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MECH0007 Topic Notes
UCL

Hasha Dar

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Contents

Chapter 1

Course Outline

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1.1 Coursework and exam

- Metallography and Microstructure - Lab week (week 26), held in Materials Lab Sub Basement Roberts.
- Manufacturing Case Study - Friday afternoon consultancy slots (14:30 onwards), Materials Lab Sub Basement Roberts.
- One three hour exam, consistent of two sections: MCQ (sort of?) and conventional. Timetabled revision slots in summer term.

Add notes about the following topics:

- Cracking - welding vs riveting, arrestment of cracks in a material.
- Casting and forging - in context of manufacturing processes, perocity of a liquid vs a solid.
- Crystalline and amorphous solids - materials which are one or the other, both or both in different capacities, look into molecular structure of each, crystallinity is a degree of structure which affects its properties.
- Plasticity and deformations in metals and other materials.

Structure - Property Relationship at the heart of all Material Science.

Manufacturing (Processing)	
Structure	Property

Categories of materials - these all have different structures and hence properties.

- Metals
- Ceramics
- Polymers
- Composites - a mix of the other three above (physical mix), provides an extra level of structure for scientists to work with.

Chapter 2

Properties of materials

2.1 Metals

2.1.1 General Properties

- High electrical conductivity - "thermal".
- Heavy and plastically deformable.
 - Plastic - permanent change in dimension.
- Shiny when polished.

All of these properties are a function of the atomic bonding ("metallic bond"). A metallic bond is traditionally thought to be a sea of delocalised electrons "orbiting" a *regular* array of ions. A regular array is known as a *crystal*. In this structure, we see repulsive and attractive forces from the atoms and subatomic particles. These are all balanced and thus in *equilibrium*. The interatomic distance can be defined as a_0 . The interatomic distance can be modelled as a spring. Initially a tensile (or a compressive) force will generate deformation and thus a_0 but will attempt to restore to its original shape; i.e. the deformation is recoverable. This is the definition of *elastic* behaviour.

Beyond a certain deflection/deformation, *permanent* deformation is achieved. When the deforming force is removed, only some of the deformation is recovered (the elastic portion) and the plastic deformation remains.

2.1.2 Mechanisms of plastic deformation in metals

Slip

This is where planes of atoms (ions) slip/slide past each other. Planes orientated at 45° to the tensile or compressive load will slip first. Slip (under tension) gener-

ates lengthening of the specimen. However, the *volume* of the specimen does not *change* i.e. the intermolecular distance stays the same. This means that under a tensile force, the specimen becomes *thinner*. Under compression, metals become *shorter/fatter*.

2.2 Polymers

2.2.1 Thermoplastics and Thermosets

General Properties

- Thermally and electrically poor conductors.
- Low density.
- Poor reflectors.
- Often flexible (low stiffness).
- Often deformable.
 - "Slip" is possible.
 - Behave plastically.

These properties (including the mechanical properties) are due to the *bonding* occurring in polymers. These bonds are *covalent* within a polymer molecule but the existence of secondary bonding (e.g. Van der Waals and H bonding) are very influential on the properties.

Polyethene (or PE) is a chain structure molecule made up of carbon and hydrogen atoms. This structure is *thermoplastic* or *thermopolymer*. Often these chains can be 100,000 carbon atoms long. The carbon-carbon bond is tetrahedral in reality. If such a polymer was to be stretched out linearly, its length would be approximately 20 μm . Each molecule is *stable* i.e. all the covalent bonds are satisfied but there must be interaction between molecules; else PE would have no physical strength. Hence, intermolecular bonding *must* be present. There will be a degree of mechanical interaction with such "massive" molecules but secondary bonds (dipole interactions) dominate.

Not all polymers have this structure e.g. *thermosets*. Epoxy resin such as urea-formaldehyde are thermosetting. The molecular structure of thermosets are similar to thermoplastics. However, there are *real* covalent bonds between the chains instead of secondary bonding. These are called *crosslinks*. Crosslinks are created through chemical reaction during the *polymerisation* process. This creates a new substance and have no chemical formula. Thermoplastics are polymerised at the factory. Thermosets are sold as two products (*pre-polymers*), which are to be reacted together to make the thermoset. As a consequence of the crosslinks, the properties differ to those of thermoplastics such as being stiffer, harder and they can also be stronger. They are also brittle (which can lead to weak behaviour).

2.2.2 Elastomers

General Properties

- Massive elastic deformation.
- No plastic deformation.
- Non recyclable (by melting).

Elastomers are effectively a subset of thermosets; they contain covalent cross links (not as many) and thus cannot be melted once formed. The crosslinks permit *freedom* of deformation (movement) of the carbon chains but ultimately restrict it and thereby stop *plastic* deformation. The degree of crosslinking *strongly* affects the stiffness of the elastomer. The stiffness increases with the number of crosslinks.

2.3 Ceramics

2.3.1 General Properties

- High electrical resistivity (insulators).
- Highly thermally insulating.
- Hard.
- Brittle (not necessarily weak).

Ceramics are inorganic chemical compounds, usually between two or more elements: a metallic and non metallic element. The above properties are all a function of the atomic bonding; often a mix of ionic and covalent bonding. Alumina (Al_2O_3), silica (Quartz) (SiO_2) and silicon carbide (SiC) (hard, abrasive) are all examples of ceramics. Note: the way in which a material fractures is important - brittle failure is rapid and 'clean' such that the pieces fit back together.

Consider the case of NaCl, which has non-directional ionic bonds. Thus, the ionic bond should (in theory) allow some form of slip to occur along planes - hence plastic deformation. Slip is possible but much more difficult than with the metallic bond. This is due to the repulsion of ions and the need to slip in two atom jumps (alternating + - structure between planes).

A covalent bond is very 'rigid' and resists breakage - hence no slip is possible. Very high strengths are observed but also brittle behaviour

2.4 Composites

A physical mixture of the three previous categories (not chemical). GFRP (glass fibre reinforced polymer) and CFRP (carbon fibre reinforced polymer) are examples of composites.

Individual constituents will have their own properties governed by structure and bonding. In some cases, overall properties are a mathematical average of the individual properties e.g. stiffness - glass added to polymer causes an increase in stiffness. However, many properties e.g. stiffness, strength and toughness are also a function of how the constituents are mixed e.g. arrangement, shape and orientation.

Natural composites do exist e.g. wood, which is mixture of cellulose and lignin (both polymers). Cellulose is crystalline and acts as a fibre. Lignin is amorphous and acts as the 'matrix'. A structural composite is a structure optimised to improve the stiffness to weight ratio. Properties of a composite are also about *how* the two constituents *interact* with each other.

2.5 Properties

2.5.1 Stress and strain

Stress a.k.a load, strain a.k.a deflection. Doubling the stress will double the deflection. Deflection will depend on the specimen size. In order to compare these properties, we need to normalise for differences in dimension e.g. $\delta L/L = \epsilon$ - strain. For stress, we divide the force by the area its being applied over i.e. $F/A = \sigma$. Strain is sometimes represented as percentage.

Note: stress is a variable. Strength is not, it is a fixed property of a material.

2.5.2 Hardness

Often quoted for metals as a design parameter as it is easy to measure and can be related to strength. Dimensions of indent can be related to the strength in compression, which can be measured in various ways. In the UK, Vickers hardness H_v (triangular indenter) is a test for the hardness of the material. Other systems, such as Rockwell and Brinell hardness (circular indenter) exist. Scratching a specimen can also be used to test the hardness of a material e.g. Mohs scale, where diamond is at 10 and arbitrary hardness at the other end of the scale.

Indentation techniques are not suitable for brittle materials and is normally used for metals as they slip (plastically deform). They are also difficult to use on elastomers, where we use abrasion test or "bouncing ball" tests.

2.5.3 Stiffness

Also known as - Elastic Modulus, Modulus of Elasticity or the Young's Modulus (tension). May also be referred to as the opposite of floppiness. Refers to the flexibility of a material. Units are in Pascals Pa or Nm^{-2} . The following equation

gives us the Young's Modulus of a material.

$$E = \frac{\sigma}{\epsilon} \quad (2.1)$$

This equation relates the normalised load and its normalised deflection. It measures how far something deflects per unit load. These only apply in the elastic regime of a material's behaviour i.e. only for elastic strain.

2.5.4 Strength

Defined as the stress required to "break" a material (there are different types of break, hence different strengths definable).

Tensile strength

Defined as the stress required to fracture a material in tension into two bits. Symbol used is σ_{UTS} , where UTS stands for ultimate tensile strength. This has units Pa.

Compressive strength

In most cases, this is similar to σ_{UTS} , but its often difficult to measure. This is because materials such as metals don't break into two pieces under a compressive force - they just squash. Other materials such as ceramics will shatter or crush at a specific load. Hence, a compressive strength is definable for such materials.

Metals and polymers often "fail" at much lower stresses than σ_{UTS} e.g. they will suffer plastic deformation before fracture. This is always less than σ_{UTS} , if slip can occur, slip will occur first - this is a form of failure. The stress at which this happens is called the yield strength σ_y , defined as the stress required to induce plasticity in a material.

In a ceramic, there is no easy mechanism for slip and thus no noticeable plastic deformation. We define σ_f or fracture strength for such materials. As there is no plasticity, $\sigma_{UTS} = \sigma_y = \sigma_f$.

2.5.5 Ductility

Defined as the degree of plastic deformation achievable in a material before it breaks into two/fractures. It is a materials parameter and so a strain (plastic strain to fracture). It is often seen as a percentage of strain. Often 0.1% for most metals and up to even 2000% for some polymers. Ductility is very important if we want to create/shape materials through plastic deformation - extrusion, drawing, forging, bending. Ceramics have almost no observable ductility (no slip). These need to be sintered from powder.

2.5.6 Toughness

Related to the work/energy required to fracture a material, the amount of "damage" a material can take before fracturing. Very different to strength - which is the *force* required to fracture. Strength and toughness are not absolutely related from an atomic viewpoint. The opposite of tough is *brittle*, where very little energy is required to fracture.

Fractured surfaces tend to be "clean" and fit back together again. Brittle is often confused with being 'weak' i.e. a low force to break. It is true that brittle materials often appear to be weak in practice but not necessarily intrinsically weak. They behave 'weakly' due to the presence of defects - some can be visible (scratches, cracks) while others can be minute (micro-cracking at the atomic level, porosity). Defects determine the failure load (stress) of brittle materials. These act as stress concentrators, raising the globally applied load to much higher values on a local level, so much so that local bonds are broken i.e. the intrinsic strength is exceeded. so failure occurs at an apparently lower stress. Manufacturing has a huge role to play in determining the presence and severity of defects. However, if there are mechanisms for plastic deformation e.g. slip (which occurs below tensile strength), then as the stress rises at the defect, slip will begin to occur at the tip of the stress concentration and smooth it out, reducing its severity. Thus, in metals fracture at low loads is unlikely - they are tough.

THIS IS THE SAME THING REWRITTEN:

In a 'tough' material, local stress concentrators exist, so σ_{global} rises ahead of the crack to reach the point at which *plastic* deformation occurs, such that yield will occur (slip (in metals) absorbs energy because work is consumed).

Slip can slow down a crack or stop it. This work is demanded from an external load in order for the crack to propagate. It can change the shape of σ 's concentration i.e. smooth it out. Slippage and sliding can open up a defect and extra surface area is generated (blunting). Thus, in a plastically deformable material, existing defects are tolerated (no longer critical to strength). These materials are described as *tough*.

Note one: "bad" stress concentrators are sharp and long e.g. cracks and holes (which are still stress concentrators, just not to the same degree).

Note two: toughness is related to ductility: high ductility = ease of slip = high toughness. A lot of energy is absorbed in attempting to propagate a defect line or crack. THIS IS STUFF THAT I JUST SAW ON THE BOARD WHEN I CAME IN LATE:

[...] the σ can quickly build up to that necessary to break the bonds at a crack tip (i.e. exceed theoretical strength). Long, deep cracks are more severe than shallower ones and sharp cracks are worse than rounded or blunt ones. Thus, on breaking A-B bond, the crack gets longer, σ 's concentration increases and the crack propagates uncontrollably (i.e. a brittle material).

2.5.7 Fatigue strength

The ability to resist failure under a cyclical load. Fatigue occurs at loads well below σ_{UTS} and can initiate and then propagate defects (principally cracks) to a point where they cause failure by fracture. Steels typically have a lifetime of $10^6 - 10^8$ cycles for typical loads. All materials 'suffer' fatigue failure, even though the internal mechanisms vary from category to category. The amplitude of the alternating stress is a factor. Low amplitudes favour many cycles before failure - 'long lifetime' but lifetime is stress dependent.

2.5.8 Other properties

- Cost
 - Dependent on the availability (rarity) of a material.
 - Manufacturing - note: polymers are expensive in but but component cost is reduced due to ease of manufacturing.
- Corrosion resistance.
 - Rate of reaction with an environment. Most applicable to metals but polymers and ceramics also suffer from corrosion (to a degree).
- Abrasion resistance
 - The ability to avoid wear in components that are in sliding contact (bearings).
 - Usually, materials with high hardness is best for reducing wear but we must also consider frictional coefficients.
- Environmental 'credentials'
 - Recyclability and re-use. Rubber is a good example of something which is very hard to recycle.
 - Toxicity/waste.

2.5.9 Stress/strain responses

Many mechanical properties can either be measured, inferred or illustrated from a stress-strain response. We plot σ vs ϵ in tension. Doing such a test we are measuring force and deflection and using the dimensions of the specimen we can calculate σ/ϵ . Extension is measured using an extensometer (laser based or contact based). The extensometer is placed across the gauge length (distance between the two necks of a dog bone shaped specimen). It measures $L + \Delta L$. The distance between the grips is also an alternative but this is inaccurate.

Deviation from linearity normally due to extending σ_y because metals are linearly elastic, caused by slip. Drop in σ required just before failure due to 'necking'. Local failure point, material will decrease in cross section. Necking is a random instability

in the material; if at some point it gets longer faster than elsewhere. Due to the volume being conserved, specimen gets thinner. This raises the global stress applied such that further extension is focussed in this region. This is known as a positive feedback mechanism and the neck is the ultimate failure location. You can plot 'true stress' (and strain) which takes into account the decrease in cross section area.

2.5.10 Structure

Ionic bonding

The ionic bond is multi-directional and is capable of being disrupted via shear, generally sliding - "slip", but quite hard, due to the need to "slip twice" as to maintain the low energy charge distribution in the lattice structure. It is formed when one electron is donated from one atom to another, creating a positive and negative ion structure. This sort of bonding is only for compounds.

Covalent bonding

These can occur between unlike atoms (like ionic bonds) *and* like atoms. In covalent bonding, there are shared electrons in common orbits, which generates highly directional bonds. These are difficult to displace and break; it does not support slip. Hence, it is difficult to displace off equilibrium angles. Stiffness is usually high in covalently bonded materials. Some examples of covalently bonded materials are CH_4 , SiO_2 and diamond. Usually they are brittle and hence, susceptible to defects (covalent solids). Polymers are covalently bonded only in part. It is not fair to say that their properties should be similar to covalently bonded materials. For example, we might expect polyethylene to be stiff and strong but this is only partially correct. If we were to test a single molecule, this would be the case. However, it is very difficult to deal with single molecules at a time as a single molecule is only about 20 μm in length. The strength of polymers such as polyethylene, is mostly a function of the way in which each molecule interacts with its neighbours. This is done via Van der Waals H bonds and secondary bonds - a dipolar interaction. These are not whole charges; only minor charge differences and thus are weak. By controlling the level of interactions, we can then control properties of such a polymer. For example, in PVC, chlorine is substituted for hydrogen atoms. Chlorine is very electronegative and loves electrons - it generates permanent dipoles. However, in PE, the molecule only contains carbon and hydrogen bonds and it is symmetric so permanent dipoles do not exist. Instead, 'temporal' (in time) dipoles exist, which come and go. These will attract and provide mechanical properties; a sense of strength. This is the definition of Van der Waals bonding.

Metallic bonding

Occurs in elements which have insufficient valence electrons to either ionically or covalently bond i.e. middle of the periodic table. Occurs in single elements e.g. gold and in different elements e.g. copper and zinc: brass. Valence are donated to the 'common' surrounding, an array of positive ions. This is non-directional, so slip is easy. Metallic bonding importantly permits alloys - atomic level mixtures, generating 'solid solutions'. These can be random mixtures and of continuously variable concentrations. An alloy has a mix of properties generated from its constituents. The mix will also have a new level of structure, called the micro-structure, that *strongly* affects the mechanical properties.

2.5.11 Creating solids

Consider a liquid, cooling it down yields a solid. A liquid is a random arrangement of 'particles' (atoms or molecules). The particles get closer together as the temperature drops as the amplitude of the thermal vibrations are reduced. They begin to interact and eventually 'structure' themselves so as to minimise their free energy; called 'ordering'. We have two types of ordering: *short range* order and *long range* order. Short range order yields us amorphous solids and long range order yields us crystalline solids. An example of a crystalline solid is SiO_2 which can come together to form SiO_4^{4-} also known as the basic building block of silica quartz. This is a 3D structure that is electrically neutral. There are four main 'forms' of ordered SiO_2 and one irregular form, where only the short range order persists. This short order form is called silica glass and the regular form is referred to as quartz. These four long order forms of quartz have the same formula SiO_2 but have different structures. Glassy SiO_2 does not exhibit a melting point. Quartz does. Glassy SiO_2 would be described as brittle. Quartz is less brittle - the energy required for fracture is higher than that of glassy SiO_2 . Glassy materials are referred to as *amorphous* - supercooled liquids: solid. Materials 'prefer' to be crystalline as it is the lowest energy state, they like to be ordered - the most energy favourable form. To prevent crystallinity, we need to cool liquids rapidly. This is easier if the crystal structure is complex i.e. molecules but for single atoms e.g. metals it is very difficult. Amorphous metals have been produced requiring a cooling rate of six million degrees per second but these have limited use. So assume metals are crystalline. **Insert solid structure lab report here**

2.6 General link between properties and bonding

Consider two atoms bonded in a solid. Figure ?? shows two atoms bonded together at a distance x from each other - the equilibrium interatomic distance. There is a balance of two forces, the attractive "bond" and the repulsive; the nuclei are positively charged and thus repel. The distance x will affect the fundamental properties e.g. optical properties. The graphs shown in Figure ?? show the force of attraction

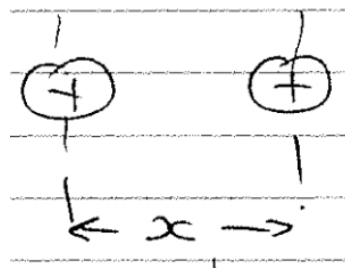


Figure 2.1: Two atoms bonded together at an equilibrium intermolecular distance x

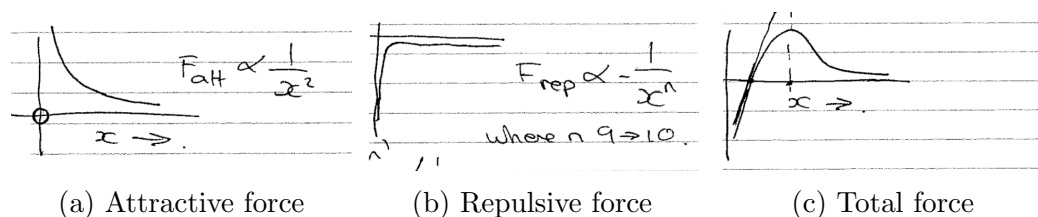


Figure 2.2: Force graphs for two atoms bonded together

(??), the force of repulsion (??) and how the total force on the particle changes with x (??). The attractive relationship (??) can be described as $F_{att} \propto \frac{1}{x^2}$. The repulsive relationship (??) can be described as $F_{rep} \propto -\frac{1}{x^n}$ where n is between 9 and 10. Integrating (??) generates an energy response.

2.6.1 Force-sum curve

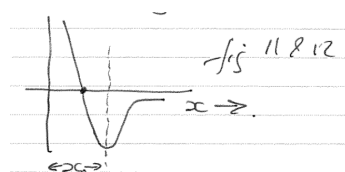


Figure 2.3: Energy response as x is varied

This crosses zero when $x = \text{interatomic distance}$ i.e. both forces are balanced - x_0 . Displacement away from x_0 requires a net force to be applied. The peak of the force-sum curve can be related to the strength of the material. The slope of the curve when $x = x_0$ can be related to the stiffness of a material.

2.6.2 Energy curve

The minimum of this curve occurs when $x = x_0$ - i.e. the material at equilibrium is at its lowest energy state. It is asymmetric about x_0 . The depth of the well is related to how 'stable' a material is in the solid state. This related to the melting point of the substance (and its chemical reactivity). Also as heat (energy) input

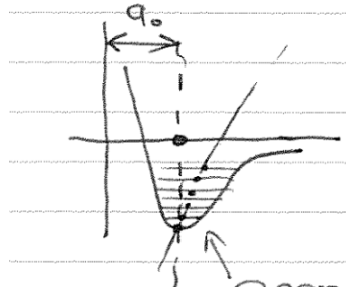


Figure 2.4: The energy "well"

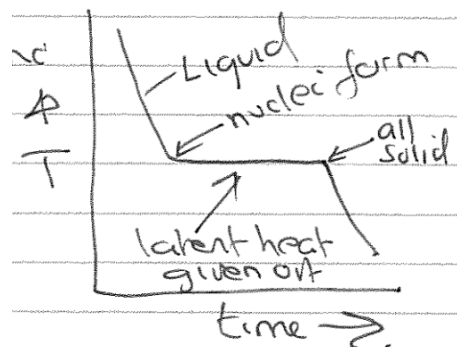


Figure 2.5: The characteristic cooling curve

into such a system, the minimum moves to the right hand side (as the well fills up). This predicts that a_0 increases as heat is input i.e. materials expands on heating - expansion coefficient.

2.7 Solidification of crystalline materials

Regular solids (crystalline), that form at freezing point, start out via formation of a nuclei (small 'areas' (embryos) of crystalline material). These are nominally 200-300 atoms in diameter. They come about randomly, via collisions; this process is called nucleation. Once a nucleus of a given critical size has been created, crystals become stable at R_{crit} and more atoms join, leading to the crystal growing. Anything smaller than R_{crit} , the crystal will remelt (because we are at the melting point as well as the freezing point). Because nuclei become stable, the heat (energy) they lose, needs to be removed, else solidification (into the surroundings) will stop (latent heat of solidification). This process is isothermal at the melting point and can be monitored using a cooling curve. Nucleating, being random, can occur anywhere and everywhere. This results in many crystals being formed and a polycrystalline solid being formed. This generates a characteristic cooling curve.

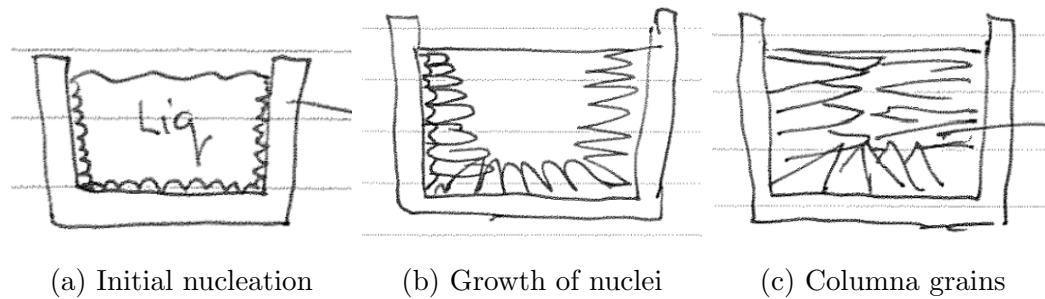


Figure 2.6: The nucleation process

2.7.1 Practical casting

Many nuclei are formed but on walls of the mould (??). Subsequently crystals grow from the nuclei into the centre of the mould (??) - long and thin "columna" crystals (grains) (??). Nuclei are formed by random means i.e. we get lots of crystals; there is no orientation relationship between each nucleus. Hence, misorientated crystals cannot join perfectly. This results in a polycrystalline solid grain structure aka a microstructure μm - mm in dimension. This strongly influences properties and can easily be altered via manufacturing processing. e.g. columnar grains - typical of an 'open' casting are not ideal - better mechanical properties can be achieved if grains are polygonal and approximately equal sized in 3 orthogonal directions: equiaxed crystals (??). This can be achieved via rapid cooling. When grains eventually

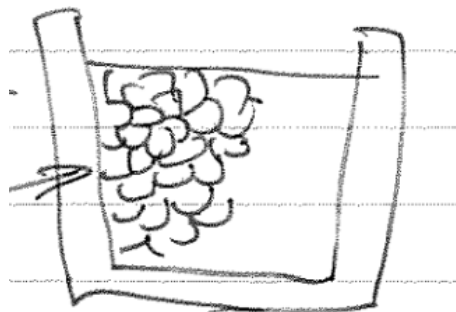
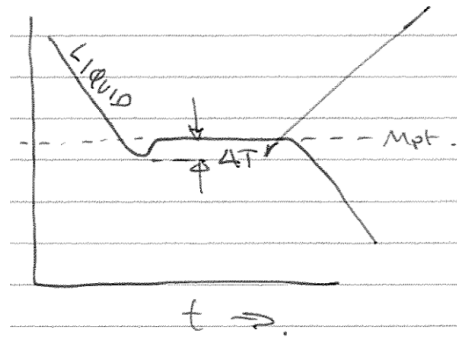


Figure 2.7: Equiaxed crystal structure

touch they cant join perfectly - so they create an area of 'disorder' - i.e. high energy (thermodynamically) - not fully crystalline. This is the grain boundary. Due to higher free energy, grain boundaries are more likely to host chemical reactions or processes that decrease free energy. e.g. oxidation/corrosion. They are also significant in determining mechanical properties.

During cooling if a material is very pure and/or the mould is extremely pure/clean, it is possible to avoid nucleation and hence cool to below freezing point. This is called undercooling. n.b. extreme undercooling - called supercooling - results in no crystalline structures forming: an amorphous solid (supercooled, high viscosity liquids) Once nucleation begins, the crystallisation process wil rapidly occur. Undercooling can be generated by rapid cooling of a mould. This is more common in



materials that find it difficult to crystallize e.g. long chain thermopolymers and SiO_2 ceramics. Undercooling, therefore, occurs more easily in complex crystal structures - in a metal, a ΔT is almost impossible to observe. It is possible to see in ultra pure metals and/or if cast into a very clean mould. Why? ΔT is related to the time it takes to create stable nuclei - i.e. reach R_{crit} . R_{crit} is a radius - achievable either by

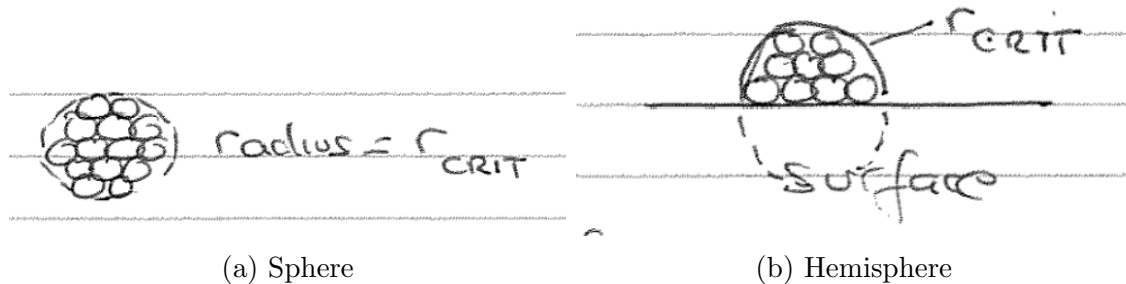


Figure 2.8: Different sorts of nuclei formation

creating a sphere of atoms or a hemisphere of atoms. Thus, if a surface is available it can reduce the requirement for the number of atoms to create a R_{crit} (is a random process - so more chance of happening) i.e. surfaces help nucleation and act as sites for nucleation. There are two types of nucleation that we can define: self nucleation (homogeneous nucleation) and heterogeneous (nucleation on something). The nucleation type affects microstructure. Commercially done by adding inoculants e.g.

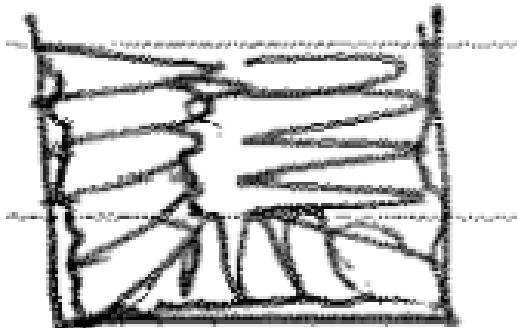


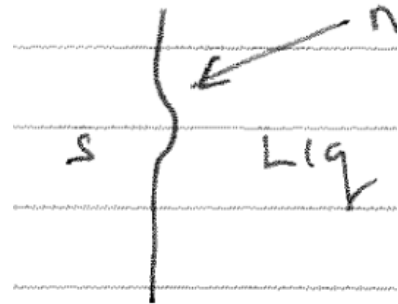
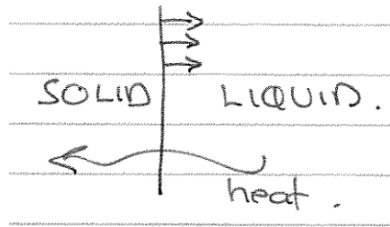
Figure 2.9: Heterogeneous nucleation
X1



Figure 2.10: Homogeneous nucleation
(or hetero if impure) X1A

TiO₂ SiO₂ powder. Also known as seeding.

In many crystalline solids, the process of solidification goes through a dendritic stage. dendrite - from greek for tree - dendra - 3D crystal Dendrites emerge from nominally



stable S-L growth fronts and would normally melt back - but under certain circumstances any protruberance becomes stable e.g. see constitutional supercooling. more likely in impure substances normally a growing dendrite will fill space gradually and become a single crystal and in disappear.

Two occasions when dendrites appear in the microstructure: coring - variation in the composition of a dendrite as it grows revealing the stages of dendritic growth e.g. as colour changes. gradual change in composition - microsegregation. every grain will be cored, can compromise corrosion resistance and mechanical properties. or if the space in between the dendrite arms are filled with another substance (phase see X6 and X7).

in casting technology, coring is regarded as a defect but there are others, principally porosity - holes in the microstructure. they can seriously degrade/affect mechanical properties. act as stress concentrators.

