## Summary + guide

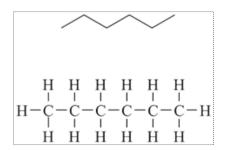
## Lecture 1

# Multiple choice section

- Stick structures and names
  - 1. Recognise amount of atoms from a stick structure
  - 2. Recognise the correct name from a list of possibilities
- · Balance reaction equations
  - 3. Be able to do simple balancing on moles
- Industrial chemicals
  - 4. Recognise the names of major chemicals (scale)
- · Fuel properties
  - 5. Recognise a good fuel component

## Method and explanation:

## 1. Recognise amount of atoms from a stick structure



Every end represents a carbon-atom linked to its correct number of hydrogen atoms

## 2. Recognise the correct name from a list of possibilities

See IUPAC Naming of organic molecules sheet on Nestor

## 3. Be able to do simple balancing on moles

$$..Fe_2O_3 + ..C \Rightarrow ..Fe + ..CO_2$$

Solve from one side, don't forget about molecules like H<sub>2</sub>O that only have one O instead of the regular O<sub>2</sub>

## 4. Recognise the names of major chemicals (scale)

Name	Formula	Principal End Use
Sulfuric acid	H <sub>2</sub> SO <sub>4</sub>	Fertilizers, chemicals, processing
Nitrogen	N <sub>2</sub>	Fertilizers
Oxygen	O <sub>2</sub>	Steel, welding
Ethylene	C <sub>2</sub> H <sub>4</sub>	Plastics, antrifreeze
Lime	CaO	Paper, chemicals, cement
Ammonia	NH <sub>3</sub>	Fertilizers
Phosphoric acid	H <sub>3</sub> PO <sub>4</sub>	Fertilizers
Sodium hydroxide	NaOH	Chemical processing, aluminium production, soap
Propylene	C <sub>3</sub> H <sub>6</sub>	Gasoline, plastics
Chlorine	Cl <sub>2</sub>	Bleaches, plastics, water purification
Sodium carbonate	Na <sub>2</sub> CO <sub>3</sub>	Glass
Methyl tert-butyl ether	(CH <sub>3</sub> ) <sub>3</sub> COCH <sub>3</sub>	Gasoline additive
Ethylene dichloride	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	Plastics, drycleaning
Nitric acid	HNO <sub>3</sub>	Fertilizers, explosives
Ammonium nitrate	NH <sub>4</sub> NO <sub>3</sub>	Fertilizers, mining
Benzene	C <sub>6</sub> H <sub>6</sub>	Chemicals, processing, solvent

## 5. Recognise a good fuel component

Bases on octane number: measure of fuel performance (higher for branched alkanes)

Higher alkanes have a higher autoignition temperature and prevent engine knocking

The percentage isooctane and heptane decides the octane number and thus the quality of the fuel (petrol cars = 95+)



- · Naming and drawing of basic hydrocarbons
- · Recognise a high vs low octane number fuel component
- · Most important chemical intermediates and their origin
- · Balancing of reactions equations
- Use of moles, Mw, density and E-factor/atom economy equations
- Reaction types
- · Conversion, yield and selectivity
- · Steam cracking, catalytic cracking, catalytic reforming
- Structural isomers (constitutional isomers)
- Other reactions like gasification, methanol synthesis and Fisher Tropsch
- Repeat everything from MC

# Multiple choice section

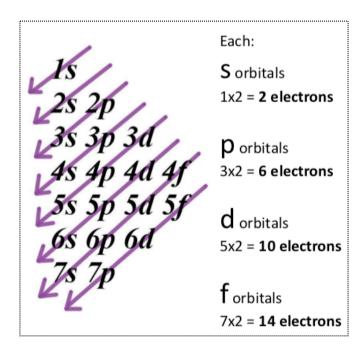
- Electron configuration and atomic structure
  - 1. Periodic table (make sure you have one)
  - 2. (Valence!) electrons, neutrons, protons
- Names of alkenes
  - 3. Names of simple alkenes (structural isomers) (1)
- 3D structure (hybridisation)
  - 4. Recognise sp, sp<sup>2</sup>, sp<sup>3</sup> carbons
- Aromaticity
  - 5. Recognise aromatic compounds (apply basic rules)
- Conjugation
  - 6. Recognise when bonds and charges are conjugated

#### Method and explanation:

#### 1. Periodic table

See BINAS last page or internet

#### 2. (Valence!) electrons, neutrons, protons



For example:

Boron =  $1s^22s^22p^1$ 

Implying that it has: 2 electrons in 1s

2 electrons in 2s1 electron in 2p

Another notation is [Ne] 3s<sup>2</sup>3p<sup>3</sup>

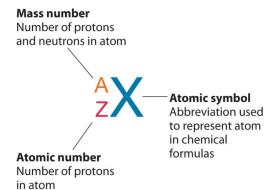
Implying that this atom has the same configuration as Neon plus the additional configuration

Valence electrons are electrons in the outer shell (orbital), they can move around.

Table 2	The Electronic Configurations of the Smallest Atoms							
Atom	Name of element	Atomic number	1s	<b>2</b> s	$2p_x$	$2p_y$	$2p_z$	3 <i>s</i>
Н	Hydrogen	1	<b>↑</b>					
He	Helium	2	$\uparrow\downarrow$					
Li	Lithium	3	$\uparrow \downarrow$	$\uparrow$				
Ве	Beryllium	4	$\uparrow\downarrow$	$\uparrow\downarrow$				
В	Boron	5	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$			
С	Carbon	6	$\uparrow \downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow$		
N	Nitrogen	7	$\uparrow\downarrow$	$\uparrow\downarrow$	<b>↑</b>	$\uparrow$	$\uparrow$	
О	Oxygen	8	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow$	
F	Fluorine	9	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	
Ne	Neon	10	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	
Na	Sodium	11	$\uparrow\downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$	1

Remember the octet rule when deciding the number of electrons

Covalent bond = a *pair* of shared electrons



The number of protons is the atomic number = Z

The number of protons and neutrons combined is the mass number = A

A = N + Z with N being the number of neutrons

## 3. Names of simple alkenes (structural isomers) (1)

Name	General formula	Number of bonds	Naming	Reactivity	sp <sup>x</sup> hydridized	Additional info
Alkanes	$C_nH_{2n+2}$	single	-ane	Relatively unreactive	sp <sup>3</sup>	Common use is fuel
Alkenes	C <sub>n</sub> H <sub>2n</sub>	double	-ene	More reactive	sp <sup>2</sup>	Location in naming before dash
Alkynes	$C_nH_{2n-2}$	triple	-yne	Most reactive	sp <sup>1</sup>	Sometimes use different naming like 'acetylene'
Cyclo- alkanes	$C_nH_{2n}$ (1 cycle) $C_nH_{2n-2}$ (2 cycles)	single	cycloane	(in most cases) similar to alkanes	sp <sup>3</sup>	-

## 4. Recognise sp, sp<sup>2</sup>, sp<sup>3</sup> carbons

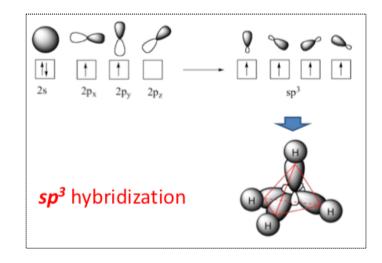
See point 2 and below:

Steps to determining hybridization:

1. Determine steric number

Steric number = Atoms + Lone pairs

2. If steric number is  $4 \rightarrow sp^3$ If steric number is  $3 \rightarrow sp^2$ If steric number is  $2 \rightarrow sp$ 



3. Check since in general an atom with all single bonds is sp<sup>3</sup> hydribized, double bonds are sp<sup>2</sup> hydribized and triple bonds are sp hydribized

## 5. Recognise aromatic compounds (apply basic rules)

A molecule is aromatic if:

- 1. They are cyclic (in a full circle/triangle/hexagon)
- 2. They are conjugated all around the ring. So, <u>every atom in the ring</u> must be able to participate in resonance. (resonance = structure that allows for movements and thus different isomers)
- 3. The molecule has an even number of electrons (also called Pi electrons)
- 4. The molecule must be flat/planar (implying that it has no tetrahedral structures = no sp<sup>3</sup>)

#### 6. Recognise when bonds and charges are conjugated

Molecules are conjugated if two double bonds are separated by a single bonds, since their orbitals will interact. This also counts for charges.

- · Atom compositions
- Electron configuration & valence electrons
- Application octet rule, draw Lewis, resonance-contributors and -hybrid structures
- Recognise sp, sp<sup>2</sup>, sp<sup>3</sup> carbons
- Recognise conjugated double bonds
- · Recognise aromatic compounds
- Balancing of reaction equations (REPEATED)
- Use of moles, Mw, density and E-factor/atom economy equations (REPEATED)
- Repeat everything from MC

# Multiple choice section

- · Stick structures and names
  - 1. Names of simple alkenes (structural isomers) (2)
- 3D structure and hybridisation
  - 2. Atoms in the same plane
- Isomers and chirality
  - 3. Amount of chiral centers
  - 4. Types of isomers
  - 5. Recognise constitutional/structural isomers

## Method and explanation:

## 1. Names of simple alkenes (structural isomers) (2)

<u>Isomerism</u> = chemical compounds have different structures but the same elemental composition.

Structural isomers (constitutional isomers):

Both have the same composition: C<sub>4</sub>H<sub>10</sub>

Yet have a different structure (and different name).

#### Properties:

- I. Same molecular formula
- II. Different connectivity
- III. Different functional groups
- IV. (Very) different chemical properties
  - e.g. boiling point, physical appearance, melting point, reactivity, stability (energy level)

Conformational isomers:\*

Have to be sp<sup>3</sup> and they can rotate.

#### **Properties:**

- I. Same molecular formula
- II. Same connectivity
- III. Same functional groups
- IV. Overall same molecule, so all identical properties

The actual molecule will be at any time a mixture of different conformers and the ratio (axial-equatorial) is determined by the relative stability and temperature.

Geometric isomers:\*

Mainly the cis (Z) or trans (E) configuration. (Z = zusammen, E = entgegen)

#### **Properties:**

- I. Same molecular formula
- II. Same connectivity
- III. Same functional groups
- IV. Different chemical properties

#### 2. Atoms in the same plane

In the same plane implies that there are no tetrahedral structures (no sp<sup>3</sup> configured atoms).

#### 3. Amount of chiral centers

Stereoisomerism = configurational isomerism (mirroring)

<u>Chiral</u> = Non-superimposable on its mirror image, e.g. hand (different in the mirror)

Achiral = Superimposable on its mirror image, e.g. sphere (same in the mirror)

A molecule will have a chiral (or asymmetric) center if an atom has 4 different groups connected to it. If a molecule has (at least) 1 chiral center it will be called chiral.

#### 4. Types of isomers

Most types are mentioned in point 1, yet two types still aren't discussed.

<sup>\*=</sup> these types of isomers aren't mentioned until point 4, but fit better in this section.

Enantiomers (stereoisomers):

These are chiral molecules.

#### **Properties:**

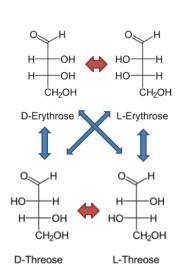
- I. Same molecular formula
- II. Same connectivity
- III. Same functional groups
- IV. Same chemical properties

Only differ in interaction with other sources of chirality:

- Chiral compounds
- Chiral light

#### Diastereoisomers:

These are chiral molecules with more than one chiral center. They differ from enantiomers since they will be the difference between a cis and trans configuration of an enantiomers.



These cis and trans configurations are called <u>erythro</u> if the chiral centers and their connections are on the same side and <u>threo</u> if the chiral centers and their connections are across from each other.

Red indicates the enantiomers.

Blue indicates the diastereoisomers.

Notice the erythro and threo configurations.

## **Properties:**

- I. Same molecular formula
- II. Same connectivity
- III. Same functional groups
- IV. Different chemical properties

#### 5. Recognise constitutional/structural isomers

See point 1, mostly look at structure or name that might differ.

- Recognise different types of isomers
- Different chemical/physical properties for different types of isomers
- · Distinguish cis and trans
- Distinguis R & S
- Difference in stability (equatorial vs axial as well as position of a double bond)
- Determine meso compounds
- Convert to chair configuration
- · Perform ring flip
- Repeat everything from MC

# Multiple choice section

- Acids and bases
  - 1. Recognise strong acids and bases
- Solubility, boiling point
  - 2. Relative strength of intermolecular forces
  - 3. Relative interaction with polar solvents (e.g. water) or hydrophobic solvents (e.g. alkanes)

## Method and explanation:

## 1. Recognise strong acids and bases

An acid is able to 'lend' a H+ to a base, whereas a base needs to 'adopt' it (it is short of a H+). A strong acid has a weak base and vice versa.

$$H_2O + H_2O \longrightarrow OH^{\Theta} + H_3O^{\Theta}$$

 $pK_a + pK_b = pK_w$  (=14 at room temperature).

**Neutral water:**  $[H_3O^+] = 1.0 \times 10^{-7} M$ 

 $pH = -\log[H_3O^+] = 7$ 

pH < 7.00 Acidic solution pH = 7.00 Neutral solution pH > 7.00 Basic solution The strength of an acid is represented by its ionisation constant (acidity constant) =  $K_a$ 

The factors that affect the pKa (acidity) are:

- Electronegativity = acidity increases with electronegativity

- Atomic size = acidity increases with size

Hybridisation = the higher the s-character the higher the electronegativity
 Resonance = acidity increases with distribution of charge (more stable)

- Inductive effects = as the number of +/ groups increase the acidity increases

<u>Electronegativity</u> = tendency of an atom to attract electrons (electron density) around itself → See BINAS 40A

Atomic size = size of atom

→ See BINAS 40A

<u>Hybridisation</u> = sp has a higher acidity than sp<sup>3</sup>

→ See 2.4

Resonance = more distribution of charge, more stable, increased acidity

→ See 2.5

<u>Inductive effects</u> = the effect where charges are passed on from atom to atom.

Since two different atoms won't have an equally distributed charge (electron positions), one of these atoms will be a bit more negative than the other.

This is called a polar atom/molecule (or dipole)

If the chain of atoms (rest of the molecule) is bound to the more electronegative (mostly carbon) atom it has a positive inductive effect +*I* 

If the chain of atoms (rest of the molecule) is bound to the less electronegative atom, it has a negative inductive effect -*l* 

In general, in increasing order of +/ these are the most common groups:

$$-NH_{3^{+}} > -NO_{2} > -SO_{2}R > -CN > -SO_{3}H > -CHO > -CO > -COOH > -COCl > -CONH_{2} > -F > -Cl > -Br > -I > -OR > -OH > -NR_{2} > -NH_{2} > -C_{6}H_{5} > -CH=CH_{2} > -H$$

As there are more +/ groups the molecule is more acidic

#### IN GENERAL:

BINAS 49 shows all bases and acids ranked on strength

#### 2. Relative strength of intermolecular forces

From strong to weak:

- Ionic interactions
- Hydrogen bonding (polar interactions)
- Dipole-dipole bonding
- Vanderwaals interactions (hydropohobic interaction)

Polar interactions are interactions between polar molecules.

→ A polar molecule has a difference in charge distribution (dipole)

Hydrophobic interactions are interactions between non-polar molecules.

→ They do not have polar molecules and the charge is equally divided.

# 3. Relative interaction with polar solvents (e.g. water) or hydrophobic solvents (e.g. alkanes)

The more polar interactions a molecule can make the more soluble it is in water and other polar solvents.

The more hydrophobic interactions can make the more soluble it is with alkanes and other hydrophobic solvents.

# Determining the boiling point of a substance:

- I. The stronger the bonds between the molecule, the higher the boiling pointII. The 'heavier' the molecule, the higher the boiling point
- I. As the number of branches decreases, the boiling point increases (straight chain has a higher boiling point)

- Intermolecular interactions
  - Relative strength
  - Polarized bonds (hydrogen bonding)
  - Relation to functional groups
- · Acid and bases
  - pKa and pKb (and pKw)
  - Factors influencing acidity
  - Resonance!!
- Which form is predominate at certain pH
- Fats and oils
- Repeat everything from MC

# Multiple choice section

- 1. Recognise precursors of biochemical materials (such as nucleotides)
- 2. Types of building blocks (for DNA and RNA)
- 3. Describe the different pathways for nucleotide synthesis
- 4. Configuration of amino-acids
- 5. Bonds between amino-acids (in DNA/RNA)
- 6. Stability of DNA and RNA
- 7. Structure of nucleotide and nucleoside (and thus of RNA and DNA)
- 8. Naming of nucleotides
- 9. Properties of biochemical materials

#### Method and explanation:

## 1. Recognise precursors of biochemical materials (such as nucleotides)

A precursor is a compound that participates in a chemical reaction that produces another compound.

This precursor will turn into another using a metabolic pathway. IMP for example is a precursor of adenine and guanine.

#### 2. Types of building blocks (for DNA and RNA)

The general building blocks of chemistry are:

- A. Sugars
- B. Amino acids
- C. Nucleotides
- D. Fatty acids
- E. Salts
- F. Waters
- G. Vitamins and trace elements

DNA & RNA are built out of RNA building blocks (nucleotides or nucleosides):

- Phosphate group
- 5-carbon sugar
- Nitrogenous base
  - ATCG amino-acids (DNA)
  - AUCG amino-acids (RNA)
- → SEE BINAS 71 (C)

The 5-carbon sugars can be either <u>D-2-deoxyribose</u> for DNA or <u>D-ribose</u> for RNA.

#### 3. Describe the different pathways for nucleotide synthesis

There are two different metabolic pathways to nucleotide biosynthesis:

- (1) **De-novo synthesis**: biochemical pathway where nucleotides are synthesised new from simple precursor molecules
- (2) **Salvage synthesis**: used to recover bases and nucleosides formed during the degradation of RNA and DNA

Nucleotides can be categorised in two categories; Purines & Pyrimidines

<u>Purines</u> are responsible for the bases: adenine & guanine <u>Pyrimidines</u> are responsible for the bases: thymine, cytosine & uracil

A purine is a heterocyclic aromatic organic compound containing 4 nitrogen atoms. It contains of *two carbon rings*.

A pyrimidine is a heterocyclic aromatic organic compound containing 2 nitrogen atoms. It contains only *one carbon ring*.

Both metabolic pathways can synthesise purines as well as pyrimidines using it's precursors (De-novo) or turnover of nucleic acids (Salvage)

## 4. Configuration of amino-acids

The amino-acids in RNA and DNA are connected to the sugar-group on one side. A sugar-group can (in general) be configured as an  $\alpha$  sugar or as a  $\beta$  sugar.

If the OH-group is pointed upwards (same direction as O-group) it is a  $\beta$  sugar. If the OH-group is pointed downwards (opposite direction of O-group) it is an  $\alpha$  sugar.

Like all amino-acid bonds, the connection between the sugar and the amino-acid is made using the OH or NH group.

## 5. Bonding of amino-acids

The amino-acids in RNA and DNA are connected to each other using hydrogen bonds.

Adenine - Thymine & Cytosine - Guanine (DNA)

Adenine - Uracil & Cytosine - Guanine (RNA)

The bonding between A-T (and A-U) uses 2 hydrogen bonds.

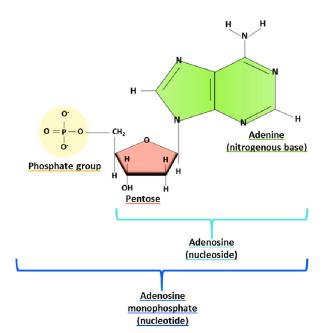
The bonding between C-G uses 3 hydrogen bonds.

#### 6. Stability of DNA and RNA

DNA is more stable than RNA because of the double helix and Thymine being a stronger nucleic acid than Uracil. However, DNA is also easier to manipulate.

Another factor is that in ribose there exists another OH-group which is less stable than a normal hydrogen atom → see point 8

## 7. Structure of nucleotide and nucleoside (and thus of RNA and DNA)



Nucleosides are used for RNA, they consists out of:

base + ribose (or deoxyribose)

Nucleotides are used for DNA, they consists out of:

phosphate + base + ribose (or deoxyribose)

## 8. Naming of nucleotides/nucleosides

If the sugar that is used is deoxyribose instead of ribose, add "deoxy" as a prefix

## • Naming of <u>nucleosides</u>:

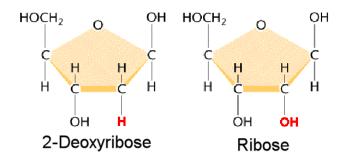
 $\begin{array}{cccc} \text{adenine} & \to & \text{adenosine} \\ \text{guanine} & \to & \text{guanosine} \\ \text{uracil} & \to & \text{uridine} \\ \text{cytosine} & \to & \text{cytidine} \\ \end{array}$ 

thymine → thymidine (yet can't be used in RNA so deoxythymidine)

## • Naming of nucleotides:

adenine → adenosine - 5' - .... phosphate
guanine → guanosine - 5' - .... phosphate
uracil → uridine - 5' - .... phosphate
cytosine → cytidine - 5' - .... phosphate
thymine → deoxythymidine - 5' - .... phosphate

#### In .... add mono-, di-, or tri- for the number of phosphates



You know if a nucleotide/nucleoside is RNA or DNA by checking the second carbon on the sugar group.

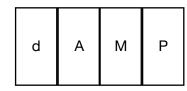
If it has a OH-group attached its Ribose and thus RNA.

If it has a H-atom attached its Deoxyribose and thus DNA.

• The short manner of naming the nucleotide (or nucleoside) is done as follows:

The first column: Enter a 'd' if DNA

Enter nothing if RNA



#### The second column:

Enter the base (A-T-C-G-U) or 'N' if you don't know the base

#### The third column:

Enter the number of phosphates (attached to 5' of the carbon sugar) → (M)ono, (D)i, (T)ri

Example:

#### The fourth column:

End the name with 'phosphate' (unless its RNA) → just the letter 'P'

# 9. Properties of biochemical materials

Enzymes end with -ase

In general an enzyme exists of many amino-acids. These amino-acids can be called the monomers. A rare case is the oligomer that exists out of 3 monomers.

An enzyme is a polymer (many monomers) of amino-acids.

- Describe the three main biomaterials and their building blocks
- · Describe and draw the chemical structure and main chemical bonds of DNA and RNA
- Explain the naming of nucleotides
- Explain nucleotides biosynthesis and regulation
- Understand transcription and translation (DNA to metabolites)
- Describe heterologous expression
- · Describe coiling and re-coiling
- Draw the Haworth projection and the chair confirmation
- · Fats and oil structures
- Disulfide bonds
- Repeat everything from MC

## Multiple choice section

- · Describe chemical properties of (mono)saccharides
  - 1. Number of carbon atoms and naming
  - 2. Physical properties
  - 3. Cyclic structures (puran & furan)
- Some extra types of isomers
  - 4. Epimers
  - 5. Anomers
- · Derive name and bond from chemical structure of carbohydrates
  - 6. Glycosidic bonds

#### Method and explanation:

#### 1. Number of carbon atoms and naming

In general we have carbohydrates also called sugars or saccharides.  $C_n(H_2O)_n\,$ 

→ 'n' is mostly 5 or 6

Sacharides can be divided into four categories: monosaccharides (1), disaccharides (2), oligosaccharides (3) and polysaccharides (many).

## Monosaccharides:

- Simple sugars
- Nature of the carbonyl group

#### Naming of monosaccharides:

- The prefixes tri-, tetra-, penta- are used to indicate the number of carbon atoms in the chain
- The suffix -ose indicates that a molecule is a carbohydrate

#### 2. Physical properties of monosaccharides

- Monosaccharides are colorless, crystalline solids
- Hydrogen bonding is possible between the polar -OH groups and H<sub>2</sub>O
- · And thus, all monosaccharides are very soluble in water
- They are only slightly soluble in alcohol
- They are insoluble in non-hydroxylic solvents such as ether, chloroform, or benzene

## 3. Cyclic structures (Pyran & Fyran)

 Six-membered hemiacetal (or hemiketal) rings are known as <u>pyranoses</u>, after the heterocycle <u>pyran</u>.



Hemiacetal (or hemiketal) = the fact that a single alcohol has been added to the carbonyl group (C=O)

 Five-membered hemiacetal or hemiketal rings are known as <u>furanoses</u>, after the heterocycle <u>furan</u>.



furan

## 4. Epimers (stereoisomer)

An epimer is one of a pair of diastereomers (SEE 3.4). The two epimers have opposite configuration at only one chiral center out of at least two. All other chiral centers in the molecules are the same in each.

Epimerization is the transformation of one epimer to the other epimer.

#### 5. Anomers (stereoisomer)

An anomer is a specific case of an epimer. It is an epimer at the hemiacetal carbon (the carbon that has an OH-group attached to it) in a *cyclic* saccharide. This specific carbon is called the anomeric carbon.

Anomerization is the transformation of one anomer to the other anomer.

The left and right form are the different anomers of glucose. The middle would be an epimer.

Like any stereoisomer; anomers and epimers have a difference in physical properties (e.g. boiling point) → see 3.4 (diastereoisomers)

## 6. Glycosidic bonds

A glycosidic bond is a covalent bond that joins a carbohydrate (saccharide) to another group (which could be another carbohydrate). It is a condensation reaction.

This bond is formed between the hemiacetal (or hemiketal) group of the saccharide and the OH-group of some compound. The resulting substance is called a glycoside.

The bond forms at the anomeric carbon and connects to the OH-group.

The naming of the bonds is depended on the molecule that is linked to the glycosidic oxygen.

O-glycosidic bonds - an oxygen is linked S-glycosidic bonds - the oxygen is replaced with a sulfur atom N-glycosidic bonds - the oxygen is replaced with a nitrogen atom (see figure)

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- Describe the general chemical properties of carbohydrates (main monosaccharides and polysaccharides)
- Describe chiral properties of carbohydrates
- Convert Fisher projection of monosaccharides to Haworth's projection
- Derive the name of carbohydrates and their bonds from their chemical structure
- Different configurations of (poly)saccharides
- · Chirality in saccharides
- · Mutarotation of monosaccharides
- Repeat everything from MC

# Multiple choice section

- Describe the process from DNA to protein
  - 1. DNA to mRNA (transcription)
  - 2. mRNA to amino acids (translation)
- Protein structure
  - 3. Covalent bonds (peptide & disulphide)
  - 4. Primary, secondary, tertiary, quaternary
  - 5. Forces stabilising protein
- · Protein functions
  - 6. Know the 6 different types of enzymes
  - 7. Describe the active site
- Acidic properties
  - 8. Isoelectric point of amino-acids

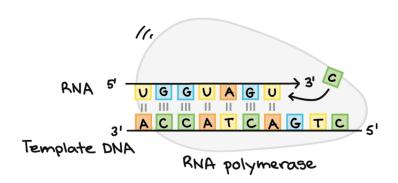
#### Method and explanation:

## 1. DNA to mRNA (transcription)

For this process, the DNA double helix unwinds near the gene that is getting transcribed. The region that is opened up, is called the <u>transcription bubble</u>.

Transcription uses the opposite of the <u>template strand</u> and turns it into an RNA strand. This mRNA strand is the same as the <u>coding strand</u> of the DNA, yet the T's are replaced with the U's.

In the process of transcription, there are enzymes that do the actual transcribing (called RNA polymerases). They will add an opposite of the <u>template strand</u> to the RNA strand.



This process can only be done in the **5' to 3' order.** Implying that it can only add RNA nucleotides (A, U, C, G) to the 3' end of the (RNA) strand.

The 5' and 3' are named after the molecule that is attached to which carbon of the sugar ring.

(phoshate = DNA; hydroxyl = RNA)

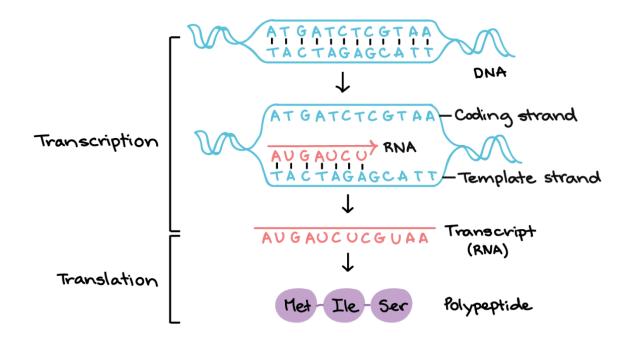
## 2. mRNA to amino acids (translation)

In this stage the mRNA is 'decoded' to build a (chunk of a) protein that contains a specific series of amino acids.

The messenger RNA (mRNA) contains the information of the genetic code that is to be written. It translates three nucleotides into <u>codons</u>.

Second letter								
		U	С	Α	G			
	U	UUU }Phe UUA }Leu UUG }	UCU UCC UCA UCG	UAU Tyr UAC Stop UAG Stop	UGU Cys UGC Stop UGG Trp	UCAG		
letter	С	CUU CUC CUA CUG	CCU CCC CCA CCG	CAU His CAC GIN CAG GIN	CGU CGC CGA CGG	UCAG	Third letter	
First letter	Α	AUU AUC AUA AUG Met	ACU ACC ACA ACG	AAU Asn AAC Lys AAG Lys	AGU Ser AGC AGA Arg	UCAG	Third	
	G	GUU GUC GUA GUG	GCU GCC GCA GCG	GAU Asp GAC GAA GAG Glu	GGU GGC GGA GGG	UCAG		

The overall process of DNA transcription and translation (so from DNA to polypeptides) is described in the following figure. *(SEE ALSO BINAS 71E and 71G)* 



6

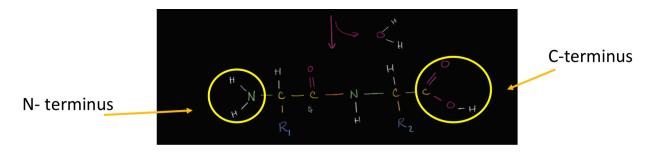
#### 3. Covalent bonds (peptides & disulphide) (protein structure)

**Peptides** are amino-acids polymers containing 2-50 individual units. If peptides > 50 units they are called *proteins*.

Two types of covalent bonds

- Peptide bond -dehydration
- Disulphide bond (between two Cys)

<u>Peptides bonds</u> are bonds between amino-acids. The connection/bond is made via the CH and NH groups. The naming is; first the N-terminal amino acid (on the left) and the C-terminal amino acid second (on the right).



<u>Disulphide bonds</u> are bonds between two Cysteine residues. This will create a sulphur-sulphur bond. They are of great importance in the shaping of proteins and make a protein very stable (nails, hair, horn).

#### **4. Primary, secondary, tertiary, quaternary** (protein structure)

The protein structure is built up of 4 categories;

#### Primary structure:

The sequence of a chain of amino acids (kind of-, number of-, order of amino acids)

#### Secondary structure:

If the structure has any hydrogen bonds that form an alpha helix or a pleated sheet.

#### <u>Tertiary structure:</u>

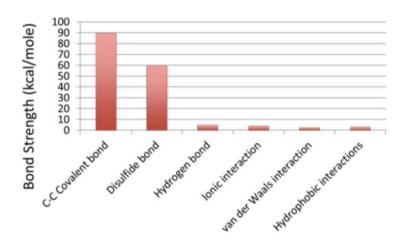
Occurs when certain connections are present between these alpha helices or pleated sheets. This is the ACTIVE state of the protein.

#### Quaternary structure:

The overall result; a protein consisting of more than one amino-acid chain.

## **5. Forces stabilising protein** (protein structure)

There are different bonds stabilising a protein. See the figure below for the order of strength of each bond.



## 6. Know the 6 different types of enzymes (protein function)

Individual subunits can transform into dimers (or higher order structures). A dimer is a combination of two proteins (quaternary structure).

These subunits can be identical or different.

An identical subunit = homomeric

A different subunit = heteromeric

Proteins have the following functions:

- I. Catalyse all metabolic pathways (enzymes)
- II. Provide structure (nails, skin, hair)
- III. Allow movement (muscles, transport within cells)
- IV. Regulate cellular process (DNA and RNA synthesis)

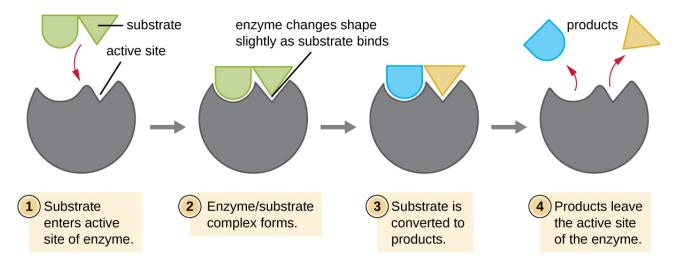
Enzymes (proteins) can be categorised into 6 major categories:

- A. **Oxidoreductases** = transfer electrons between molecules and catalyse oxidation reduction reactions
- B. **Transferase** = transfer functional groups between molecules
- C. **Hydrolases** = cleave molecules by addition of water
- Lyases = add atom or functional group to a double bond or remove them to form a double bond
- E. **Isomerases** = move functional group within a molecule
- F. **Ligases** = join two molecules at the expense of ATP hydrolysis & DNA ligase is the enzyme replication

## 7. Describe the active site (protein function)

Enzymes work as *catalyst* by using their active site. This will stabilise the transition state and lower the energy for a sequential reaction (of the substrates) that is to be catalysed.

Every enzyme has two active sites, both only fit a specific type of substrate.



The process is described above.

There are two key theories on how the substrate enters the active site.

- The <u>induced fit</u> proposes that an enzyme mutates in shape to host the substrate
- The <u>lock and key principle</u> proposes that a substrate only suits a specific enzyme (see figure)

#### 8. Isoelectric point of amino-acids

Like any acid, an amino acid also has a pKa, the lower the pKa, the stronger the acid.

 If the pH solution is lower than pK<sub>a</sub>, the compound is protonated (has an extra hydrogen-ion) → acids

$$pK_{a} = 9.6$$

$$H_{2}N - CH - C - OH$$

$$CH_{2}$$

$$C = O$$

$$OH$$

$$PK_{a} = 3.7$$
Aspartic acid

$$pI = (3.7 + 1.9)/2 = 2.8$$

•If the pH solution is higher than  $pK_a$ , the compound is deprotonated (is short off an hydrogen-ion)  $\rightarrow$  base

Amino acids (and other biological compounds) contain more than one pK<sub>a</sub> value, implying they exist in different acid/base conjugate forms depending on the pH of the solution.

**Isoelectric point (pl)** = point at which there is no net charge

This point is computed by adding the  $pK_a$  of the two groups that have the most-similar  $pK_a$  and dividing it by 2.

See figure.

- Be able to draw process of transcription and translation (of DNA)
- · Draw a peptide bond
- Describe pKa and pl and their relation
- Describe the 4 levels of structure and be able to recognise them
- · Recognise and describe forces stabilising protein structure
- Describe and draw the process of recombinant protein expression
- Be able to describe the process of protein purification
- · Describe function of proteins
- Explain and recognise 6 enzyme classifications
- · Describe the effect of pH and temperature on enzyme function
- · Describe the characteristics of an active site
- Understand enzyme catalysis
- Describe free energy
- The inhibition of enzymes
- Repeat everything from MC

# Multiple choice section

- Interatomic bonding
  - 1. Why do atoms bond
  - 2. Types of bonding (ionic, covalent, metallic)
  - 3. Van der Waals -bonding
  - 4. Mixed bonding

## Method and explanation:

#### 1. Why do atoms bond

Atoms have the tendency to form the electron configuration of (the nearest) noble gas. This tendency is otherwise referred to as the <u>octet rule</u>; implying every atom wants 8 electrons in their valence shell (outer shell).

This is because of two concepts:

- I. Since the <u>valence electrons</u> in the outer shell might be of an abundance or shortage, the atom will try to get rid of an electron or try to inherit one.
- II. The <u>electronegativity</u> is a measure on how bad it wants to attract or repel such an electron (to adhere to the octet rule)

This a reason to bond; to get an electron or share one, with another atom.

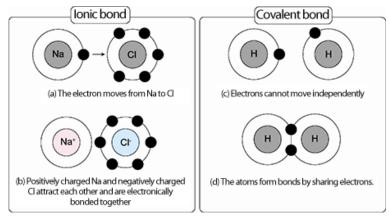
Using the rules of the Lewis structure (not part of MC exam) we can compute the number of electrons that an atom has (and thus determine if it's abides the octet rule). With this note that a covalent bond between two atoms acts as 2 electrons (one for each atom).

## 2. Types of bonding (ionic, covalent, metallic)

<u>Ionic bonding</u> = involves an electrostatic attraction between oppositely charged ions.

This is due to a large difference in electronegativity.

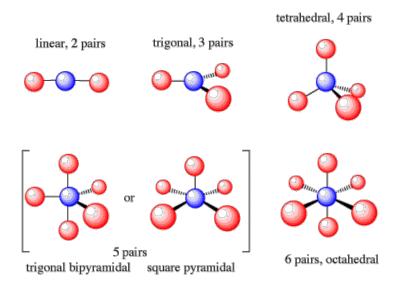
The transfer of electrons is known as electrovalence in contrast to covalence (for covalent bonding).



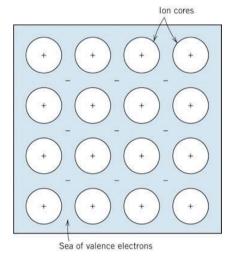
<u>Covalent bonding</u> = adjacent atoms share common electron pairs where each atom donates at least 1 electron.

The coordination number and bond angle are strongly determined by orbital geometry.

- → the coordination number is another word for the type of structure, with 3 different structure options:
- Linear (2 atoms straight across from each other) → 180°
- Trigonal (3 atoms in a triangle) → 120°
- Tetrahedral (4 atoms in a tetrahedron) → 109,5°



<u>Metallic bonding</u> = the valence electrons are delocalised from the atoms (cores) and can more or less move freely through the metal (form together an 'electron sea')



This type of bonding can only occur between two metal atoms.

Like with the ionic bonding, metallic bonds have a strong driving force for a mutual maximum coordination, implying they are often closed packs.

These form a metal cluster.

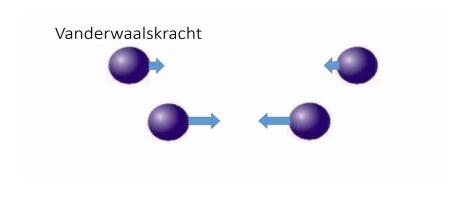
#### IN SUMMARY:

- Large difference in electronegativity gives ionic bonding
- Small difference gives covalent bonding
- Combinations of metal atoms gives metallic bonding

#### 3. Van-der-Waals bonding

This type of bonding is weak compared to the previous types. It is a distance-dependent interaction between atoms and molecules.

It's based on the interaction of dipoles (atoms that have a difference in electronegativity, the charge is divided over the core of the atom).





## 4. Mixed bonding

A bonding will usually have a mixed <u>covalent</u> and <u>ionic</u> character, where on type can strongly dominate.

Although rare, a solid can have a covalent / ionic, a metallic and a van-der-Waals bonding simultaneously.

The chemical and physical properties are determined by the type of bonding. This also means that from the material in the periodic table you can derive the type of bonding.

The summary of the different types of bonding and their properties are given in the figure below.

Bonding	Metallic	Covalent	Ionic	v.d. Waals+ Covalent
Material	Metal	Ceramic/ Semiconductor	Ceramic	Polymer
Electrical Conduction	High	Low*	Low*	Low*
Thermal Conduction	High	Low*	Low	Low
Ductility	High*	Low	Low	High
Hardness	Low*	High	High	Low
Melting point	Low-High	High	High	Low*

Take care: The indicated behavior (Low or High) holds in general, but exceptions are possible; particularly when a \* is added, there are special cases where strongly deviating behavior is possible.

- Know the three types of chemical bonding (covalent, ionic and metallic)
- Understand, with the help of the periodic table, what type of bonding will dominate if elements will be brought together in a material.
- Know in general sense how the types of bonding influence the material properties.
- Know the different categories of material properties (mechanical, electrical, magnetic, thermal, optical)
- Repeat everything from MC

- 1. Understand the concept of stress and strain in the case of isotropic elastic behaviour
- 2. Know what a tensile test is (plastic and elastic behaviour)
- 3. Know the concept of ductility and toughness
- 4. Know the difference between the normally used (engineering) stress and strain and the true stress and strain
- 5. Know the concept of hardening (and hardness test)

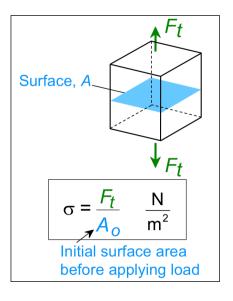
#### Method and explanation:

# 1. Understand the concept of stress and strain in the case of isotropic elastic behaviour

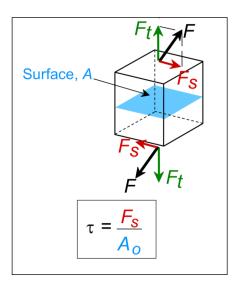
• <u>Stress</u> = the force divided by the surface area (the applied force).

There is two types of stress:

**Normal stress**  $\sigma$  (F $\perp$ A)



Shear stress  $\tau$  (FIA)



• Strain = the measure of deformation (relative change in length).

Strain has no subunit, since its length divided by length.

There is three types of strain:

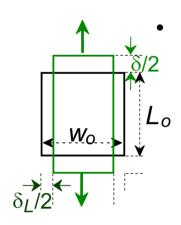
**Tensile strain** = fractional increase in length

$$\varepsilon_{//} = \frac{\delta}{L_o}$$
 The formula is: { change in length / original length }

**Compressive strain** = fractional decrease in length (width)

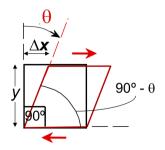
The formula is: { -change in width / original width }

The figure below illustrates these two types of strain.



**Shear strain** = the ratio of the change in deformation to its original length (sideways)

$$\gamma = \Delta x/y = \tan \theta$$
 It's the tangent of the angle, since the strain is the hypothenuse of the triangle.



### 2. Know what a tensile test is

It tests the tension a certain material can withstand. Consists out of three parts:

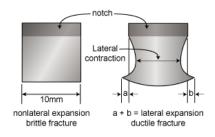
#### Part 1: Elastic

If the stress disappears, so does the strain. This is because of the linear behaviour between stress and strain (the constant of proportionality is E).

$$arepsilon_{//}=rac{oldsymbol{\sigma}}{E},\quad arepsilon_{\perp}=-
urac{oldsymbol{\sigma}}{E}$$

E: Elastic modulus (Young's modules) = measure of stiffness

v : Poisson's ration (in case of <u>lateral</u> <u>contraction</u>)



This image shows the meaning of lateral contraction or (in this case also) lateral expansion

If the volume doesn't change, the **tensile strain** (which is parallel to stress) will only change in one direction. Yet, the **compressive strain** is in two orthogonal directions. This can be seen in the formula below:

$$\begin{split} \Delta V = 0 \Longrightarrow \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \varepsilon_{//} + 2\varepsilon_{\perp} = 0 \Longrightarrow \nu = \frac{1}{2} \\ \text{In practice:} \qquad \Delta V > 0 \Longrightarrow \nu < \frac{1}{2} \quad \text{( 0.2 - 0.25: ceramics, glass } \\ 0.25 - 0.35: \text{ metals, } 0.5: \text{ elastomers )} \end{split}$$

E, v: Constants for elastically isotropic materials

For ceramics, glass and metal volume increases with strain, therefore the Poisson ratio is smaller than 0.5.

#### Part 2: Plastic

If the stress disappears, the non-elastic part of the strain remains. This causes for a permanent change in length.

The transition from elastic to plastic behaviour:

- The highest stress possible without plastic deformation is called elastic limit
- Yielding, the stress at which yielding occurs is called *yield strength*
- → yield strength = the point where there is a large permanent change in length with no extra load force

The transition is because of atomic planes that slide along each other, causing permanent change in length.

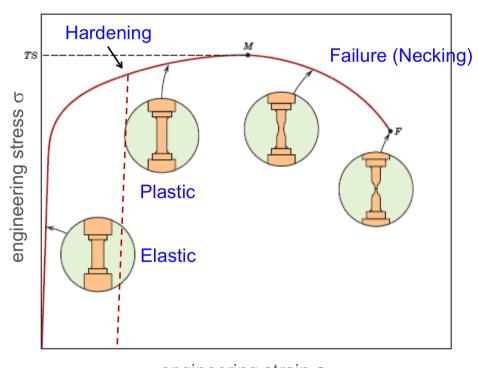
## Part 3: Failure (breaking)

The maximum stress that a material can withstand is the (ultimate) tensile strength.

In this phase, stress decreases, yet strain will remain increasing. This increase in strain causes for a rapid thinning and elongation called *necking*.

Fracture strain is the point where fracture occurs (also called elongation).

The three phases of the tensile test are described in this figure.



engineering strain  $\epsilon$ 

#### 3. Know the concept of ductility and toughness

<u>Ductility (brittleness)</u> = the deformability of a material, can be measured with fracture strain or elongation.

Brittle/ductile materials have a fracture strain that is substantially larger than the maximum elastic strain and is brittle if the fracture strain is mostly elastic.

<u>Toughness (U)</u> = work/energy

$$U = \int F ds = V_0 \int \sigma d\varepsilon$$

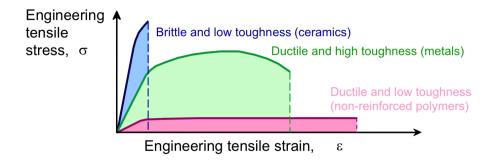
The energy needed is the integral of the force times the distance (through the material) [ex. car crash]

Easy to calculate for elastic part (triangle area):

$$U_e = \frac{V_0}{2}\sigma\varepsilon = \frac{V_0}{2}\frac{\sigma^2}{E}$$

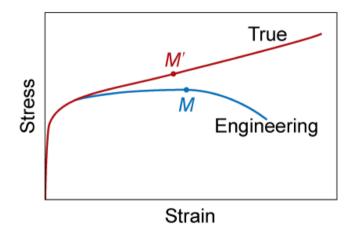
The energy needed is not only about the stress applied but also the Young's modulus (how much strain it can take before it breaks).

Both is needed for a big area under the curve. [ex. diamond breaks fast due to strain]



# 4. Know the difference between the normally used (engineering) stress and strain and the true stress and strain

Due to necking the area decreases, therefore the true stress increases



Formula true stress:

$$\sigma_T = \sigma(1+\varepsilon)$$

Formula true strain:

$$\varepsilon_T = \int_{l_0}^{l_i} \frac{dl}{l} = \ln(\frac{l_i}{l_0}) = \ln(1 + \varepsilon)$$

#### 5. Know the concept of hardening (and hardness test)

Hardening creates a resistance against local plastic deformation.

There are standardised tests for this concept (Vickers/Knoop/Brinell/Rockwell).

These tests use a hard object with a certain shape, pressing it into a test material with a specific load and loading time. The size of the resulting indentation is measured and converted into a hardness number using: *P/A*.

With P being the load (kg) and A the total surface (in mm<sup>2</sup>) of the residual indentation

- Be able to calculate stress and strain in the case of isotropic elastic behaviour
- · Know what a tensile test is
- · Know the difference between plastic and elastic behaviour
- Know that work per unit volume is equal to the surface below the stress-strain curve
- Know the difference between the normally used (engineering) stress and strain and the true stress and strain
- · Know the concept of hardening
- · Know what is meant by a hardness test
- · Know what is meant by dislocations
- Types of dislocations
- Understand the difference in the size of substitutional atoms and the consequences
- Repeat everything from MC

- 1. Understand the concept of dislocations and know the different types
- 2. Know the concept of fatigue, fracture and creep
- 3. Obstacles of dislocation movement

#### Method and explanation:

#### 1. Understand the concept of dislocations and know the different types

Dislocations are line defects in a material. They exist along a dislocation line. This line can never end in a crystal. Another vector exists, Burgers vector  $\overrightarrow{b}$  and is constant along a dislocation line.

Two different types of dislocations:

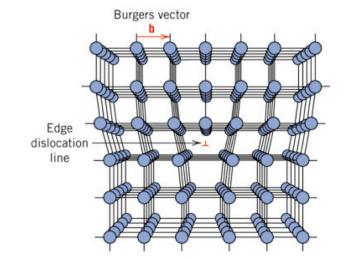
<u>Edge dislocation:</u> displacements of half a crystal plane. Burgers vector is perpendicular to the dislocation line.

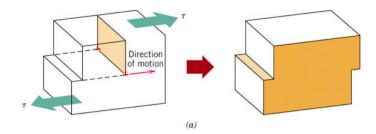
**Screw dislocation:** displacement of one crystal with every 360° turn. Burgers vector is parallel to the dislocation line.

Edge and screw dislocation can be seen in the figure on the right.

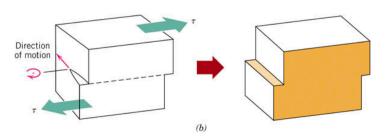
There is also another form of dislocation, called the **mixed dislocation**.

If the dislocation density is very high, the dislocations can't move. The only option for the material is to break.





Difference between dislocation type: edge (above) and screw (below)



#### 2. Know the concept of fatigue, fracture and creep

**Fatigue** = when applying a cyclic load (mean stress, stress amplitude and frequency of stress cycle) a material which is loaded far below the yield strength can still fail/break after a large amount of stress cycles.

Origin of fatigue is usually another initial problem like a notch.

#### Fatigue limit:

Below a certain stress level some materials can handle an infinite amount of cycle without fracture (ex. Steel).

Other materials like aluminium don't have this limit and can never made completely safe from fatigue (number of cycles until fracture increases with lower stress level).

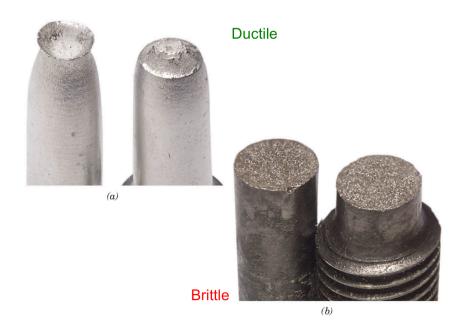
#### **Fracture** comes in two categories:

#### Brittle (e.g. ceramics):

- Small (permanent) strain, almost no necking
- Fracture surface is smooth
- Fracture surface is, for tension, perpendicular to the loading direction
- Fracture can occur intercrystalline (between grains) or intracrystalline (through grains)

#### Ductile (e.g. metals):

- High (permanent) strain, necking involved
- Fracture surface is rough
- Fracture surface is, for tension, in a 45° angle with respect to loading direction
- In thick sample with a ductile fracture, the central part usually still has brittle fracture, with only the outside ductile, giving a conic fracture surface.



**Creep** = with a static load at relatively high temperature (>0.4Tmelt) a material, that is loaded far below its yield strength, can break in time due to continuous straining.

Higher stress and/or temperature lead to more creep strain (earlier fracture).

#### 3. Obstacles of dislocation movement (strengthen materials)

The obstacles to the dislocation movement are:

- Other dislocations
- II. Interstitial or substitutional atom
- III. Grain boundaries
- IV. Precipitates

All these obstacles reduce dislocation mobility, increases the strength of the materials. Yet, this hardened material is also more brittle.

#### Other dislocations:

- Strain fields around dislocation lines cause dislocations to mutually hamper each other's movement, because they attract or repel each other
- Dislocation density increases but simultaneously dislocation mobility strongly decreases (called hardening).

#### Interstitial or substitutional atom

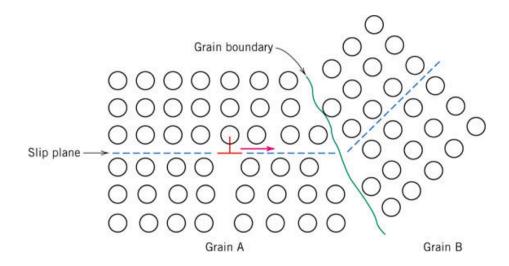
→ likes to be in compressive- or tensile strain regions of dislocation and restricts further sliding of dislocations

Smaller substitutional atoms:		Larger substitutional atoms:	
Prefer to be in compressive region around dislocation and hinder further slip of the dislocation		Prefer to be in tension region around dislocation and also hinder further slip of the dislocation	
(a)	000000 000000 000000 00000		

#### **Grain boundaries**

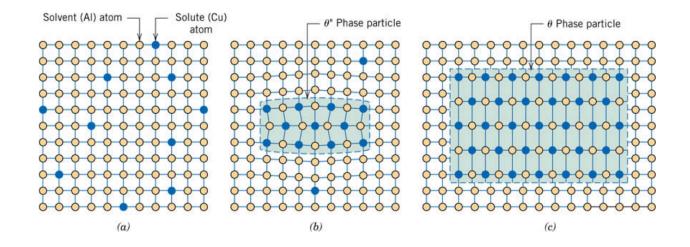
→ by disorientation and disordered space between grains, crossing of dislocations is strongly restricted

Smaller grains, results in an increasing strength of the material



### **Precipitates**

→ slip can usually not occur through precipitate and will have to move around it



Precipitates are technologically important for high strength in many metal alloys.

Many small ( $\theta$ ') particles provide much higher strength than a few big ( $\theta$ ) particles. Small particles usually have (semi-)coherent interfaces, which generate relatively large and long-range stress fields, while bigger particles usually have incoherent interfaces which hardly produce stress fields.

These obstacles can increase the strength, yet there are other methods. All are summarised below:

1. **Cold work/hardening** – dislocation is brought to a higher density which increases strength. Also, more brittle (lower ductility)

- 2. **Add substitutional atoms** add smaller atoms: smaller atoms prefer to be in compressive regions around dislocation, which hinder dislocation mobility. Add larger atoms: larger atoms prefer to be in tension regions around dislocation and hinder the dislocation mobility.
- 3. **Grain boundaries** by disorientated and disordered space between the grains, further slip of dislocation is strongly hampered.
- 4. **Precipitates** Many small particles provide more strength than large particles, since they have coherent interfaces. Mainly used in metal alloys.

- Know the difference between brittle and ductile fracture.
- Know the phenomenon of stress concentrations at 'defects' and the important role played by the radius of curvature of the crack tip.
- Understand, coupled to the previous point, why (a certain degree of) ductility is
  essential for making safe constructions and why the strongest material can turn out
  useless!
- Know that concerning fatigue there are materials with and without fatigue limit; know globally what the effect is of stress amplitude in combination with the average stress value on the fatigue behaviour.
- · Know when creep can occur.
- Know in general that materials under several special conditions can fail (fracture) while their load was considered sufficiently safe below the yield strength.
- · Repeat everything from MC

- 1. Understand the electrical properties of materials
- 2. Describe the different band structures of materials
- 3. Know the different types of semi-conductors

#### Method and explanation:

#### 1. Understand the electrical properties of materials

There are different electrical properties for any material.

- Ohm's law: V = IR (Voltage = Current x Resistance)
- Resistivity (measurement of resistance):  $\rho = \frac{RA}{l}$

with A = cross-sectional area and l = length of the wire

• Conductivity:  $\sigma = 1/\rho$ 

With electron conduction:  $\sigma = n|e|\mu_e$ 

with n number of free (=conduction) electrons per unit volume, |e| the absolute charge of an electron en  $\mu_e$  the electron mobility:  $\mu_e = \frac{v_d}{E}$ 

with  $v_d$  the average velocity of electrons in the the direction of the applied electrical field E (=  $-\frac{dV}{dx}$ )

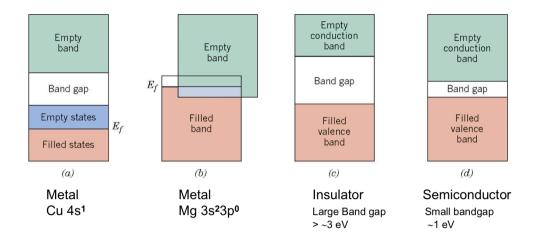
#### 2. Describe the different band structures of materials

The electron conductivity of materials differ significantly. This is due to the number of free electrons per unit → the conductivity difference between silver and diamond is 10<sup>24</sup>

The 'n' in the equation stands for this number of free electrons and the huge variances in 'n' can be explained using band structures.

Materials without bandgap between filled and empty states are metals and have enormous amount of free electrons per unit, whereas materials with a large bandgap between states have an extremely low number of free electrons per unit.

The size of the bandgap and thus the number of free electrons make up the difference between insulators and (semi-)conductors.



With increasing temperature, the conductivity increases.

## 3. Know the different types of semi-conductors

<u>Intrinsic semi-conductor</u> = the number of free electrons n is exactly equal to the number of holes (bandgaps) p.

$$\sigma = n|e|\mu_e + p|e|\mu_h$$

<u>Extrinsic n-type semi-conductor</u> = n >> p, in this case an '+1 element' enters the semi-conductor, which is an electron donor to the conduction band.

$$\sigma \approx C_a n = C_b \exp\left(-\frac{E_g - E_d}{kT}\right)$$

<u>Extrinsic p-type semi-conductor</u> = p >> n, in this case an '-1 element 'enters the semi- conductor, which is an electron acceptor to the valence band.

$$\sigma \approx C_c p = C_d \exp\left(-\frac{E_a}{kT}\right)$$

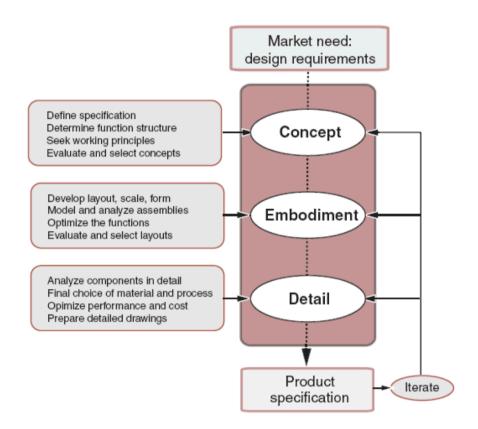
- The electrical properties of materials
  - Electron conduction
  - Metals
  - Semiconductors (different types)
- Know the difference between piezo-, pyro- and ferroelectrics
- Know the properties and usage of insulators and dielectrics
- · Repeat everything from MC

- 1. Describe the design process
- 2. Understand what materials data is available and how the selection works
- 3. Materials selection without shape
- 4. Materials selection with shape

#### Method and explanation:

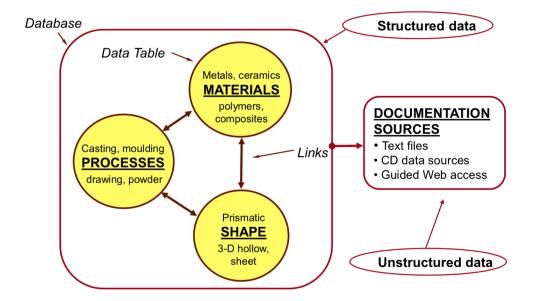
#### 1. Describe the design process

The design process describes how a product is made.

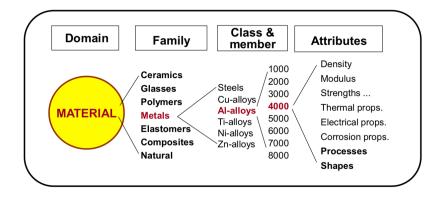


#### 2. Understand what materials data is available and how the selection works

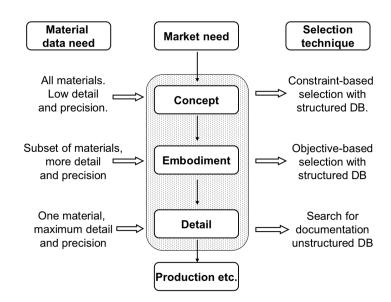
Materials data can be found in a structured database and consists of different categories; *materials*, their *processes* and the *shapes*.



The overall structure of a data table (one of yellow circles) is done in an order.  $\underline{Domain \rightarrow Family \rightarrow Class \& member \rightarrow Attributes}$ 

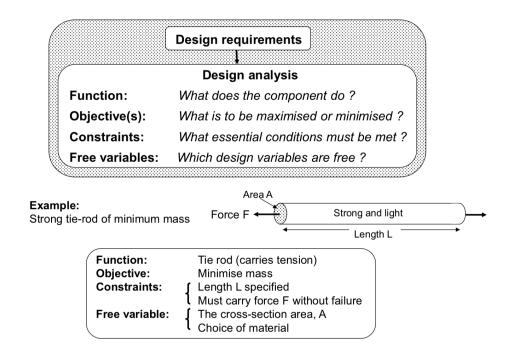


The selection of materials is based on the selection needs, as described in the figure below.



After a selection is made, the design can be configured (see design process in point 1).

The design will have certain requirements and an analysis can be made to determine these certain requirements.



The design analysis together with an example is shown in the figure above.

#### 3. Materials selection without shape

A materials selection has four categories: Process, Material, Function and Shape

In materials selection without shape, only the *Function* and the *Material* are used to select an alternative.

For this selection the **performance** is used: P = F(f, g, m) also described as  $P = F(functional\ requirements,\ geometric\ parameters,\ materials\ properties)$ 

Separable they can be used as:  $P = F_1(f) F_2(g) F_3(m)$ 

<u>Functional requirements</u> = the requirements in terms of function, such as safety factors and safe design

Geometric parameters = geometric measurements, such as length, height and area

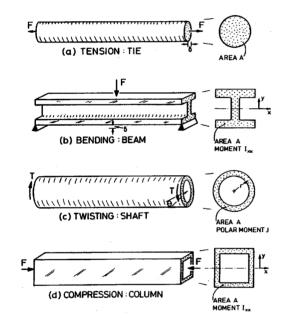
Material properties = properties like mass, density and stiffness.

#### 4. Materials selection with shape

In materials selection with shape, the *Function*, *Material* and *Shape* are used to select an alternative.

There exist standard structural members when it comes to the shape of a material.

Standard structural members in design



Area A matters, not shape!!!

Area A and shape I<sub>xx</sub> matter

Area A and shape J matter

Area A and shape I<sub>min</sub> matter in case of buckling; with pure compression shape does not matter!

There is a measurement for the efficiency gain by shaping a material, called the shape factor  $\phi \rightarrow \phi = \frac{4\pi l}{A^2}$ , with A = area and l = length

The shape factor can be divided in two different kinds, Bending and Torsion. The higher the shape factor, the higher the efficiency of shaping this material.

Bending:

**Torsion**:

$$\phi_B^e = \frac{4\pi I_{xx}}{A^2} = \frac{4\pi}{A^2} \int y^2 dA \qquad \qquad \phi_T^e = \frac{2\pi J}{A^2} = \frac{2\pi}{A^2} \int r^2 dA$$

With y is the distance of the bending axis and r is the length of the rotation axis (distance to the rotation centre).

- Understand the design process
- Understand what materials data is available and how the selection works
- Determine the best material based on design analysis
- Materials selection without shape
- · Materials selection with shape
- · Repeat everything from MC