension = $\frac{4R}{\sqrt{2}}$
- APF = 0.74 = 74%

2.1.3 Hexagonal Close Packed

Hexagonal Close Packed (HCP) is a prism shape with hexagonal arrangements of atoms layered up.



Smith, McGraw-Hill, 1959, p.79

- Number of Atoms = 6
- Co-ordination Number = 12
- APF = 0.74 = 74%

2.2 Density

Density is the degree of compactness of a substance. The amount of mass you get for a given volume. The density of a material is its mass divided by its volume.

$$\rho = \frac{n \cdot A}{V_c \cdot N_a}$$

Where n is the number of atoms per unit cell, A is the atomic mass of the material, V_c is the volume of the unit cell (a^3) and N_a is Avogadro's Number.

Example

Iron

$$\begin{aligned} a &= 0.286 \text{ nm}, n = 2 \\ \rho &= \frac{2 \times 55.85}{(2.86 \times 10^{-8})^3 \times 6.023 \times 10^{23}} \\ \rho &= 7.92 \text{ g.cm}^{-3} \end{aligned}$$

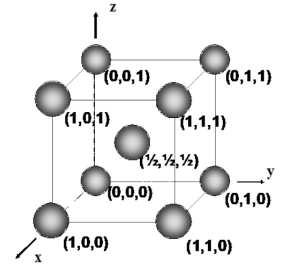
The real density of iron is 7.87 g.cm^{-3} so this is a good estimate.

2.3 Polymorphism

Materials that can exist in more than one crystal form (can have lattices made up of different unit cells) are called polymorphic. For example, Iron at room temperature has a BCC structure but at 912°C it has an FCC structure.

2.4 Planes, Directions and Positions

Navigation around our crystal structures is based on a typical x,y,z orthogonal axis. We can denote the position of an atom using a typical three dimensional vector. By convention, positions are denoted with round brackets.



2.4.1 Directions

Directions in the lattice are defined with square brackets $[u, v, w]$.

1. Draw a vector from the origin for the direction
2. Project the length of the vector onto the unit cell axes
3. Put this in terms of the coefficients
4. Convert to integers (multiply by a constant)
5. Put in square brackets

Example

Projecting the length of the vector onto axes: $1a \ 0b \ \frac{1}{2}c$

Put this in terms of co-efficients: $1 \ 0 \ \frac{1}{2}$

Convert to integers (multiply by two): $2 \ 0 \ 1$

Put in square brackets: $[201]$

Note: Negative directions will have a bar over them (read ‘bar’).

$$[1\bar{1}0]$$

2.4.2 Planes

Planes in the lattice are defined by **Miller Indices** (h, k, l) .

1. Work out the intercepts of the plane on the unit cell
2. Take reciprocals of the intercepts
3. Convert to integers (multiply by a constant)
4. Put in round brackets

Example

Intercepts: $1 \ -1 \ \infty$

Reciprocals: $1 \ -1 \ 0$

Integers: $1 \ -1 \ 0$

Round Brackets: $(1\bar{1}0)$

2.4.3 Families

You can denote the ‘family’ of a plane (all of the planes made up with these values). Families of planes are denoted with curly brackets e.g. Cube Faces $\{100\}$. Families of directions are denoted with angle brackets e.g. $\langle 100 \rangle$.

2.5 Slip, Theoretical Strength and Defects

Recall that there are two types of deformation: Elastic and Plastic (In-elastic). Elastic Deformation springs back (recovers), Plastic Deformation does not. At the atomic level, Elastic Deformation is merely stretching the atomic bonds. Any further deformation is permanent (plastic, past the yield point) and results from a process called **slip**. In plastic deformation, atomic bonds are broken (and remade).

2.5.1 Theoretical Strength

We can calculate the *theoretical* strength of a material by evaluating the amount of energy needed to break and remake the atomic bonds. This is not a very good approximation. For example, the theoretical shear strength of pure iron is 10,000MPa but the measured shear strength of pure iron is 20MPa... Why is this? Imperfections.

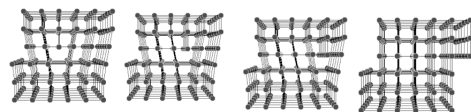
2.6 Imperfections

There are a number of different imperfections that DO happen within a lattice containing millions of atoms. This is what causes our theoretical strength and theoretical density to be off. It is EXTREMELY difficult to get 'pure' anything so this is true for any sample.

- Point Defects
 - Vacancy
 - Substitution
 - Interstitial Atom
- Planar Defects (Dislocations, \perp)
 - Edge Dislocation
 - Screw Dislocation

A vacancy is simply a missing atom in the lattice. A substitution is when a different atom is in the place of the atom that should be there. Interstitial atoms are atoms that occupy a normally unoccupied site in a crystal lattice.

2.7 Slip



Explaining how Slip works is a common exam question. Draw these!

The model of slip we will use is the movement of dislocations. The movement of dislocations means that slip can occur more easily than in a perfect arrangement of atoms. Easy slip means that a material is easily plastic deformed, this means it is *ductile*.

2.7.1 Slip Systems

Slip (dislocation movement) occurs most easily on closepack planes and in closepacked directions. Not all systems have closepacked planes so slip happens on the *closest* packed plane

A slip system is a combination of planes and directions. For FCC, the closepacked planes are $\{111\}$ ¹. The closepacked directions on these planes are $\langle 110 \rangle$ ².

¹ A family of planes

² A family of directions

Hence, the main slip system for FCC is: $\{111\} \langle 110 \rangle$

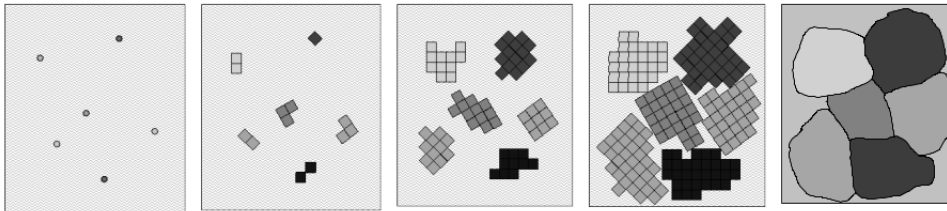
The main slip system for BCC is: $\{110\} \langle 111 \rangle$

HCP structures have closepacked planes but they are all parallel. Slip is very difficult so HCP metals are often brittle.

2.8 Microstructure

Engineering components are very rarely single crystals, this means they are polycrystalline (many crystals). Most metals have at some point been molten and as they solidify they form many crystals.

Solidification:



The name for the individual pieces is nucleus. If they have lost enough energy (cooling down) they might form nuclei when they bump together. This happens in the 2nd panel, you can call them "Baby Crystals".

The separate sections are 'perfect crystals' (but they still contain defects) and in the 4th panel they are **equiaxed**. This means they are roughly equal in each axis and of the same size (roughly spherical/of the same size). Each one of these crystals is called a 'grain'. We can then talk about **Grain Structures** within a metal and **Grain Boundaries**.

When one grain meets another, the atoms are not perfectly aligned. This means there is a little extra energy due to the atomic bonds being incomplete or out-of-equilibrium. This makes the grain boundary a 'high energy region'.

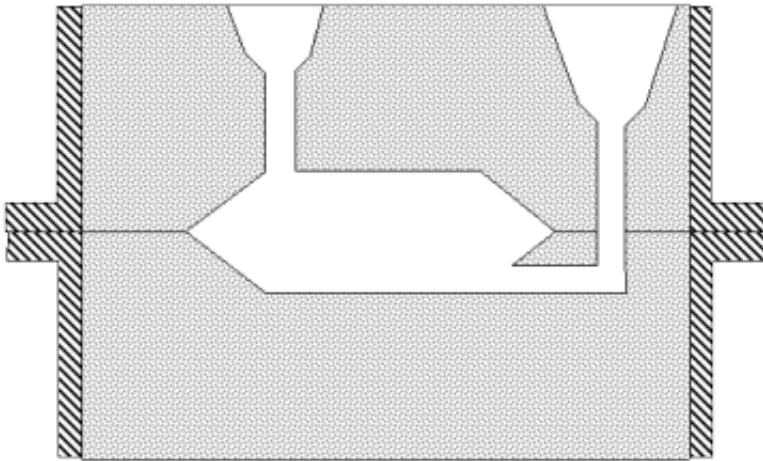
2.8.1 Nucleation

When the grains form from a molten state it is called **nucleation**. This can occur on another solid material or in solution. It is quite rare to occur in solution on its own but it is called **Homogeneous Nucleation**. When it forms on a surface e.g. the side of a mould it is called **Heterogeneous Nucleation**.

2.9 Casting

2.9.1 Sand Casting

Sand Casting is an ancient method of casting. You use something (foam etc) to make a hole in the sand and then fill your 'runner' (input) with molten metal until it burns away all the filler. This will then set in the sand you can take off the 'cope' or 'drag' (bottom or top) and access your new sword or cannon or frypan!



2.9.2 Die Casting

Die casting is a much more expensive modern method of casting. In die casting, a permanent mould is created using machining tools out of another metal. These moulds can be hundreds of thousands of dollars. All forms of casting are prone to porosity however, weakening the part.

2.10 Grain Structure Development

Grains will mostly nucleate on the sides (walls) of the mould. The first grains you will get are equiaxed grains. Columnar grains will form in 'columns' and stretch across the mould, possibly touching the grains on the other side. Sometimes columnar grains will form branches, these are called dendrite formations.

Frost will also form dendrites when it goes from gas to solid.

2.11 Metallography

Metallography is the study of the structure of metals. We use a reflective-light microscope (instead of a transmission microscope) because the metal is far too opaque to use a transmission scope. Before we can use a microscope however you must prepare the surface. This is to make the rough, cut surface smooth and reflective.

To allow us to see the grain boundaries, we ‘etch’ the metal with an acid or alkali that selectively ‘attacks’ the boundaries. This means the boundaries will scatter light instead of reflecting it so they appear dark under the microscope.

The general preparation process is

1. Grinding
2. Polishing (using finer and finer abrasives)
3. Etching
4. Cleaning (with hair-dryer, water, etc)

Some of the grains appear darker because they are also attacked by etching

2.12 Grain Boundaries and dislocation movement

More grains strengthen the metal because the grain boundaries stop dislocation movement (slip). There is hence a relationship between the grain diameter and yield stress. This relationship is described by the *Hall-Petch Equation*.

$$\sigma_y = \sigma_o + kd^{-\frac{1}{2}}$$

From high school maths, you can see that this equation is linear (of the form $y = mx + c$). On the graph $d^{-\frac{1}{2}}$ is (typically) on the x-axis so grain size is decreasing as you move right.

2.13 Grain deformation

Plastically deforming grains results in work hardening. People do this using rollers and it is called ‘rolling’. Rolling gives a rolling texture (grains are stretched out/thinner).

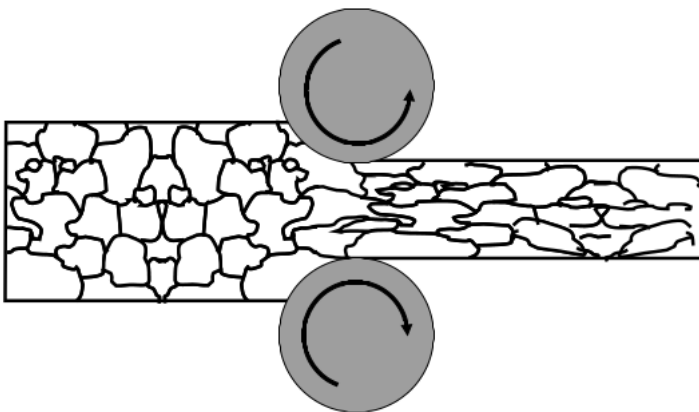


Figure 1. Rolling (note the thinner grains)

2.14 Work Hardening

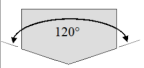


As seen previously, work hardening occurs when a material is plastically deformed and released before it inevitably fractures. Plastic deformation introduce many new dislocations. Dislocations stop dislocations moving (and create new dislocations when moving). The more dislocations there are, the harder it will be for them to move. This is, very scientifically, called a ‘traffic jam’ and is what causes the strengthening due to work hardening.

Cold work is a name for the process of work hardening without heat i.e. rolling. This causes a reduction in area as the material is because it is lengthening. Percentage cold work is hence the change in area over the original area.

$$\frac{\Delta A}{A} \times 100$$

2.15 Hardness

Hardness is a resistance to a localised deformation. Hardness can be measured in many different ways, one popular one is the Rockwell Hardness Scales. Geologists use Moh’s which is basically "rate my rock 1-10" where 10 is diamond and 1 is Talc.

Rockwell Hardness Scales		
	Load	Scale
	60kg	R_A
	100kg	R_D
	150kg	R_C
	Load	Scale
	60kg	R_F
	100kg	R_B
	150kg	R_G
	Load	Scale
	100kg	R_H

The scales go from R_a to R_e , where the different scales measure different levels of hardness. Hardness has no units but you must state the scale you used i.e. $60R_c$

You can test hardness with an indenter. Where you make a plastic deformation with a known force behind it.

2.16 Electrical Properties of Metals

Electrical properties depend on atomic and crystal structures just as much as mechanical ones. Resistivity depends on resistance (R), area (A) and length (L). Resistance changes with temperature and so there is a second equation that has ρ_0 (the resistivity at room temperature), α (thermal co-efficient, given for each material) and T (temperature).

$$\rho = \frac{RA}{L}$$

$$\rho_{\text{temp}} = \rho_0(1 + \alpha T)$$

Remember that resistivity will increase with cold work. This is because conduction in metals is due to electron drift and the velocity of that drift. Because work hardening causes increased dislocation density, electron movement is impeded.

Conductivity can be expressed as the product of n (the number of electrons), $|e|$ (the size of the charge on an electron) and μ which is the ‘mobility of electrons’.

$$\sigma = n \times |e| \times \mu$$

2.17 Annealing

Annealing is a heat treatment that allows you to recover the ductility of a material (while sacrificing yield strength). Annealing has three stages: Recovery, Recrystallisation and Grain Growth. We will discuss each.

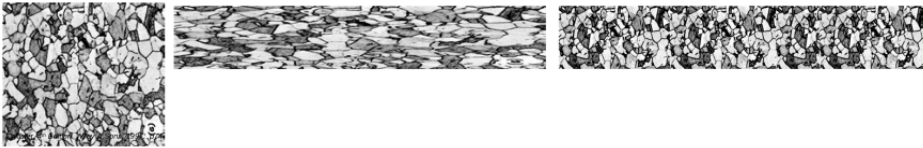


Figure 2. From left to right: untreated, rolled, rolled and annealed

2.17.1 Recovery

In this stage, the material recovers from the work-hardening. The dislocation density does not change but rearranges to a lower energy configuration.

2.17.2 Recrystallisation

In the second stage, the metal is strain free. New ‘baby grains’ nucleate at the grain boundaries. The driving force is the stored strain in the dislocations. These new grains expand until they are equiaxed with low dislocation density. Total recrystallisation occurs when just fully equiaxed.

2.17.3 Grain Growth

You can leave them to continue to grow for maximum ductility but this step is optional. You can choose to make the metal more ductile with larger grains or leave it to be stronger.

2.18 Recrystallisation Temperature

The rate of recrystallisation is proportional to temperature. There exists a ‘recrystallisation temperature’ at which: a 50% cold worked metal will just

fully recrystallise in one hour. Cold work less than 50% will take longer. CW=50% but lower temp will take longer. Some examples are:

Metal	Melting temperature ($^{\circ}\text{C}$)	Recrystallisation temperature ($^{\circ}\text{C}$)
Lead	327	-4
Aluminium	660	80
Copper	1085	120
Iron	1538	370

2.18.1 Hot Work

Hot work (i.e. forging) is work done to a metal above the recrystallisation temperature. At this point, plastic deformation and recrystallisation happen at the same time. This means it won't be work hardened or it will be but it will be done at the same time.

2.18.2 Diffusivity

Diffusion is the movement of atoms through the lattice. Lattice atoms (or substitutes) move via vacancy diffusion. Interstitials 'jump' positions by interstitial diffusion.

Diffusivity is a measure of how easily atoms can move. Diffusivity (D) behaves according to the Arrhenius equation (just like recrystallisation).

$$D = D_0 e^{\frac{-Q}{RT}}$$

3 Phase diagrams and Alloying

3.1 Phases

A phase is a component within a system that has uniform physical characteristics. In high school (and before) you were introduced to the typical Gas, Liquid and Solid (and maybe Plasma and Bose-Einstein Condensate).

3.2 Solid Solutions

There are two types of solid solution (in this course). Interstitial Solid Solutions and Substitutional solid solutions. These two types have a number of different properties:

Interstitial Solid Solutions

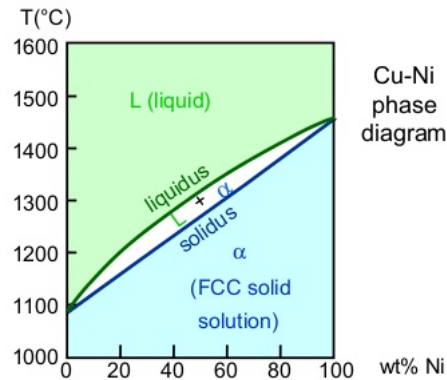
1. Solute atom must be small (relative to solvent atom)
2. Always have a solubility limit (limited interstitial spots)

Substitutional Solid Solutions

1. Similar Atomic Radius
2. Similar Crystal Structure (HCP, FCC etc.)
3. No Solid Solubility limit for some metals

3.3 Binary Isomorphous Phase Diagram

This is a two metal (binary) single shape (i.e. FCC, isomorphous) phase diagram. Here you can see the graph of temperature against weight percent Ni for a Cu solution. Clearly, when α is 100% copper it melts at the melting point of copper, 1085°C but when α is 100% nickel, it melts at the melting point of nickel 1453°C . For any other composition, α will melt at a range of temperatures. This is what we are graphing in a phase diagram.



3.4 The Lever Rule

The lever rule lets you calculate percentage makeups of the alloys and their phases. To calculate the percentage of each phase at a given temperature:

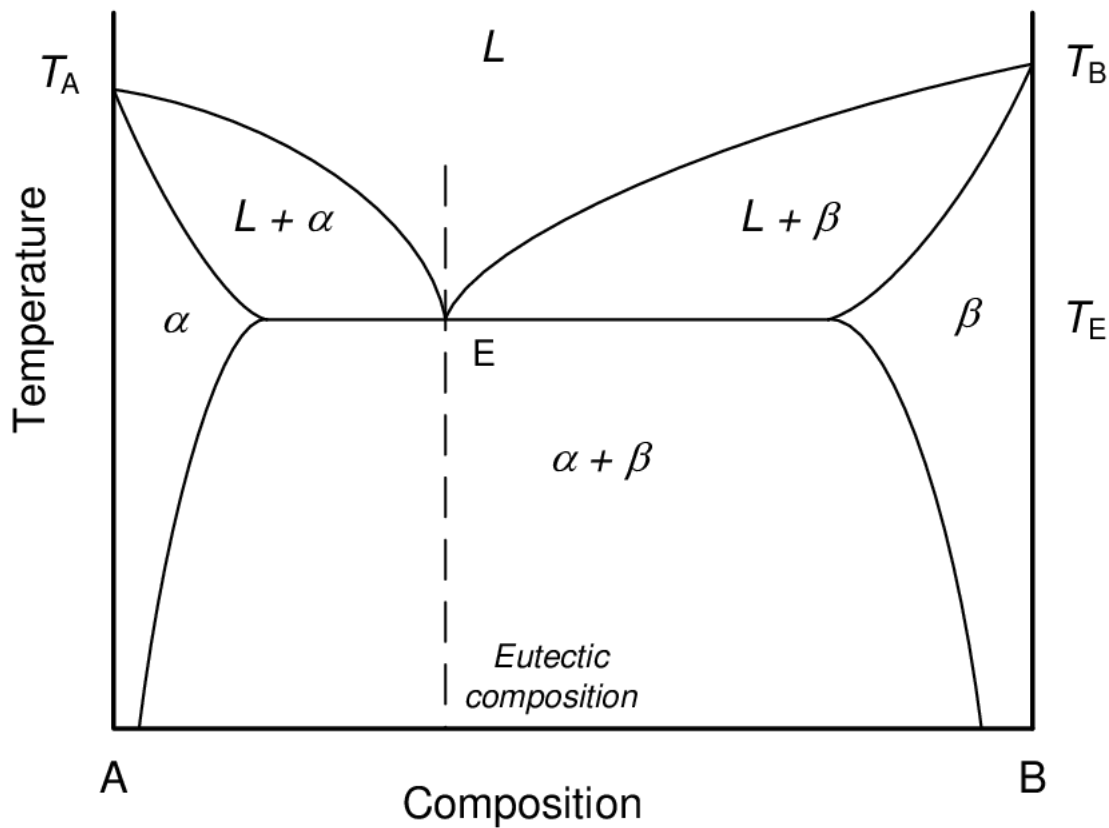
1. Place Pivot (always at the overall alloy composition)
2. Draw the tie-line
3. Draw on the phase symbols (opposite)
4. Calculate Lengths

3.4.1 What are the compositions of each phase?

To calculate the amount of each alloy in each phase, look at where the tie-line intersects with the solidus, that will be the percentage amount of Ni (or whatever is on the x axis). You can then calculate the amount of the other metal by subtracting from 100.

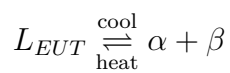
The intersection with the liquidus will give you the percentage of Ni in the liquid state and so on. This is a useful tool for all phase diagrams but is especially easy to use in this case.

3.5 Binary Eutectic Phase Diagram



3.5.1 The Eutectic Point

The Eutectic Point is a point at which the alloy has its own freezing or melting point. This is clearly seen on the graph where the two lines meet with the α and β section. The Eutectic reaction is when a liquid phase transforms into two solid phases ($\alpha + \beta$)



3.5.2 Microstructure Development

The microstructure of metals formed will vary greatly but noticeably will form equiaxed grains of one element with grains of the other at the boundaries or layers of each metal.

- 4 Strengthening mechanisms**
- 5 Engineering ceramics and glasses**
- 6 Polymers**
- 7 Failure of materials**
- 8 Corrosion of metals**
- 9 Engineering composites**