

Structure and Properties of Materials

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Metals

M5x01185

Level 420 credits

JACS CODE J511

Aims

- ▶ To enable the student to analyse structure-property relationships in materials and predict behaviour for given structures

Learning outcomes

- ▶ Upon successful completion of this module, the student should be able to demonstrate:
 - ▶ 1 knowledge and understanding of the structure of crystalline and non-crystalline materials (component A)
 - ▶ 2 analytical skills in the application of appropriate laws to determine phase composition and both equilibrium and non-equilibrium structures and corresponding properties (components A and B)
 - ▶ 3 an in-depth understanding of the role of crystal defects in the behaviour of crystalline materials at both the microscopic and macroscopic level (component B)

Materials Science

- ▶ What is Materials Science?

Materials Science

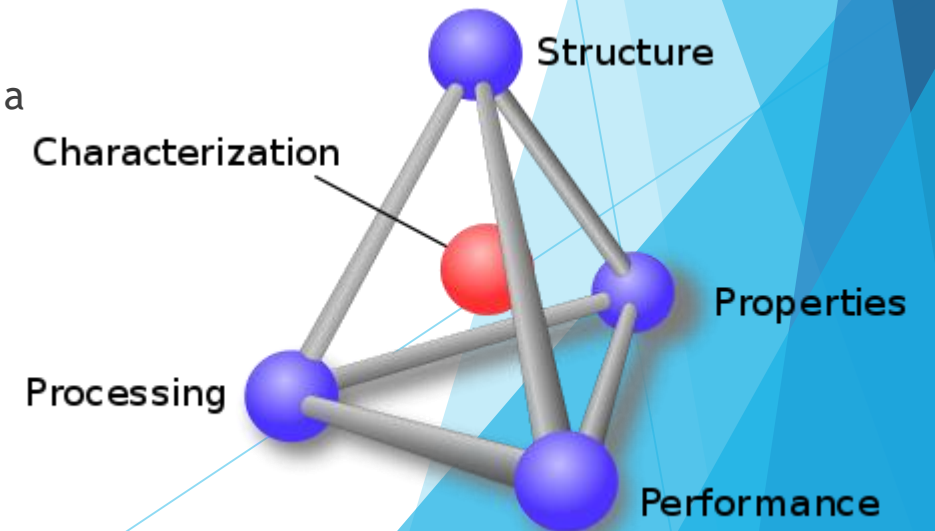
► What is materials science?

“Materials Science is an interdisciplinary subject, spanning the physics and chemistry of matter, engineering applications and industrial manufacturing processes.”
University of Oxford

This diverse programme subject had its foundations in physics and chemistry and covers the mechanical, electrical, magnetic and optical properties of materials, and the design, manufacture and applications of metals, alloys, ceramics, polymers, composites and biomaterials.

What is the relevance of Materials to Engineering and Manufacturing?

- ▶ A material is a substance, usually a solid, that is used to make anything from buildings to spacecraft.
- ▶ Materials can generally be divided into two classes: crystalline and non-crystalline. The traditional examples of materials are metals, semiconductors, ceramics and polymers. New and advanced materials that are being developed include nanomaterials and biomaterials.
- ▶ Materials science involves studying the structure of materials, and relating them to their properties.
- ▶ Materials scientists can use structure-property correlation to determine how a material will perform.
- ▶ Structure of a material consists of chemical elements and processing.
- ▶ Microstructure controls the material's properties.



Questions

- ▶ How do atoms assemble into solid structures?
- ▶ (for now, focus on metals)
- ▶ • How does the density of a material depend on its structure?
- ▶ • When do material properties vary with the sample (i.e., part) orientation?

Measures of length - fill in the blanks

- | | | | |
|------------|-----------------|-------------|------------------|
| ▶ M (mega) | 10 | ▶ | 10 ⁻³ |
| ▶ T (Tera) | 10 | ▶ μ (micro) | 10 |
| ▶ k (kilo) | 10 ³ | ▶ | 10 ⁻⁹ |
| ▶ p (pico) | 10 | ▶ G (Giga) | 10 ⁹ |
- ▶ 1 Ångström is equal to ? Nm = 10

Measures of length

- ▶ k (kilo) 10^3
- ▶ M (mega) 10^6
- ▶ G (Giga) 10^9
- ▶ T (Tera) 10^{12}

Measures of length

- ▶ k (kilo) 10^3
- ▶ M (mega) 10^6
- ▶ G (Giga) 10^9
- ▶ T (Tera) 10^{12}

- ▶ m (milli) 10^{-3}
- ▶ μ (micro) 10^{-6}
- ▶ n (nano) 10^{-9}
- ▶ p (pico) 10^{-12}

Measures of length

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|------------|-----------|-----------------|------------|
| ▶ k (kilo) | 10^3 | ▶ m (milli) | 10^{-3} |
| ▶ M (mega) | 10^6 | ▶ μ (micro) | 10^{-6} |
| ▶ G (Giga) | 10^9 | ▶ n (nano) | 10^{-9} |
| ▶ T (Tera) | 10^{12} | ▶ p (pico) | 10^{-12} |
-
- ▶ 1 Ångström is equal to $0.1\text{nm} = 10^{-10}$

Basic Chemistry Revision

- ▶ What is a mole?



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Basic Chemistry Revision

- ▶ What is a mole?
- ▶ In chemistry terms a mole is the unit for amount of substance
- ▶ What is molar mass?
- ▶ Molar mass is the relative formula mass in g, M_r (units g/mol)
- ▶ Relative formula mass (M_r) is mass of a molecule or compound (on a scale compared to carbon-12). It is calculated by adding up the relative atomic masses (A_r) of all the atoms present in the formula. Example:
The relative formula mass (M_r) for water (H_2O) is 18. Water = H_2O .
Atoms present = $(2 \times H) + (1 \times O)$



Calculating relative formula mass

- ▶ The relative formula mass of a substance made up of molecules is the sum of the relative atomic masses of the atoms in the numbers shown in the formula.
- ▶ Relative formula mass has the symbol, Mr. To calculate the Mr for a substance:
- ▶ work out how many atoms of each element there are in the chemical formula
- ▶ add together the Ar values for all the atoms of each element present
- ▶ For example, the formula for carbon dioxide is CO₂. It consists of one carbon atom (Ar = 12) and two oxygen atoms (Ar = 16):
- ▶ Mr of CO₂ = 12 + 16 + 16 = 44
- ▶ It could also be calculated this way:
- ▶ Mr of CO₂ = (1 × 12) + (2 × 16) = 12 + 32 = 44
- ▶ Like Ar values, Mr values are just numbers. They have no units because they are relative masses.

Relative formula masses of ionic compounds

- ▶ Ionic compounds such as sodium chloride do not exist as molecules. However, their relative formula masses are calculated in the same way, from the numbers shown in the formula.

Question

Calculate the relative formula mass, M_r , of calcium hydroxide, Ca(OH)_2 .
(A_r of Ca = 40, A_r of O = 16, A_r of H = 1)

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(A_r of Ca = 40, A_r of O = 16, A_r of H = 1)

- ▶ $M_r = 40 + (2 \times 16) + (2 \times 1)$
- ▶ $= 40 + 32 + 2$
- ▶ $= 74$
- ▶ It could also be calculated this way:
- ▶ $M_r = 40 + 2 \times (16 + 1)$
- ▶ $40 + 34 = 74$

Question

Calculate the relative formula mass, M_r , of magnesium nitrate, $\text{Mg}(\text{NO}_3)_2$.
(A_r of Mg = 24, A_r of N = 14, A_r of O = 16)

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(A_r of Mg = 24, A_r of N = 14, A_r of O = 16)

- ▶ $M_r = 24 + (2 \times 14) + (2 \times 3 \times 16)$
- ▶ $= 24 + 28 + 96$
- ▶ $= 148$
- ▶ It could also be calculated this way:
- ▶ $M_r = 24 + 2 \times [14 + (16 \times 3)]$
- ▶ $= 24 + 124$
- ▶ $= 148$

Law of conservation of mass

- ▶ The law of conservation of mass states that no atoms are lost or made in a chemical reaction. Instead, the atoms join together in different ways to form products. This is why, in a balanced symbol equation, the number of atoms of each element is the same on both sides of the equation.
- ▶ Since atoms are not lost or made in a chemical reaction, the total mass of the products is equal to the total mass of the reactants. The sum of the relative formula masses of the reactants is equal to the sum of the relative formula masses of the products.
- ▶ Eg. $2\text{Cu} + \text{O}_2 = 2\text{CuO}$
- ▶ 2 atoms of copper **added** to 1 molecule of oxygen consisting of 2 atoms reacts to form 2 molecules of copper oxide containing 4 atoms.

Calculations using the law

- ▶ The mass of one substance in a reaction can be calculated if the masses of the other substances are known. For example:
- ▶ $\text{CaCO}_3 = \text{CaO} + \text{CO}_2$
- ▶ Calcium Carbonate = Calcium Oxide + Carbon dioxide
- ▶ How many g? 28g 22g

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- ▶ $\text{CaCO}_3 = \text{CaO} + \text{CO}_2$
- ▶ Calcium Carbonate = Calcium Oxide + Carbon dioxide
- ▶ How many g? 28g 22g
- ▶ The calcium carbonate contains the same atoms in the calcium oxide + the carbon dioxide. The overall mass won't change so $28+22=50\text{g}$
- ▶ The calcium carbonate has a mass of 50g

Question

- ▶ $2\text{Mg} + \text{O}_2 = 2\text{MgO}$
- ▶ $48\text{g} + ? = 80\text{g}$
- ▶ 48 grams of magnesium and an unknown amount of oxygen make 80 grams of magnesium oxide
- ▶ How many grams of oxygen?

Reactions in closed systems

- ▶ No substances can enter or leave a closed system, such as a stoppered flask. Sometimes, reactions that happen in open beakers are closed systems, for example acid-alkali neutralisation reactions. Since all the reactants and products stay in the beaker, the total mass of the beaker and the substances in it stay the same during the reaction.

Reactions in non-enclosed systems

- ▶ Substances can enter or leave a non-enclosed system. These systems include open flasks, boiling tubes or crucibles that let gases enter or leave. For example:
- ▶ copper carbonate decomposes on heating to make solid copper oxide, which stays in the boiling tube, and carbon dioxide gas, which escapes
- ▶ magnesium reacts with oxygen, gained from the air, to produce magnesium oxide
- ▶ If a gas escapes, the total mass will look as if it has decreased. If a gas is gained, the total mass will look as if it has increased. However, the total mass stays the same if the mass of the gas is included.

Question

10.0 g of calcium carbonate, CaCO_3 , was heated in a **thermal decomposition** reaction. 5.60 g of solid remained after heating. The equation below represents the reaction:



Explain the change in mass.

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Explain the change in mass.

The mass appears to have decreased because one of the products, carbon dioxide, escapes to the air.

The total mass of the solid and gas products will be 10.0 g.

Chemical measurements

- ▶ Whenever a measurement is made in chemistry, there is always some uncertainty in the result obtained. There are many causes of uncertainty in chemical measurements. For example it may be difficult to judge:
 - ▶ whether a thermometer is showing a temperature of 24.0°C , 24.5°C or 25.0°C
 - ▶ exactly when a chemical reaction has finished
- ▶ There are two ways of estimating uncertainty:
 - ▶ by considering the resolution of measuring instruments
 - ▶ from the range of a set of repeat measurements

Estimating uncertainty from measuring instruments

- ▶ The resolution of a measuring instrument is the smallest change in a quantity that gives a change in the reading that can be seen. A thermometer with a mark at every 1.0°C has a resolution of 1.0°C . It has a higher resolution than a thermometer with a mark at every 2.0°C .
- ▶ The uncertainty of a measuring instrument is estimated as plus or minus ($\pm$) half the smallest scale division. For a thermometer with a mark at every 1.0°C , the uncertainty is $\pm 0.5^{\circ}\text{C}$. This means that if a student reads a value from this thermometer as 24.0°C , they could give the result as $24.0^{\circ}\text{C} \pm 0.5^{\circ}\text{C}$.
- ▶ For a **digital** measuring instrument, the uncertainty is half the last digit shown on its display. For a timer reading to 0.1 s, the uncertainty is ± 0.05 s.

Estimating uncertainty from sets of repeat measurements

- ▶ For a set of repeat measurements, the uncertainty is $\pm$ half the range. This means that the value can be given as the mean value $\pm$ half the range.

Question

The table shows five measurements for the volume of acid required in a neutralisation reaction. Calculate the mean volume and estimate the uncertainty.

Test number	1	2	3	4	5
Volume	24.0	24.5	23.5	25.0	23.0

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The table shows five measurements for the volume of acid required in a neutralisation reaction. Calculate the mean volume and estimate the uncertainty.

Test number	1	2	3	4	5
Volume	24.0	24.5	23.5	25.0	23.0

$$\text{mean} = \frac{24.0 + 24.5 + 23.5 + 25.0 + 23.0}{5}$$

$$= 24.0 \text{ cm}^3$$

$$\text{range} = (\text{biggest value} - \text{smallest value})$$

$$= 25.0 - 23.0$$

$$= 2.0 \text{ cm}^3$$

$$\text{uncertainty} = \pm \text{half the range}$$

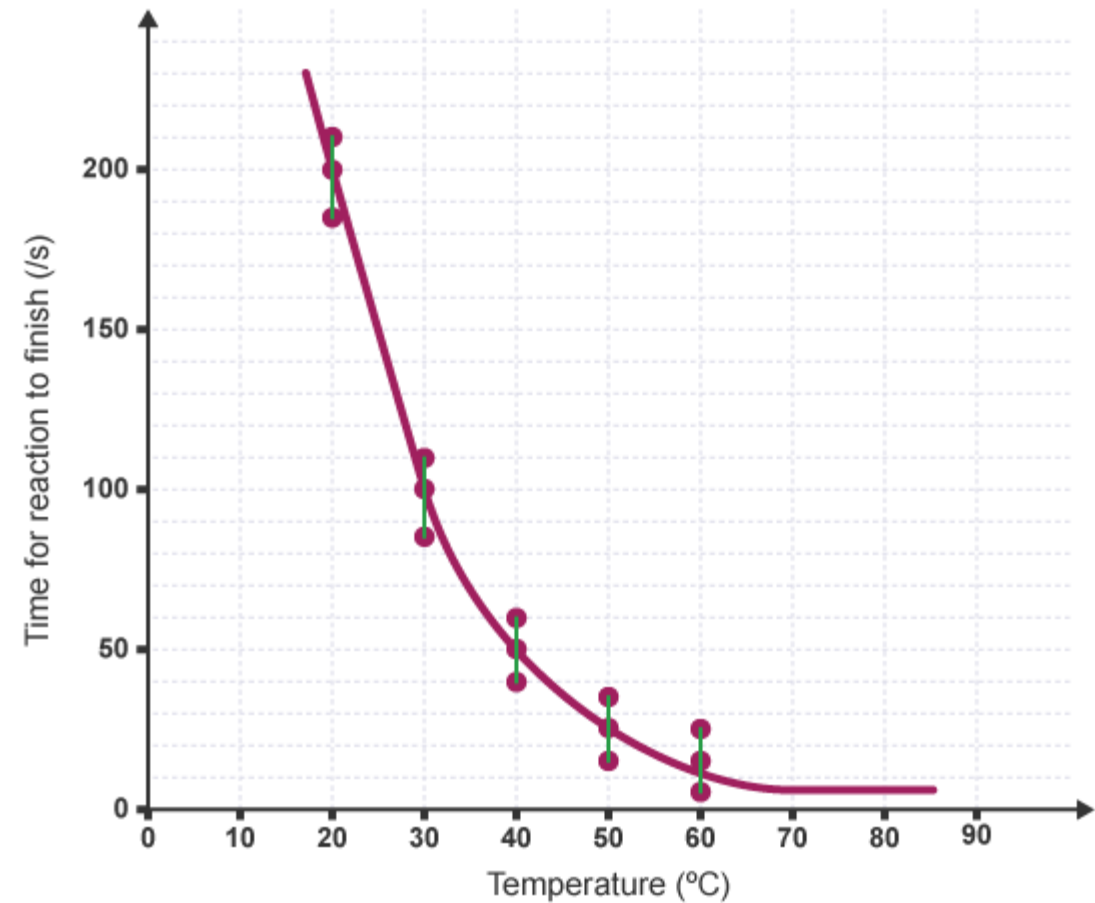
$$= \frac{2.0}{2} \text{ cm}^3$$

$$= \pm 1.0 \text{ cm}^3$$

$$\text{So the volume is } 24.0 \text{ cm}^3 \pm 1.0 \text{ cm}^3.$$

Showing uncertainty on a graph

- Uncertainty can also be shown on a graph. All the repeat readings for each value of the independent variable are plotted. Vertical lines joining these values represent the uncertainty.



A graph showing the repeat readings for each value of the independent variable. The short vertical lines represent uncertainty.

Concentration of solutions

- ▶ A solution forms when a solute dissolves in a solvent. The concentration of a solution is a measure of how 'crowded' the solute particles are. The more concentrated the solution, the more particles it contains in a given volume.
- ▶ **Calculating concentration**
- ▶ The concentration of a solution can be calculated using:
- ▶ the mass of dissolved solute in grams, g
- ▶ the volume of solution (or solvent) in cubic decimetres, dm³
- ▶ The units for concentration can also be shown as g dm⁻³, but this means the same as g/dm³.

$$\text{concentration in g/dm}^3 = \frac{\text{mass of solute in g}}{\text{volume in dm}^3}$$

Worked example

8 g of sodium hydroxide is dissolved in 2 dm³ of water. Calculate the concentration of the sodium hydroxide solution formed.

Concentration =

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Concentration =

$$\frac{\text{mass of solute in g}}{\text{volume in dm}^3}$$

$$= \frac{8 \text{ g}}{2 \text{ dm}^3}$$

$$\text{concentration} = 4 \text{ g/dm}^3$$

Volume units

- ▶ Apparatus used to measure volumes is usually marked in cm^3 or ml. Although these are different units, they describe the same volume.
- ▶ For example, $250 \text{ ml} = 250 \text{ cm}^3$.
- ▶ Volumes used in concentration calculations must be in dm^3 , not in cm^3 or ml. It is useful to know that $1 \text{ dm}^3 = 1000 \text{ cm}^3$. This means:
 - ▶ divide by 1000 to convert from cm^3 to dm^3
 - ▶ multiply by 1000 to convert from dm^3 to cm^3
- ▶ For example, 250 cm^3 is 0.25 dm^3 ($250 \div 1000$). It is often easiest to convert from cm^3 to dm^3 before continuing with a concentration calculation.

Question

100 cm³ of dilute hydrochloric acid contains 0.5 g of dissolved hydrogen chloride.
Calculate the concentration of the acid in g/dm³.

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Calculate the concentration of the acid in g/dm³.

$$\begin{aligned}\text{volume of acid} &= 100 \div 1000 = 0.1 \text{ dm}^3 \\ \text{concentration of acid} &= 0.5/0.1 \\ &= 5 \text{ g/dm}^3\end{aligned}$$

Calculating the mass of solute

- ▶ Rearranging the equation for concentration allows the mass of solute to be calculated:
- ▶ mass of solute in g = concentration in $\text{g/dm}^3 \times \text{volume in dm}^3$
- ▶ **Worked example**
- ▶ A solution of sodium chloride has a concentration of 10 g/dm^3 . What mass of sodium chloride is dissolved in 2 dm^3 of the solution?

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- ▶ **Worked example**
- ▶ A solution of sodium chloride has a concentration of 10 g/dm^3 . What mass of sodium chloride is dissolved in 2 dm^3 of the solution?
- ▶ mass of solute in g = concentration in $\text{g/dm}^3 \times \text{volume in dm}^3$
- ▶ $= 10 \text{ g/dm}^3 \times 2 \text{ dm}^3$
- ▶ $= 20 \text{ g}$

Elements are Materials too!

The Periodic Table puts elements in order of the structure of their atoms (how many protons they have and how many electrons they have in their outer shell) They are listed in the order of their atomic number, which is the number of protons in each atom.

Periodic Table of Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H Hydrogen 1.00794	Atomic # Symbol Name Atomic Mass																2 He Helium 4.002602
[C] Solid		[Hg] Liquid						[H] Gas		[Rf] Unknown							
3 Li Lithium 6.941		4 Be Beryllium 9.012182															
11 Na Sodium 22.98976928		12 Mg Magnesium 24.3050															
19 K Potassium 39.0983		20 Ca Calcium 40.078		21 Sc Scandium 44.955912		22 Ti Titanium 47.887		23 V Vanadium 50.9415		24 Cr Chromium 51.9961		25 Mn Manganese 54.938045		26 Fe Iron 55.845		27 Co Cobalt 58.933195	
37 Rb Rubidium 85.4678		38 Sr Strontium 87.62		39 Y Yttrium 88.90585		40 Zr Zirconium 91.224		41 Nb Niobium 92.90638		42 Mo Molybdenum 95.96		43 Tc Technetium (97.9072)		44 Ru Ruthenium 101.07		45 Rh Rhodium 102.90550	
55 Cs Cesium 132.9054519		56 Ba Barium 137.327		57-71		72 Hf Hafnium 178.49		73 Ta Tantalum 180.94788		74 W Tungsten 183.84		75 Re Rhenium 186.207		76 Os Osmium 190.23		77 Ir Iridium 192.222	
87 Fr Francium (223)		88 Ra Radium (226)		89-103		104 Rf Rutherfordium (261)		105 Db Dubnium (262)		106 Sg Seaborgium (266)		107 Bh Bohrium (264)		108 Hs Hassium (277)		109 Mt Meitnerium (268)	
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.																	
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57 La Lanthanum 138.90547		58 Ce Cerium 140.116		59 Pr Praseodymium 140.90765		60 Nd Neodymium 144.242		61 Pm Promethium (145)		62 Sm Samarium 150.36		63 Eu Europium 151.964		64 Gd Gadolinium 157.25		65 Tb Terbium 158.92535	
89 Ac Actinium (227)		90 Th Thorium 232.03806		91 Pa Protactinium 231.03688		92 U Uranium 238.02891		93 Np Neptunium (237)		94 Pu Plutonium (244)		95 Am Americium (243)		96 Cm Curium (247)		97 Bk Berkelium (247)	
												</					

Periodic Table of Elements

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18						
1	1 H Hydrogen 1.00794	Atomic # Symbol Name Atomic Mass C Solid Hg Liquid H Gas Rf Unknown Metals Alkali metals Alkaline earth metals Lanthanoids Actinoids Transition metals Poor metals Other nonmetals Noble gases																2	2 He Helium 4.002602					
2	3 Li Lithium 6.941	4 Be Beryllium 9.012182																	5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.0067	8 O Oxygen 15.9994	9 F Fluorine 18.9984032	10 Ne Neon 20.1797
3	11 Na Sodium 22.98976928	12 Mg Magnesium 24.3050																	13 Al Aluminum 26.9815386	14 Si Silicon 28.0855	15 P Phosphorus 30.973762	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948
4	19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.887	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.796						
5	37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.96	43 Tc Technetium (97.9072)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.293						
6	55 Cs Cesium 132.9054519	56 Ba Barium 137.327	57-71		72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98040	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)					
7	87 Fr Francium (223)	88 Ra Radium (226)	89-103		104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (277)	109 Mt Meitnerium (268)	110 Ds Darmstadtium (271)	111 Rg Roentgenium (272)	112 Uub Ununbium (285)	113 Uut Ununtrium (286)	114 Uuq Ununquadium (289)	115 Uup Ununpentium (288)	116 Uuh Ununhexium (292)	117 Uus Ununseptium (291)	118 Uuo Ununoctium (294)					

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

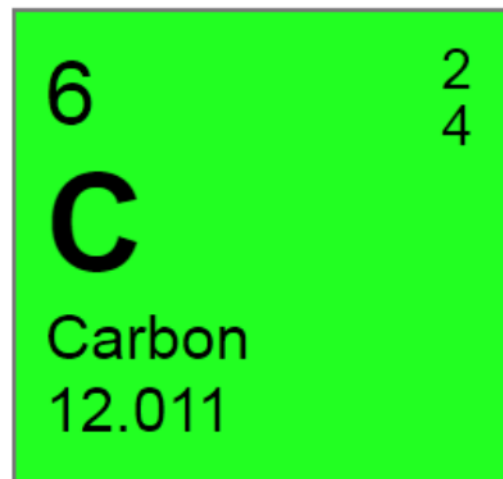
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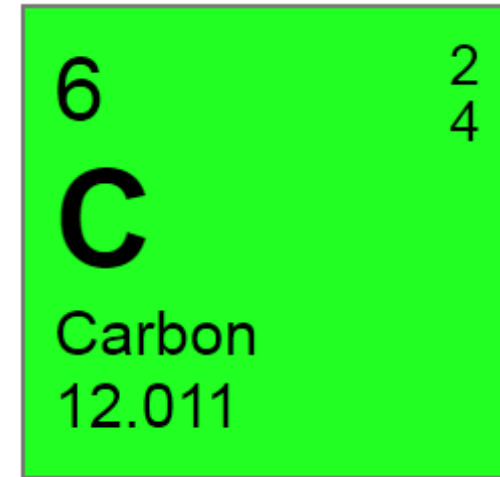
57	La Lanthanum 138.90547	58	Ce Cerium 140.116	59	Pr Praseodymium 140.90768	60	Nd Neodymium 144.242	61	Pm Promethium (145)	62	Sm Samarium 150.36	63	Eu Europium 151.964	64	Gd Gadolinium 157.25	65	Tb Terbium 158.92535	66	Dy Dysprosium 162.500	67	Ho Holmium 164.93032	68	Er Erbium 167.259	69	Tm Thulium 168.93421	70	Yb Ytterbium 173.054	71	Lu Lutetium 174.9668
89	Ac Actinium (227)	90	Th Thorium 232.03806	91	Pa Protactinium 231.03688	92	U Uranium 238.02891	93	Np Neptunium (237)	94	Pu Plutonium (244)	95	Am Americium (243)	96	Cm Curium (247)	97	Bk Berkelium (247)	98	Cf Californium (251)	99	Es Einsteinium (252)	100	Fm Fermium (257)	101	Md Mendelevium (268)	102	No Nobelium (259)	103	Lr Lawrencium (262)

1 electron in its outer shell

Full shell

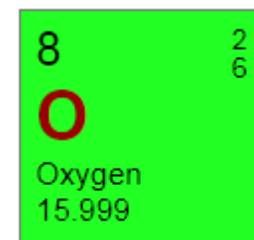
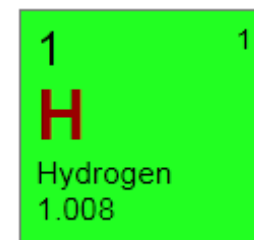


- ▶ Atomic number (No. protons=No. electrons) C=6
- ▶ No neutrons can vary giving different isotopes
- ▶ Electron shells 2,4
- ▶ Relative atomic mass (atomic weight) is an average of the atomic masses of all the different isotopes weighted by abundance C=12.011
- ▶ Mass number =No. protons + No. neutrons
- ▶ For C the No. neutrons =12 - 6 = 6



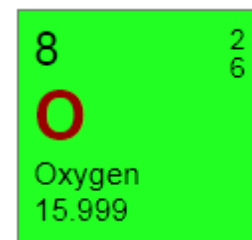
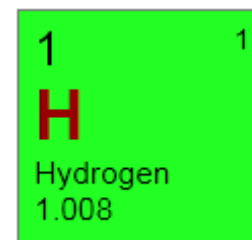
Example

- ▶ Atomic number (No. protons=No. electrons) $C=6$
- ▶ Relative atomic mass (atomic weight) is an average of the atomic masses of all the different isotopes weighted by abundance $C=12.011$
- ▶ To find Relative formula mass (M_r) add the relative atomic masses for all the atoms in its chemical formula
- ▶ What is the relative formula mass of water?



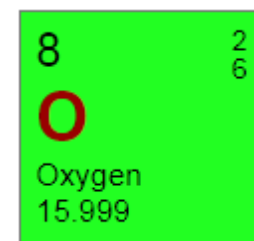
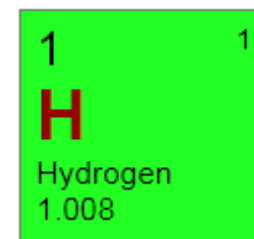
Example

- ▶ Atomic number (No. protons=No. electrons) $Z=6$
- ▶ Relative atomic mass (atomic weight) is an average of the atomic masses of all the different isotopes weighted by abundance $A_r=12.011$
- ▶ To find Relative formula mass (M_r) add the relative atomic masses for all the atoms in its chemical formula
- ▶ What is the relative formula mass of water?
- ▶ H_2O so $H + H + O$



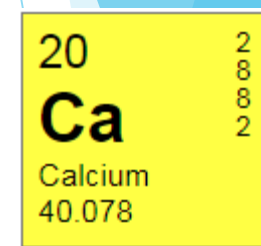
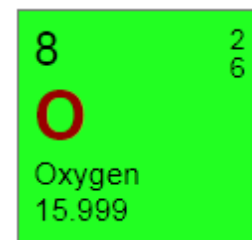
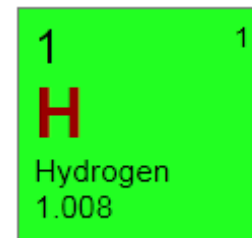
Example

- ▶ Atomic number (No. protons=No. electrons) $Z=6$
- ▶ Relative atomic mass (atomic weight) is an average of the atomic masses of all the different isotopes weighted by abundance $A_r=12.011$
- ▶ To find Relative formula mass (M_r) add the relative atomic masses for all the atoms in its chemical formula
- ▶ What is the relative formula mass of water?
- ▶ H_2O so $H + H + O$
- ▶ $M_r = 1+1+16 = 18$



Example 2

- ▶ What is the relative formula mass of Ca(OH)_2 ?
- ▶ $\text{Ca} + \text{O} + \text{H} + \text{O} + \text{H}$
- ▶ $M_r = 40 + 16 + 1 + 16 + 1 = 74$



Mole

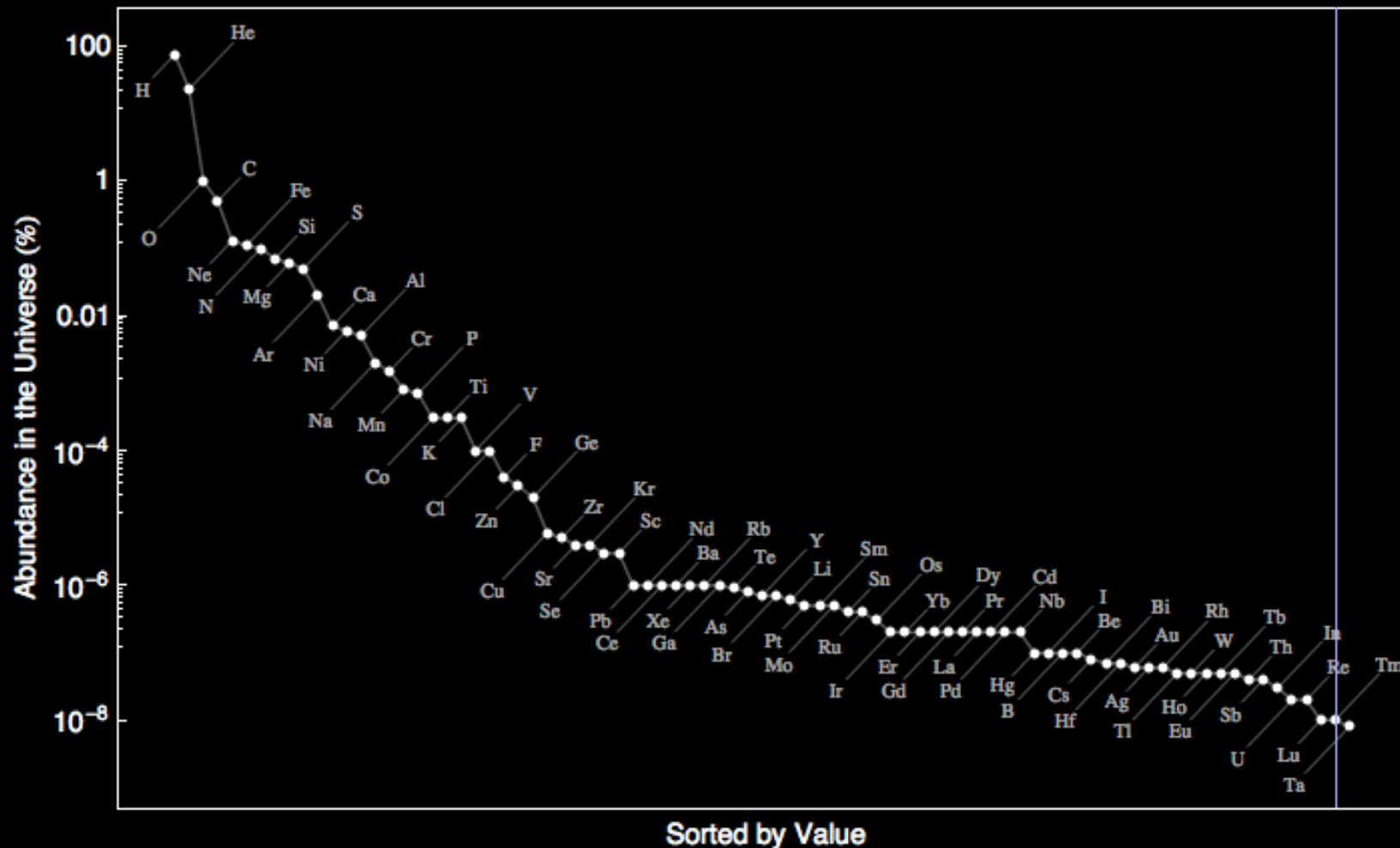
- ▶ One mole (mol) = $6 \times 10_{23}$ (Avagadro's number)
- ▶ This is equal to the number of carbon atoms in 12g of carbon
- ▶ Mr of water is 18
- ▶ Molar mass of water is 18g/mol
- ▶ Mr of calcium hydroxide is 74 so its molar mass is 74g/mol

Periodic Table Facts

- ▶ The rows of the periodic table are called periods
- ▶ An element's period number is the highest unexcited energy level for an electron of that element.
- ▶ Columns of elements form groups, elements in a group share common properties and have the same outer electron arrangement
- ▶ Most of the elements are metals
- ▶ Size of an atom is determined by the diameter of the outer shell so atoms don't always get larger as their atomic number increases, in fact element atoms decrease in size as you go from left to right
- ▶ As you go down, the melting point tends to decrease.
- ▶ As you go down or right the ionization energy increases. (energy to remove the most weakly bound electron).
- ▶ Francium is the rarest element on earth.
- ▶ The only letter not in the periodic table is the letter J.
- ▶ The country Argentina is named after the element silver (symbol Ag) which is argentum in Latin.
- ▶ Although there is helium on Earth, it was first discovered by observing the sun.

Table 1.1 Relative Abundance of Elements in the Universe

Element	Relative Abundance (Si = 1)
Hydrogen (H)	12,000
Helium (He)	2,800
Oxygen (O)	16
Nitrogen (N)	8
Carbon (C)	3
Iron (Fe)	2.6
Silicon (Si)	1
Magnesium (Mg)	0.89
Sulfur (S)	0.33
Nickel (Ni)	0.21
Aluminum (Al)	0.09
Calcium (Ca)	0.07
Sodium (Na)	0.045
Chlorine (Cl)	0.025



Elements used in making mechanical parts

- ▶ Aluminium
- ▶ Iron -Used to make steel
- ▶ Copper

Elements with high temperature properties

- ▶ Tungsten
- ▶ Platinum
- ▶ Molybdenum
- ▶ Tantalum

Silicon

25% of the earth's crust is silicon

“Silicon is the seventh most abundant element in the universe and the second most abundant element on the planet after oxygen” - Royal Society of Chemistry

Silica - an oxide of silicon is the most common component of sand.

Silicon is a metalloid, neither metal nor non-metal. It looks metallic but unlike metal it gets better at conducting electricity with higher temperatures.

Silicon is a semiconductor

Uses - transistors, solar cells, computer chips (with trace elements of boron or phosphorous)

Silicone is a polymer of **silicon**, oxygen, carbon and hydrogen. Don't confuse the two.

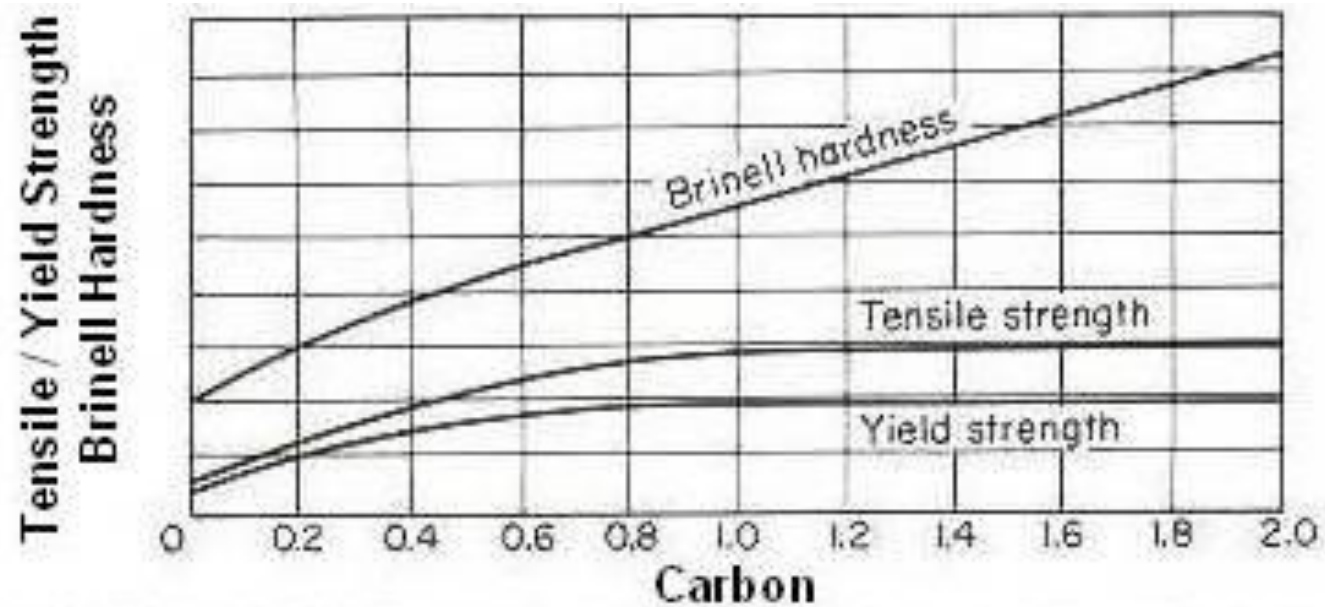
Silicon = cement, bricks, glass, computers, chips

Silicone = moulds, foam, coatings, cookware

Carbon

- ▶ Element with the highest melting point.
- ▶ Carbon is the main element in polymers together with Hydrogen
- ▶ Carbon is unique in that it is known to form up to 10 million different compounds. Carbon is important to the existence of life

Carbon



Effect of Carbon on Mechanical Properties of Steel

Metals

- ▶ What is a metal?
- ▶ Example of a metal?
- ▶ What do we know about metals?

Metals

1 H Hydrogen												2 He Helium								
		Metals Metalloids Non-Metals																		
3 Li Lithium		4 Be Beryllium												5 B Boron		6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon
11 Na Sodium		12 Mg Magnesium		Transition Metals										13 Al Aluminium	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon	
19 K Potassium		20 Ca Calcium		21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton	
37 Rb Rubidium		38 Sr Strontium		39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon	
55 Cs Cesium		56 Ba Barium		57 La Lanthanum	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon	
87 Fr Francium		88 Ra Radium		89 Ac Actinium	104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Berkelium	108 Hs Hassium	109 Mt Mendelevium	110	111	112	113	114					

Metal Properties Worksheet

Property	Metals	Non-metals
Appearance		
State at room temperature		
Density		
Strength		
Malleable or brittle		
Conduction of heat		
Conduction of electricity		
Magnetic material		
Sound when hit		

Metal Properties Worksheet Answer

Property	Metals	Non-metals
Appearance	Shiny	Dull
State at room temperature	Solid (except mercury, which is a liquid)	About half are solids, about half are gases, and one (bromine) is a liquid
Density	High (they feel heavy for their size)	Low (they feel light for their size)
Strength	Strong	Weak
Malleable or brittle	Malleable (they bend without breaking)	Brittle (they break or shatter when hammered)
Conduction of heat	Good	Poor (they are insulators)
Conduction of electricity	Good	Poor (they are insulators, apart from graphite)
Magnetic material	Only iron, cobalt and nickel	None
Sound when hit	They make a ringing sound (they are sonorous)	They make a dull sound

Metals-Properties

All metals are:

- ▶ Solid
- ▶ Shiny
- ▶ Ductile
- ▶ Malleable
- ▶ Good conductors
- ▶ Lose electrons easily

Most metals:

- ▶ Are solid at room temperature
- ▶ Are hard and strong
- ▶ Have a high density
- ▶ Are sonorous

- ▶ Three metals are magnetic

Metals-Properties

All metals are:

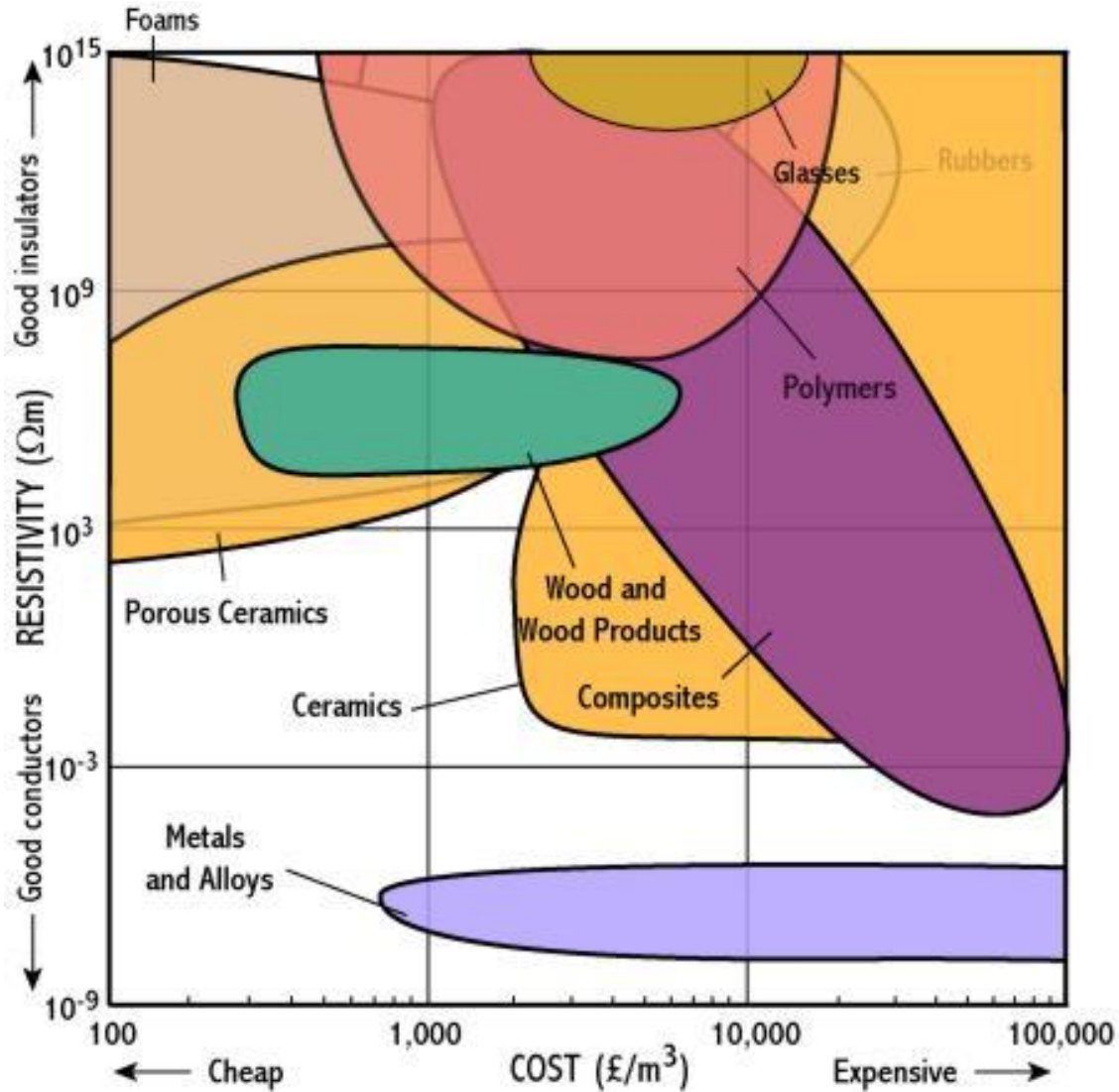
- ▶ Solid
- ▶ Shiny
- ▶ Ductile
- ▶ Malleable
- ▶ Good conductors
- ▶ Lose electrons easily

Most metals:

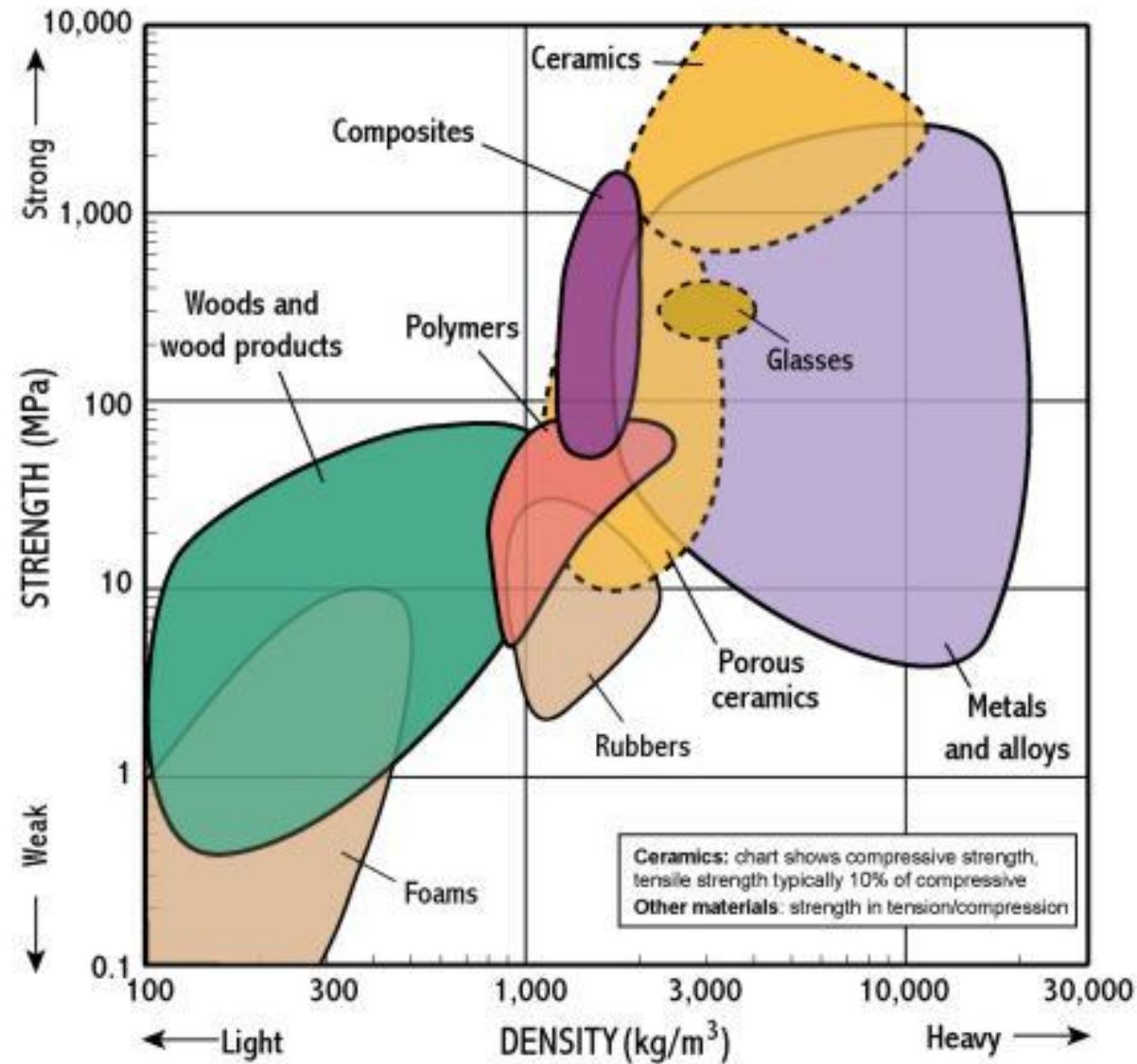
- ▶ Are solid at room temperature
- ▶ Are hard and strong
- ▶ Have a high density
- ▶ Are sonorous

- ▶ Three metals are magnetic
–Iron, Cobalt, Nickel

Electrical resistivity against cost



Strength against Density



Metals-properties

- ▶ Crystal Structure
- ▶ Large number free electrons
- ▶ Metallic bond
- ▶ Good electrical conductivity
- ▶ Opaque
- ▶ Uniform atoms
- ▶ High tensile strength
- ▶ Low shear strength
- ▶ Good ductility
- ▶ Plastic flow
- ▶ Impact strength
- ▶ Relatively high weight
- ▶ Moderate hardness
- ▶ Non porous
- ▶ High density

Metals-properties of ferrous metals

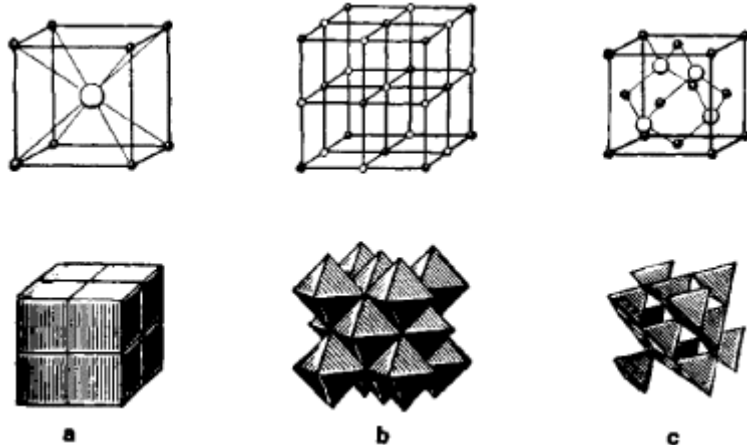
- ▶ Ferrous metals mild steel, carbon steel, stainless steel, cast iron, and wrought iron.
- ▶ used for their tensile strength and durability, especially mild steel which helps hold up the tallest skyscrapers and the longest bridges in the world.
- ▶ also find ferrous metals in housing construction, industrial containers, large-scale piping, automobiles, rails for railroad and transportation, most of tools and hardware you use around the house, and the knives you cook with at home.
- ▶ Due to the high amounts of carbon used when creating them, most ferrous metals and alloys are vulnerable to rust when exposed to the elements. While this isn't true of wrought iron, which is so iron pure that it resists oxidization, or stainless steel, which is protected thanks to its high chromium content, it's a good rule of thumb that if you see rust, it's a ferrous metal.
- ▶ Most ferrous metals also have magnetic properties, which makes them very useful in the creation of large motors and electrical appliances.
- ▶ Steady price - usually cheaper than non-ferrous metals.

Metals-properties of non-ferrous metals

- ▶ Non-ferrous metals aluminum, brass, copper, nickel, tin, lead, and zinc, as well as precious metals like gold and silver. While non-ferrous metals can provide strength, they are primarily used where their differences from ferrous metals can provide an advantage.
- ▶ much more malleable than ferrous metals.
- ▶ much lighter, making them well-suited for use where strength is needed, but weight is a factor, such as in the aircraft or canning industries.
- ▶ Higher resistance to rust and corrosion, which is why you'll find these materials in use for gutters, water pipes, roofing, and road signs.
- ▶ non-magnetic, which makes them perfect for use in small electronics and as electrical wiring.
- ▶ Varying price - usually more expensive than ferrous metals

Crystal Structures

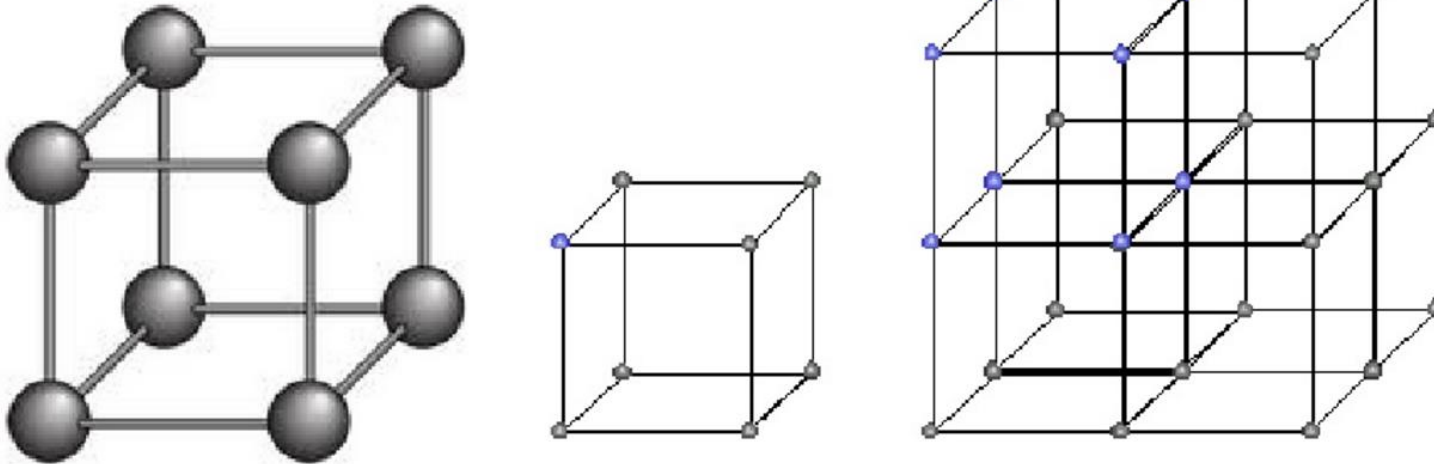
- ▶ Atoms form into a crystal lattice
- ▶ Structures that are not crystalline are called amorphous
- ▶ Metals are crystalline
- ▶ Polymers and ceramics can be crystalline and amorphous



Co-ordination Number

Co-ordination number is the number of nearest equidistant neighboring atoms surrounding an atom under consideration

1. Simple Cubic Structure:

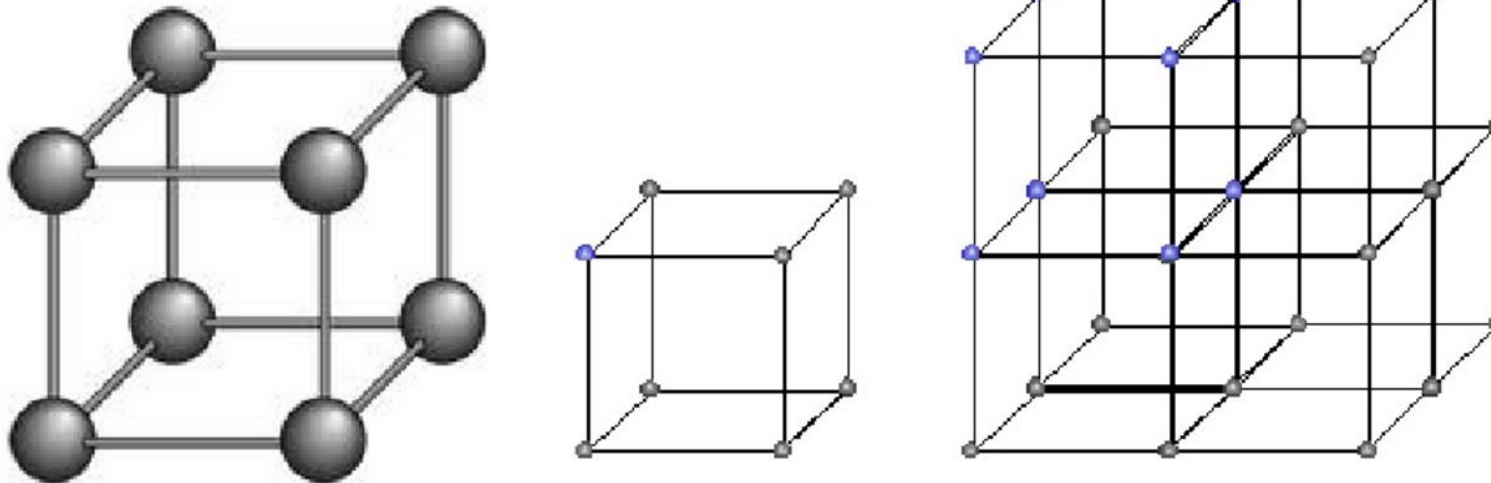


What is the coordination number of this cube?

Co-ordination Number

Co-ordination number is the number of nearest equidistant neighboring atoms surrounding an atom under consideration

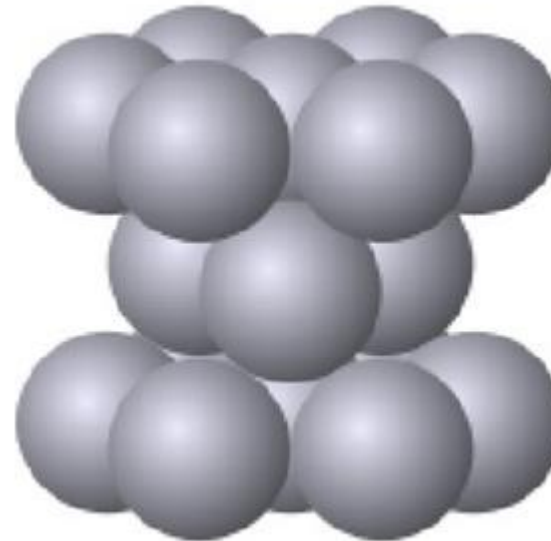
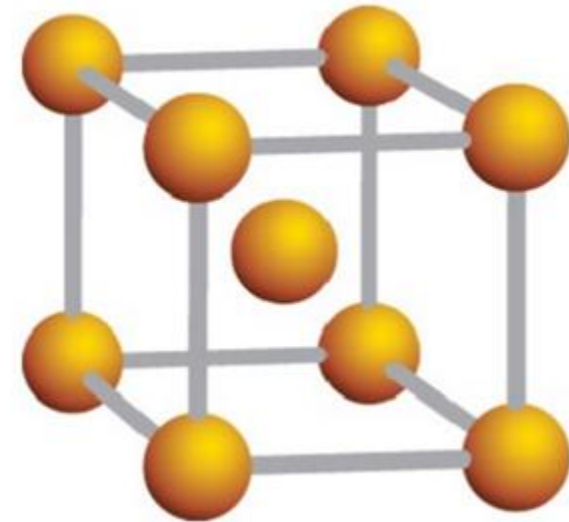
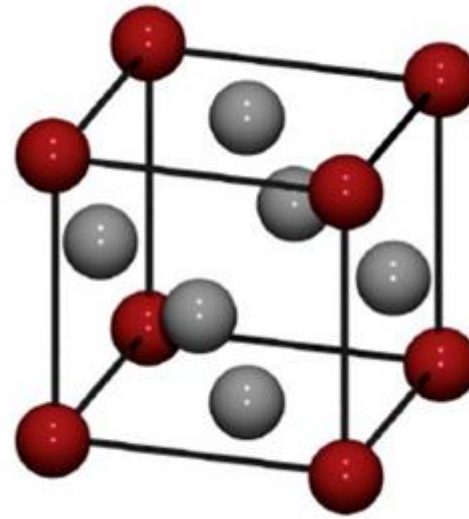
1. Simple Cubic Structure:



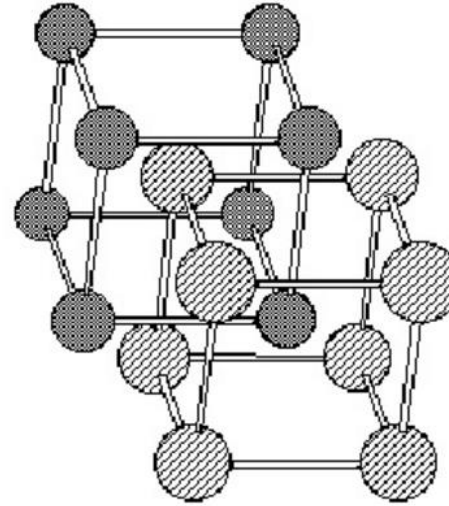
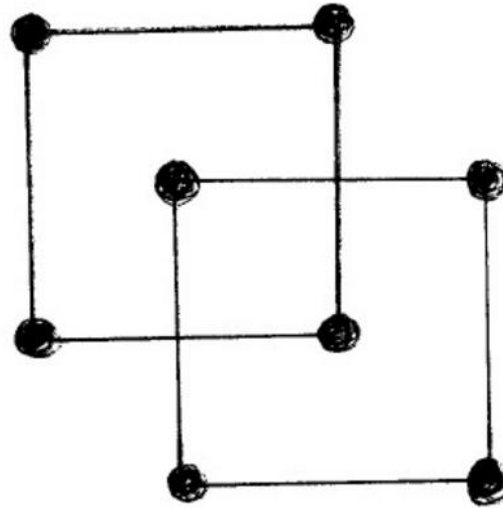
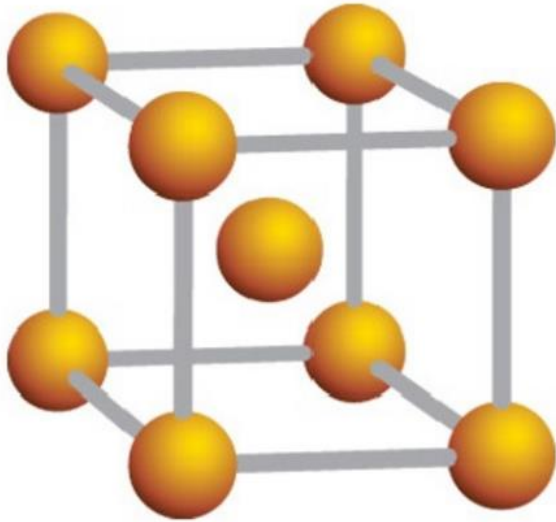
Simple cubic structure has a coordination number of **6**

Metals - Structure

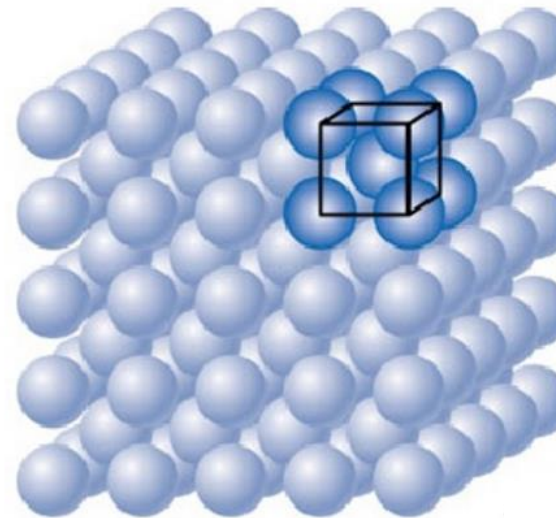
- ▶ The properties of some materials are related to their crystal structures.
- ▶ Body centred cubic structure BCC
- ▶ Face centred cubic structure FCC
- ▶ Hexagonal close-packed HCP



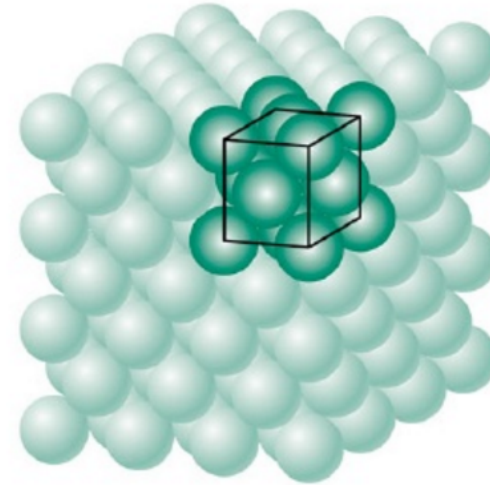
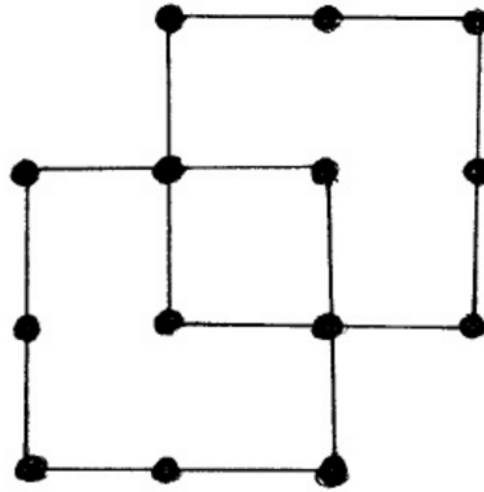
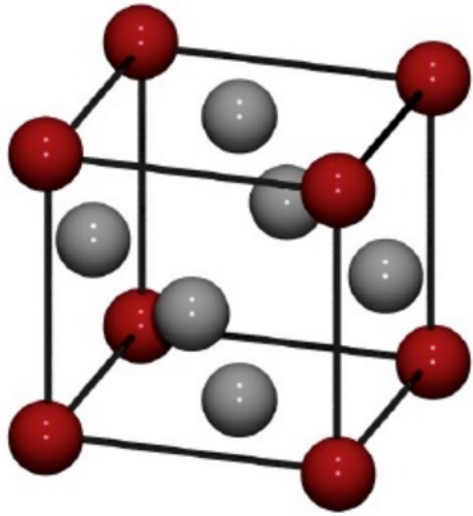
2. Body Centered Cubic Structure:



Body centered cubic structure has a coordination number of **8**



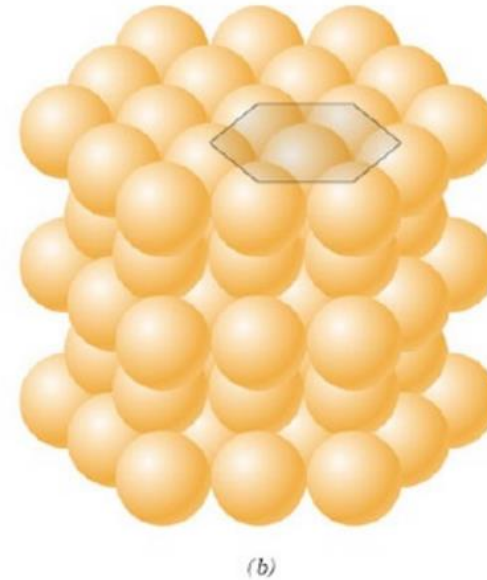
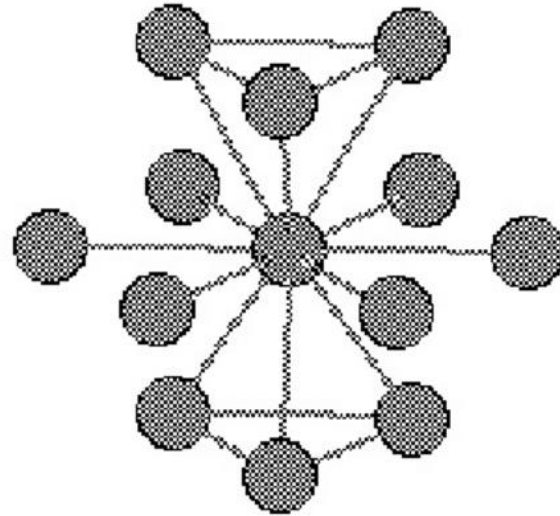
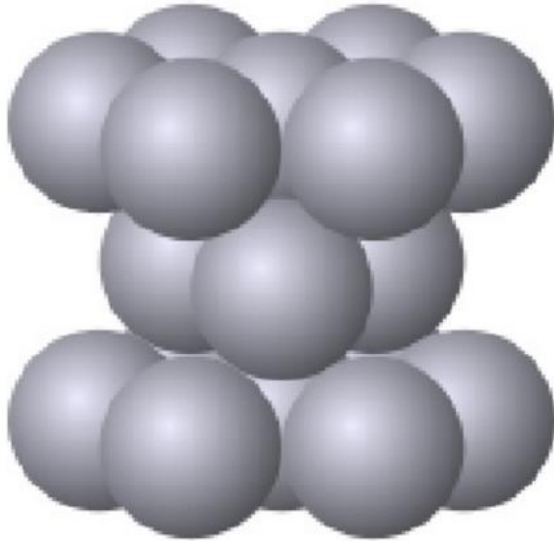
3. Face Centered Cubic Structure:



(c)

Face centered cubic structure has a coordination number of **12**

4. Hexagonal Close Packed Structure:



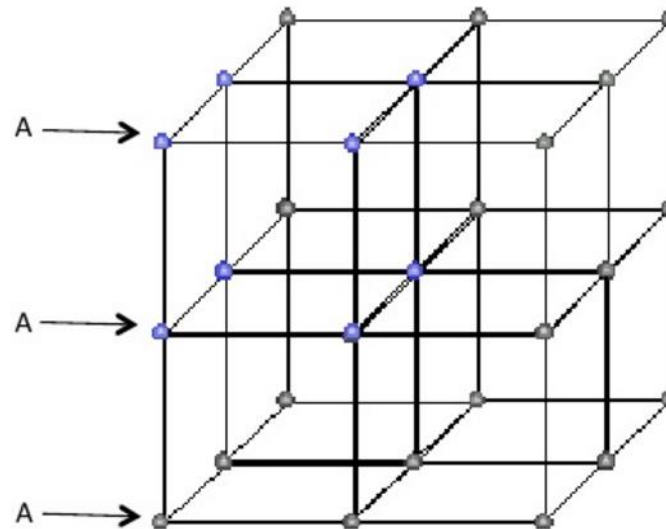
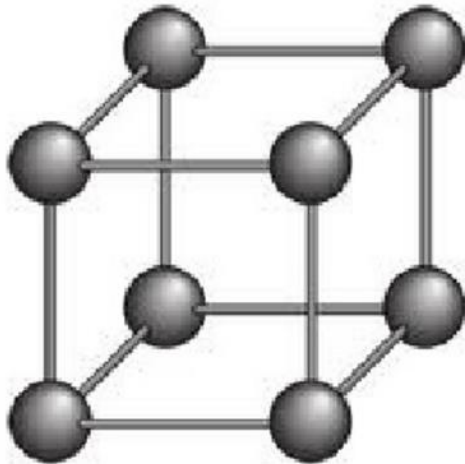
Hexagonal close packed structure has a coordination number of **12**

Stacking Sequence for SC, BCC, FCC and HCP

- Lattice structures are described by stacking of identical planes of atoms one over the other in a definite manner
- Different crystal structures exhibit different stacking sequences

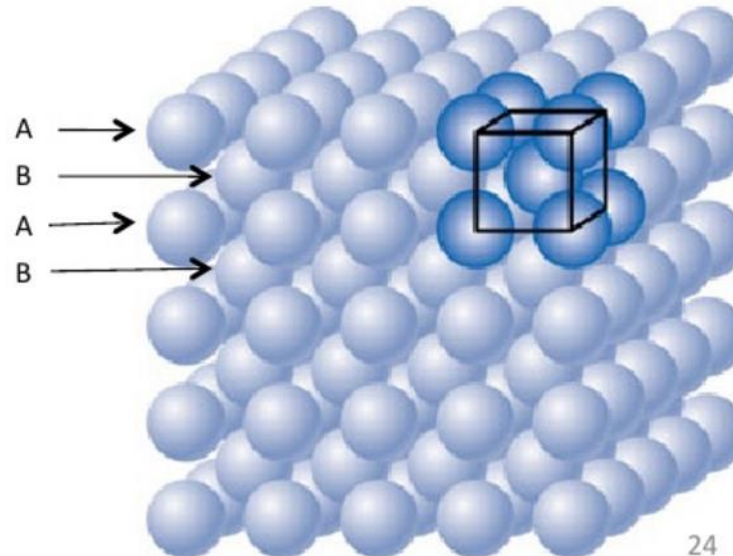
1. Stacking Sequence of Simple Cubic Structure:

Stacking sequence of simple cubic structure is AAAAAA....since the second as well as the other planes are stacked in a similar manner as the first i.e. all planes are stacked in the same manner.



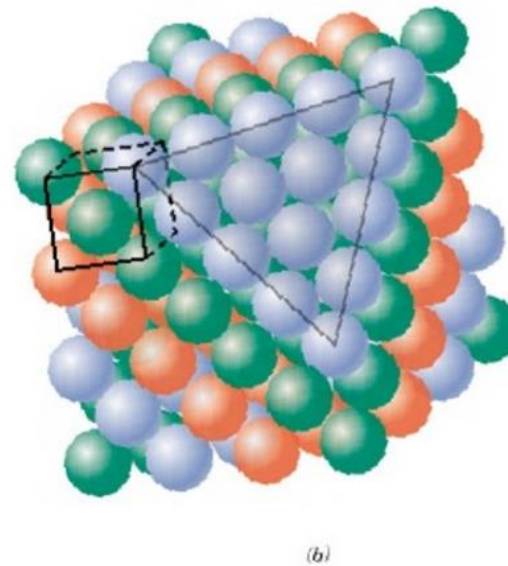
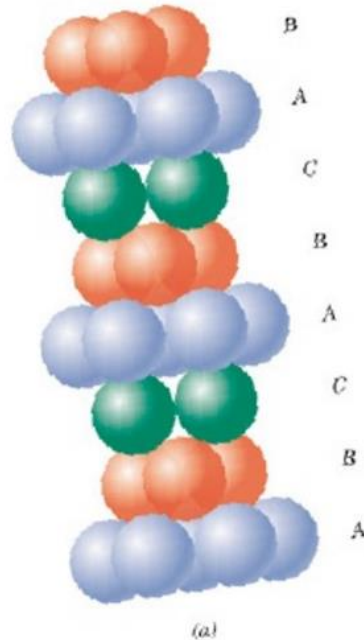
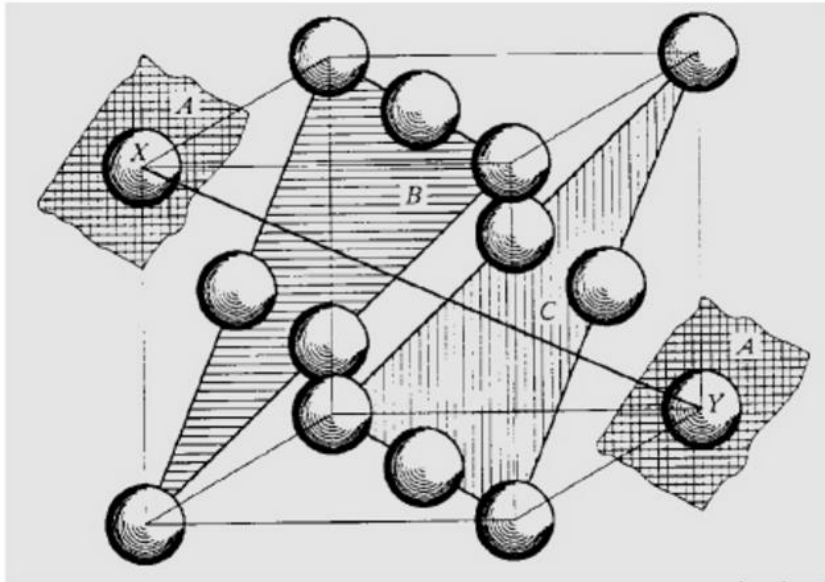
2. Stacking Sequence of Body Centered Cubic Structure:

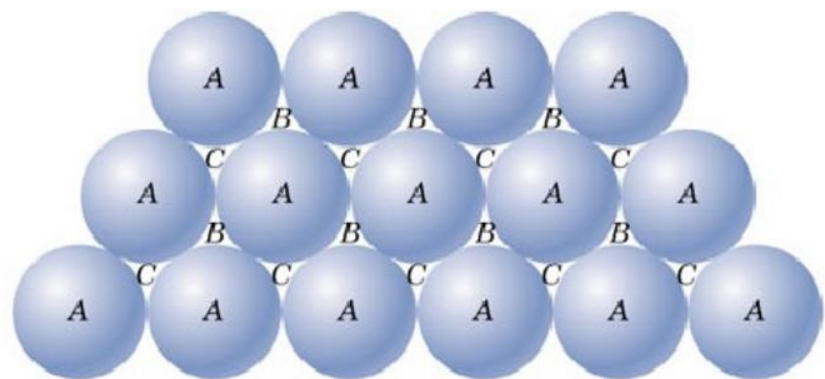
- Stacking sequence of body centered cubic structure is ABABAB....
- The stacking sequence ABABAB indicates that the second plane is stacked in a different manner to the first.
- Any one atom from the second plane occupies any one interstitial site of the first atom.
- Third plane is stacked in a manner identical to the first and fourth plane is stacked in an identical manner to the second and so on. This results in a bcc structure.



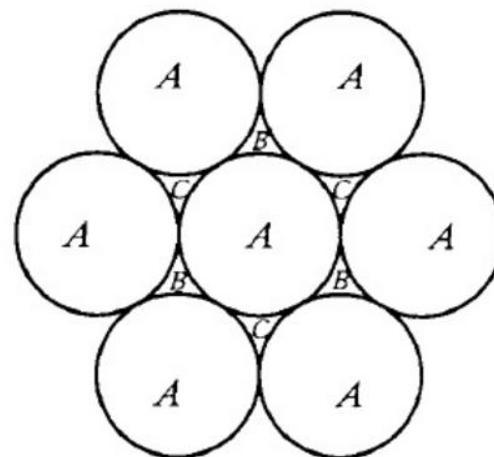
3. Stacking Sequence of Face Centered Cubic Structure:

- Stacking sequence of face centered cubic structure is ABCABC....
- The close packed planes are inclined at an angle to the cube faces and are known as octahedral planes
- The stacking sequence ABCABC... indicates that the second plane is stacked in a different manner to the first and so is the third from the second and the first. The fourth plane is stacked in a similar fashion to the first

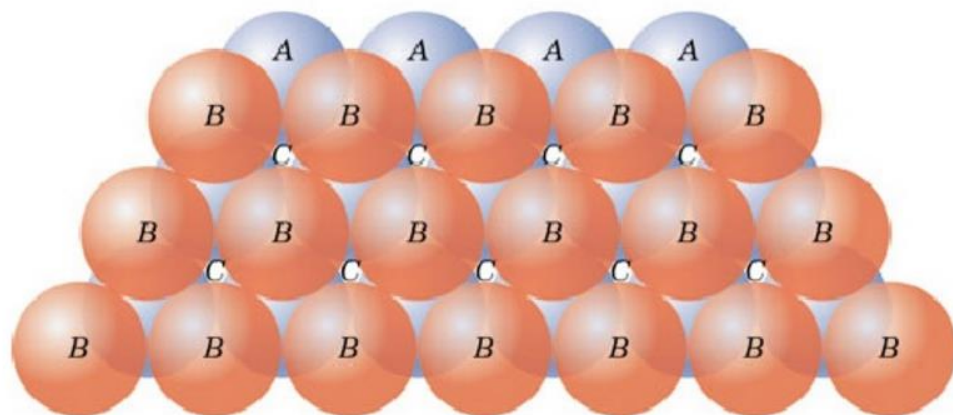




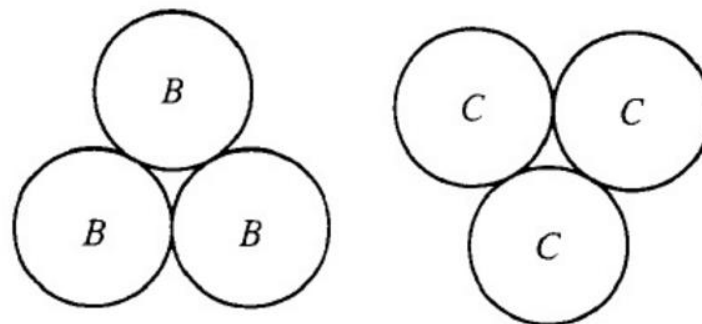
(a)



a

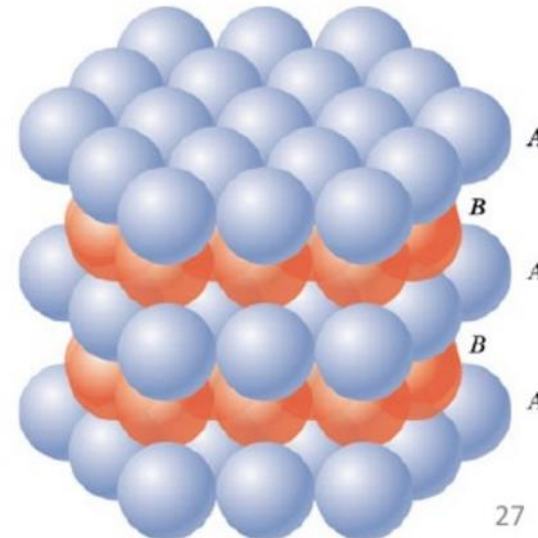
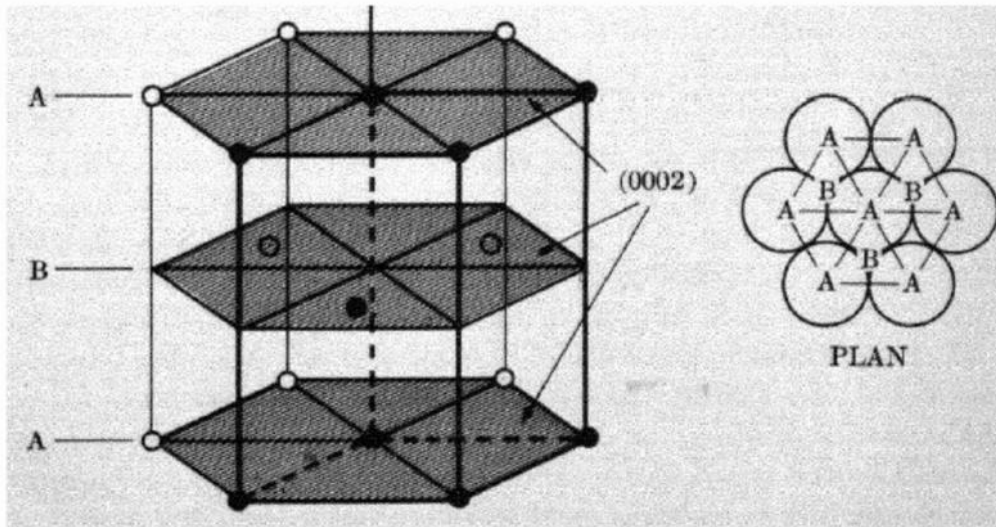


(b)



4. Stacking Sequence of Hexagonal Close Packed Structure:

- Stacking sequence of HCP structure is ABABAB.....
- HCP structure is produced by stacking sequence of the type ABABAB.....in which any one atom from the second plane occupies any one interstitial site of the first plane.
- Third plane is stacked similar to first and fourth similar to second and so on.

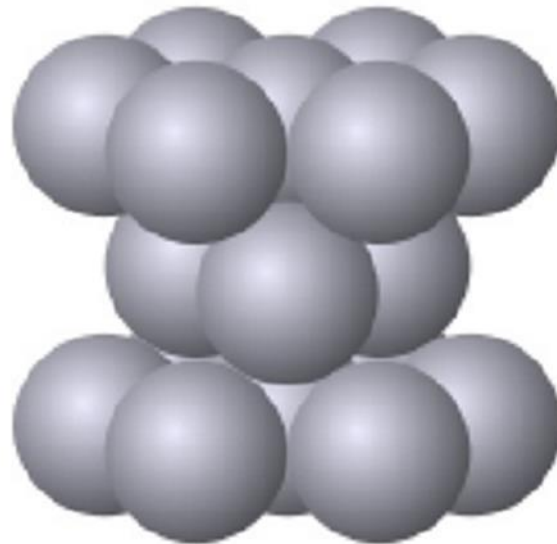
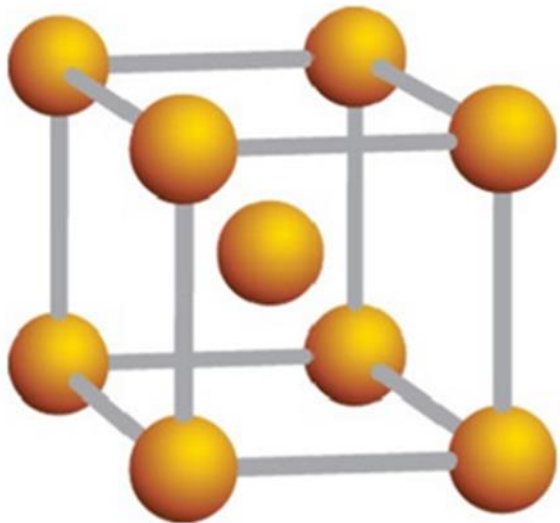
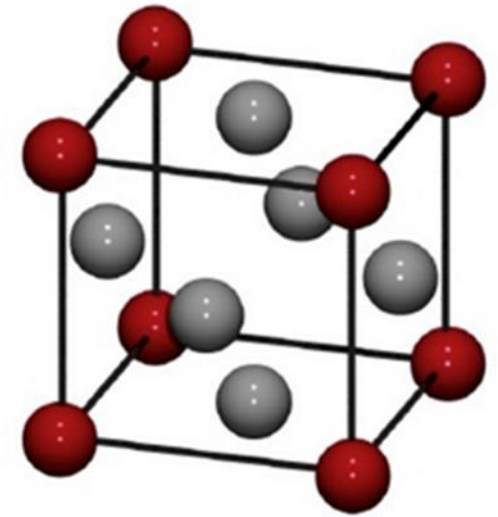


Of the three close-packed cell formations, which is most efficient?

► FCC or BCC or HCP?

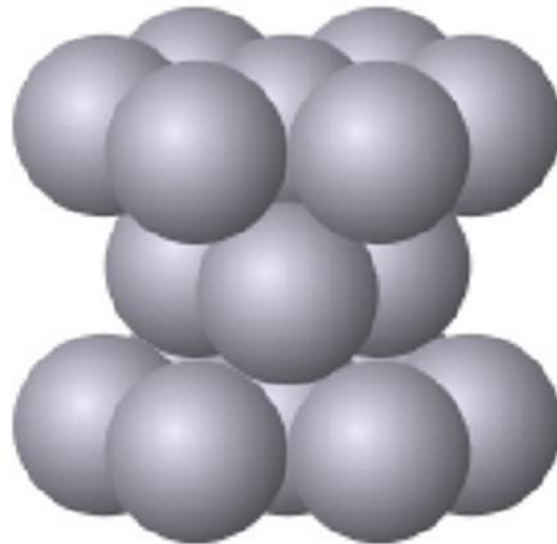
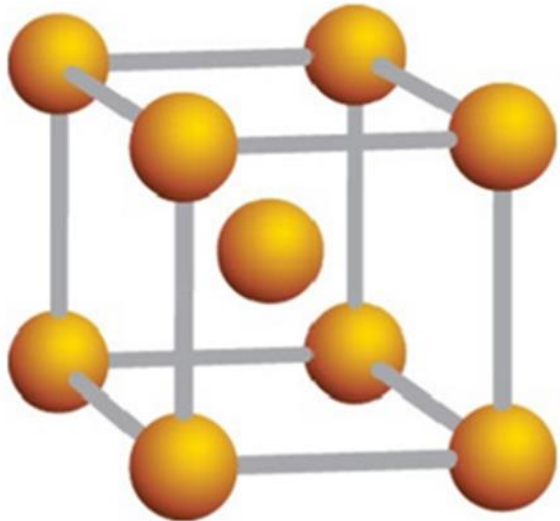
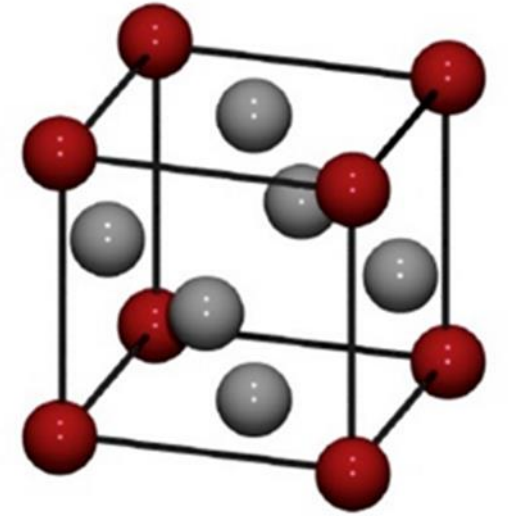
Of the three close-packed cell formations, which is most efficient?

- ▶ FCC or BCC or HCP?
- ▶ How can we work out a measure of how much space is in the unit cell compared to how much space is taken up with atoms?



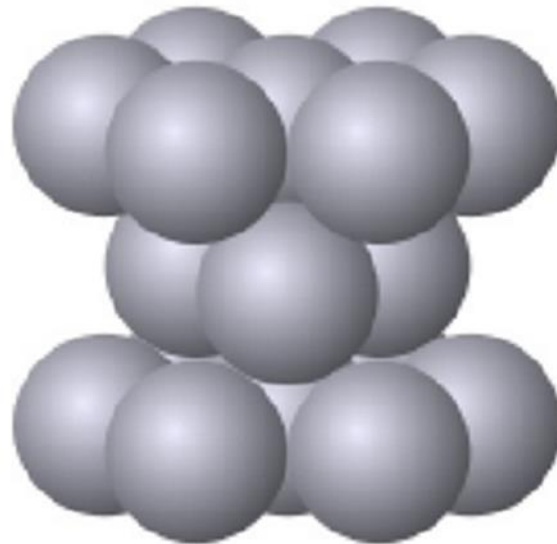
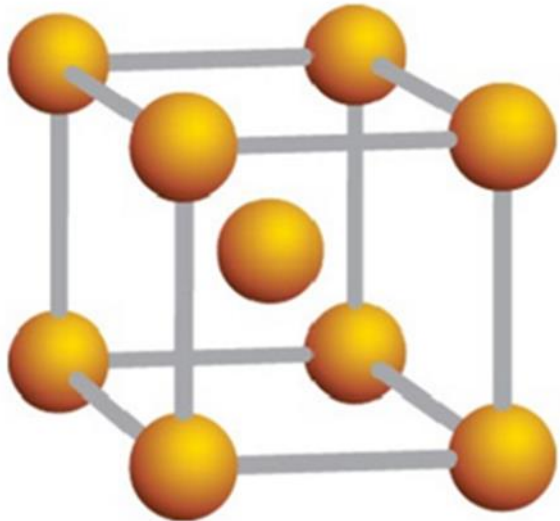
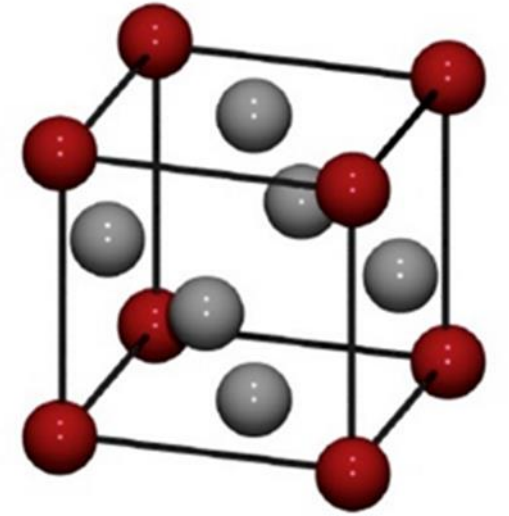
Of the three close-packed cell formations, which is most efficient?

- ▶ FCC or BCC or HCP?
- ▶ How can we work out a measure of how much space is in the unit cell compared to how much space is taken up with atoms?
- ▶ What do we need to know?



Of the three close-packed cell formations, which is most efficient?

- ▶ FCC or BCC or HCP?
- ▶ How can we work out a measure of how much space is in the unit cell compared to how much space is taken up with atoms?
- ▶ What do we need to know? How big is the unit cell? How many atoms are inside the unit cell?

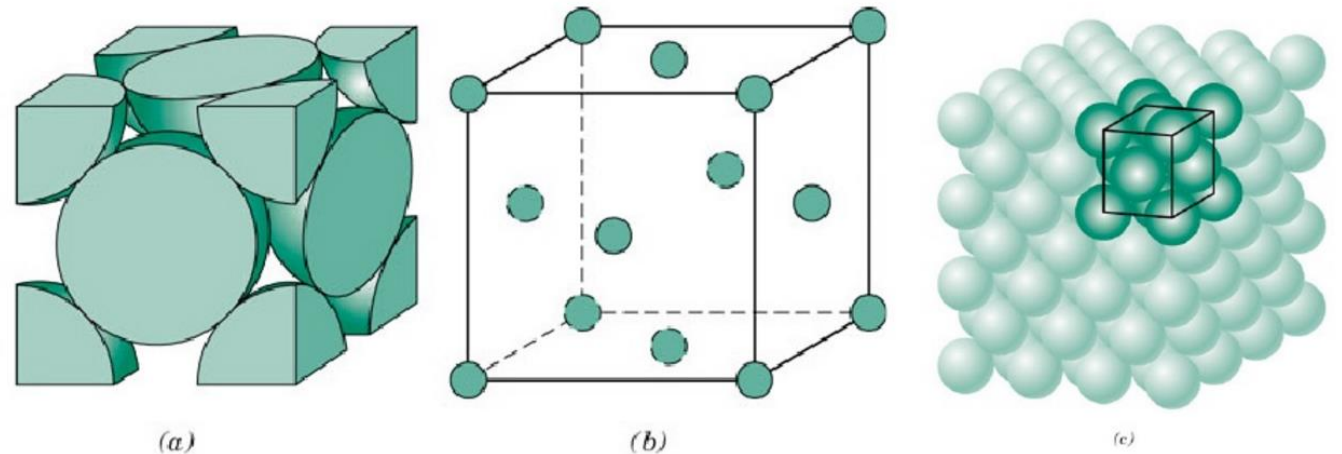


Atomic Packing Factor and Coordination Number

- ▶ Atomic Packing Factor– measure of packing efficiency or packing fraction of the volume in the structure occupied by particles.
- ▶ $APF = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$
- ▶ Coordination number- the number of nearest neighbour or touching atoms

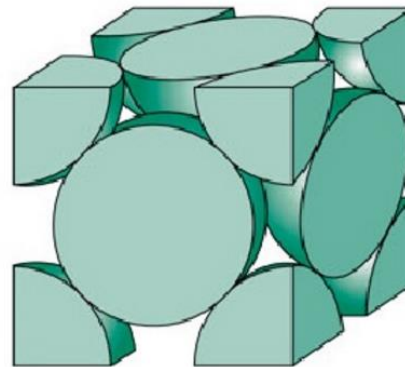
Question

- ▶ 1) Build a FCC unit cell
- ▶ 2) Calculate the volume of an FCC unit cell in terms of the radius R
- ▶ 3) What is the coordination number of an FCC unit cell
- ▶ 4) Determine the atomic packing factor for the FCC crystal structure



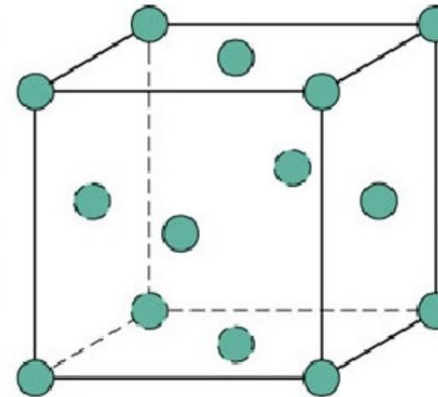
Face Centred Cubic Crystal Structure FCC

- ▶ Closely packed, stacking sequence ABCABC
- ▶ 6 half atoms, one per face
- ▶ 6 faces $(6 \times \frac{1}{2})=3$
- ▶ 8 corners $(8 \times \frac{1}{8})=1$
- ▶ 4 atoms per unit cell
- ▶ Coordination number 12
- ▶ Eg. copper, aluminium, silver, gold



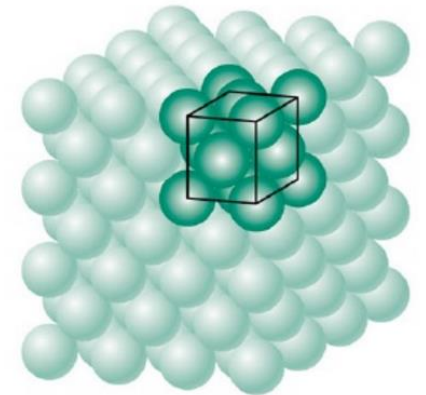
(a)

A unit cell



(b)

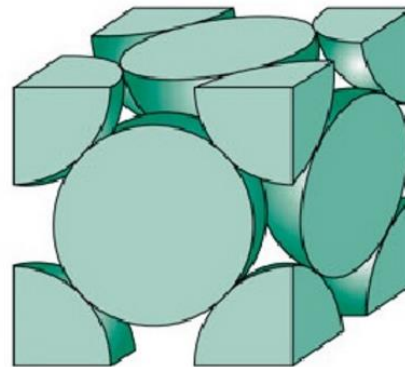
A reduced sphere unit cell



(c)

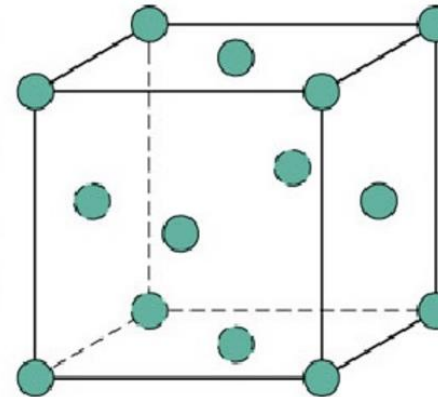
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- ▶ 8 corners $(8 \times \frac{1}{8})=1$
- ▶ 4 atoms per unit cell
- ▶ If length of unit cell is a and R is the radius of an atom, then $a = 2R\sqrt{2}$
- ▶ Coordination number 12
- ▶ Eg. copper, aluminium, silver, gold



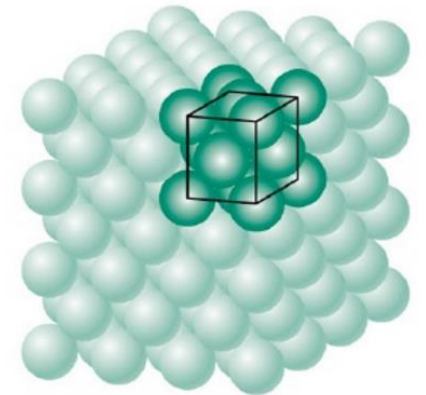
(a)

A unit cell



(b)

A reduced sphere unit cell



(c)

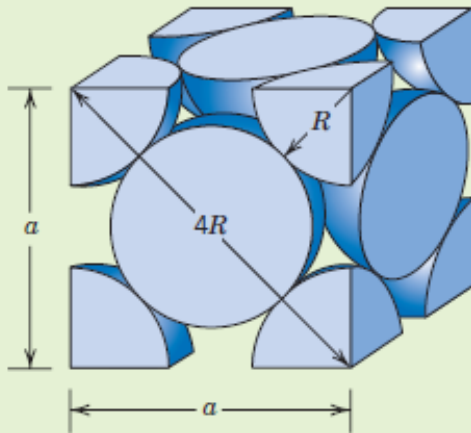
Problem 3.1

Determination of FCC Unit Cell Volume

Calculate the volume of an FCC unit cell in terms of the atomic radius R .

Solution

In the FCC unit cell illustrated,



the atoms touch one another across a face-diagonal the length of which is $4R$. Since the unit cell is a cube, its volume is a^3 , where a is the cell edge length. From the right triangle on the face,

$$a^2 + a^2 = (4R)^2$$

or, solving for a ,

$$a = 2R\sqrt{2} \quad (3.1)$$

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \quad (3.4)$$

Callister,
Materials Science
and Engineering

Computation of the Atomic Packing Factor for FCC

Show that the atomic packing factor for the FCC crystal structure is 0.74.

Solution

The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total atom and unit cell volumes may be calculated in terms of the atomic radius R . The volume for a sphere is $\frac{4}{3}\pi R^3$, and since there are four

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atoms per FCC unit cell, the total FCC atom (or sphere) volume is

$$V_S = (4)\frac{4}{3}\pi R^3 = \frac{16}{3}\pi R^3$$

From Example Problem 3.1, the total unit cell volume is

$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

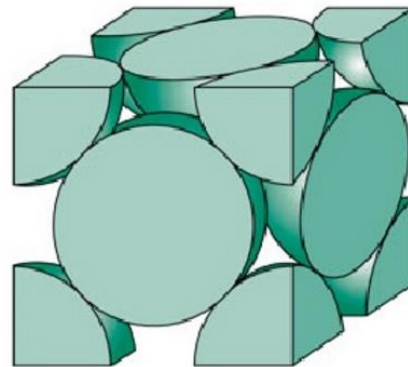
$$\text{APF} = \frac{V_S}{V_C} = \frac{(\frac{16}{3})\pi R^3}{16R^3\sqrt{2}} = 0.74$$

Callister

Materials Science and Engineering

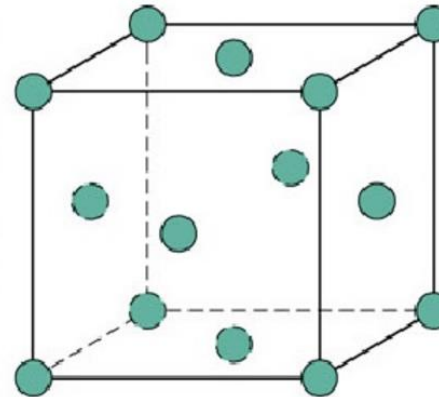
Face Centred Cubic Crystal Structure FCC

- ▶ Closely packed, stacking sequence ABCABC
- ▶ 6 half atoms, one per face
- ▶ 6 faces $(6 \times \frac{1}{2})=3$
- ▶ 8 corners $(8 \times \frac{1}{8})=1$
- ▶ 4 atoms per unit cell
- ▶ If length of unit cell is a and R is the radius of an atom, then $a = 2R\sqrt{2}$
- ▶ Atomic Packing Factor 0.74
- ▶ Coordination number 12
- ▶ Eg. copper, aluminium, silver, gold



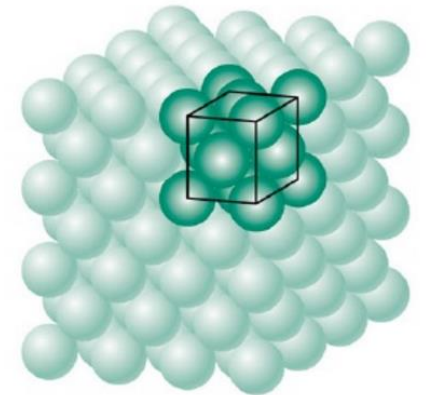
(a)

A unit cell



(b)

A reduced sphere unit cell



(c)

Question

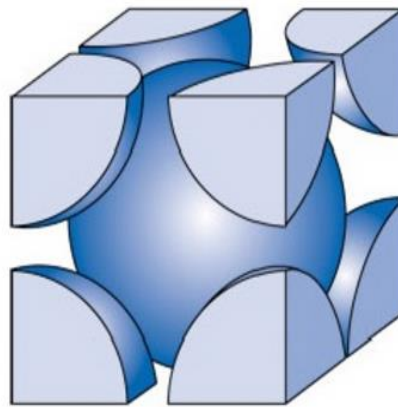
- ▶ An element crystallizes in a face centred cubic lattice and has a density of 1.45 g cm^{-3} . The edge of its unit cell is $4.52 \times 10^{-8} \text{ cm}$.
- ▶ a) How many atoms are in each unit cell?
- ▶ b) What is the volume of a unit cell?
- ▶ c) What is the mass of a unit cell?
- ▶ d) Calculate the approximate atomic mass of the element

Question - Answer

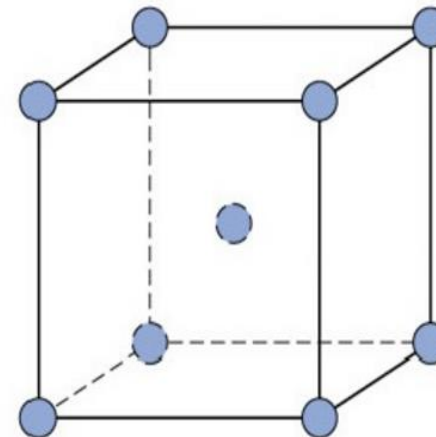
- ▶ An element crystallizes in a face centred cubic lattice and has a density of 1.45 g cm^{-3} . The edge of its unit cell is $4.52 \times 10^{-8} \text{ cm}$.
- ▶
- ▶ a) How many atoms are in each unit cell? 4
- ▶
- ▶ b) What is the volume of a unit cell? $(4.52 \times 10^{-8} \text{ cm})^3 = 9.23 \times 10^{-23}$
- ▶
- ▶ c) What is the mass of a unit cell? $\text{Mass} = d \times v = 1.45 \text{ g cm}^{-3} \times 9.23 \times 10^{-23} = 1.338 \times 10^{-22} \text{ g}$
- ▶
- ▶ d) Calculate the approximate atomic mass of the element. $1.338 \times 10^{-22} \text{ g} / 4 = 3.346 \times 10^{-23} \text{ g}$

Question

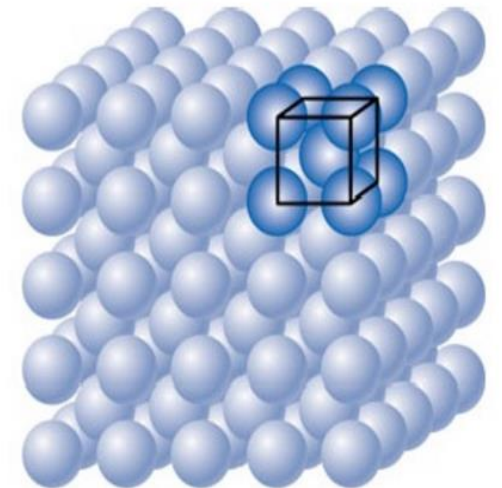
- ▶ 1) Build a BCC unit cell
- ▶ 2) Calculate the volume of an BCC unit cell in terms of the radius R
- ▶ 3) What is the coordination number of an BCC unit cell
- ▶ 4) Determine the atomic packing factor for the BCC crystal structure



(a)



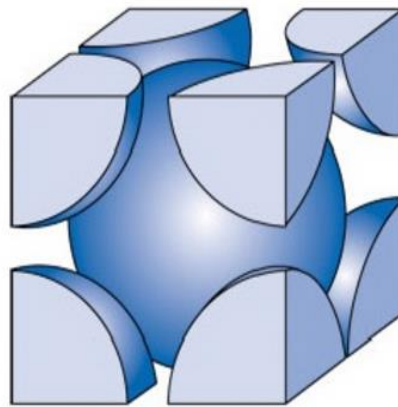
(b)



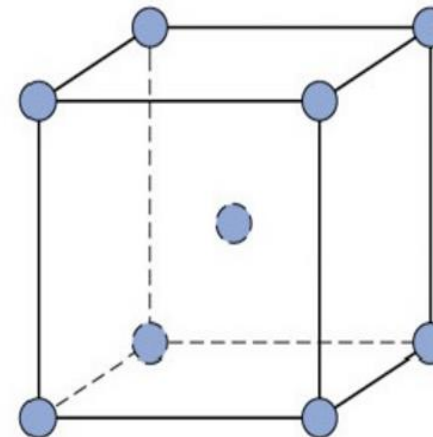
(c)

Question

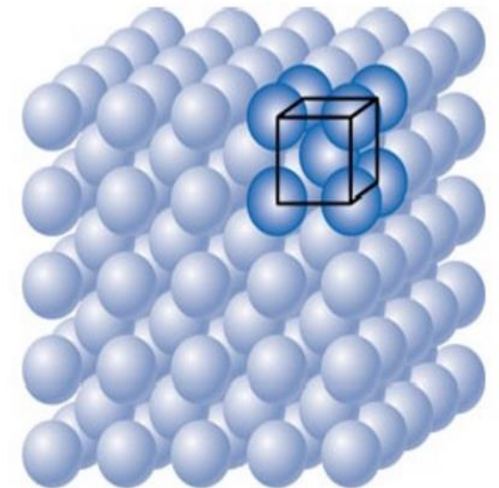
- ▶ 1) Build a BCC unit cell
- ▶ 2) Calculate the volume of an BCC unit cell in terms of the radius R
- ▶ $a = 4R/\sqrt{3}$ and $\text{vol} = (4R/\sqrt{3})^3 = 64R^3 / 3\sqrt{3}$
- ▶ $V_s = 8/3 \pi R^3$
- ▶ 3) What is the coordination number of an BCC unit cell
- ▶ 4) Determine the atomic packing factor for the BCC crystal structure



(a)



(b)

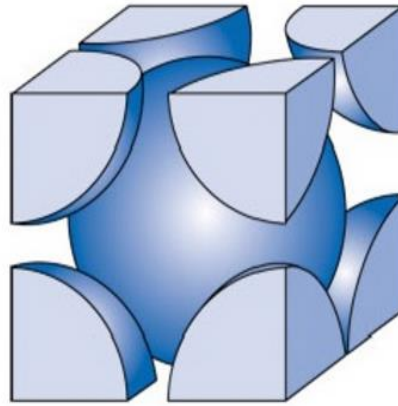


(c)

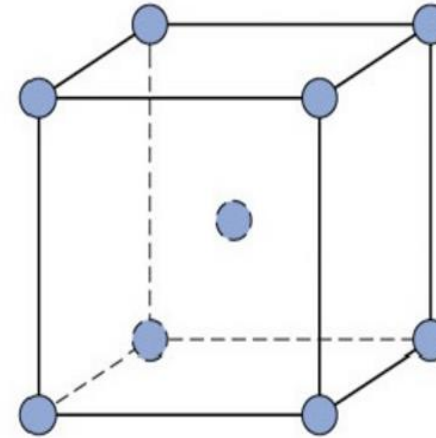
Body Centred Cubic Crystal Structure

BCC

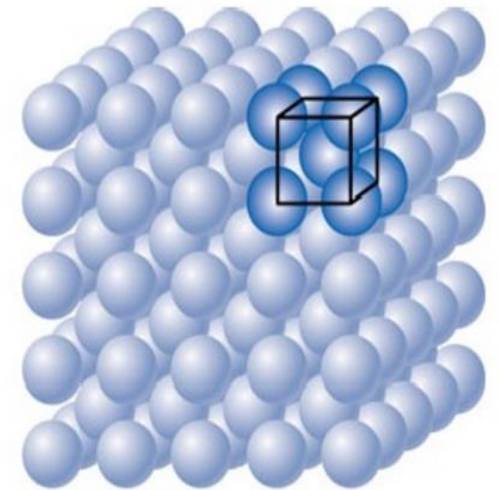
- ▶ Stacking sequence ABABAB
- ▶ 8 corners($8 \times \frac{1}{8}$)=1
- ▶ 1 central =1
- ▶ 2 atoms per unit cell
- ▶ Atomic Packing Factor 0.68
- ▶ Coordination number 8
- ▶ Eg chromium, iron, tungsten



(a)



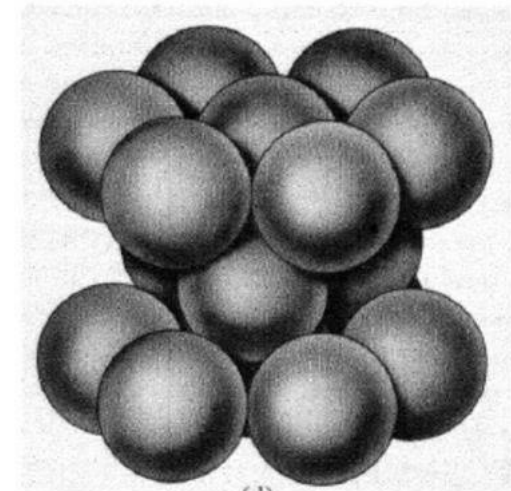
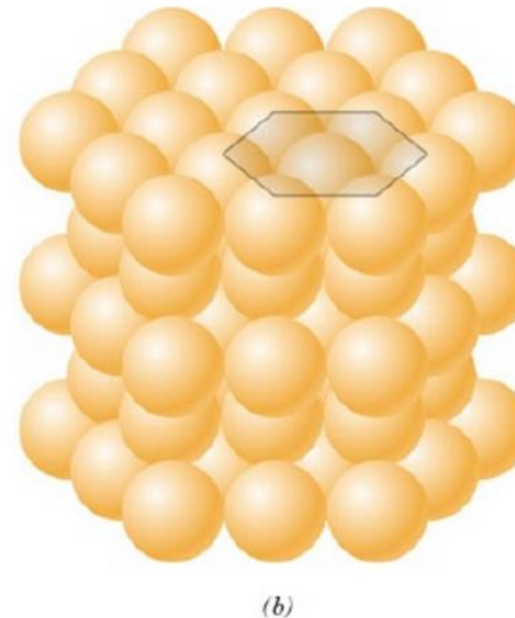
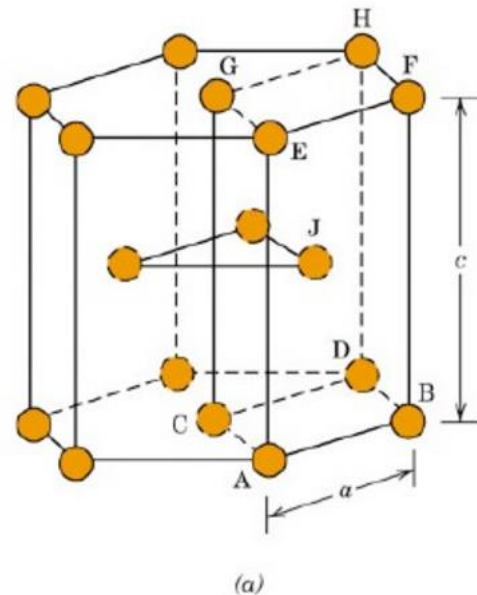
(b)



(c)

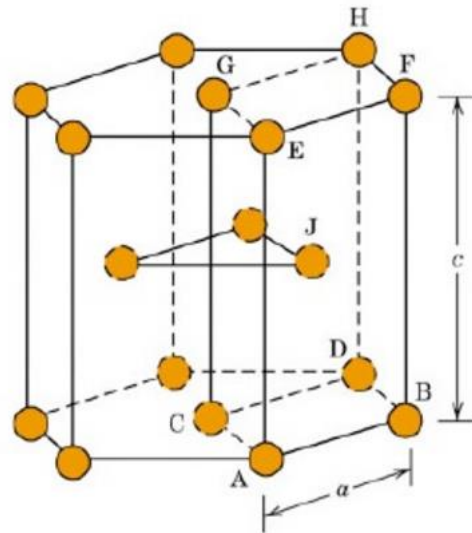
Question

- ▶ 1) Build a HCP unit cell
- ▶ 2) Calculate the volume of an HCP unit cell in terms of the radius R
- ▶ 3) What is the coordination number of an HCP unit cell
- ▶ 4) Determine the atomic packing factor for the HCP crystal structure

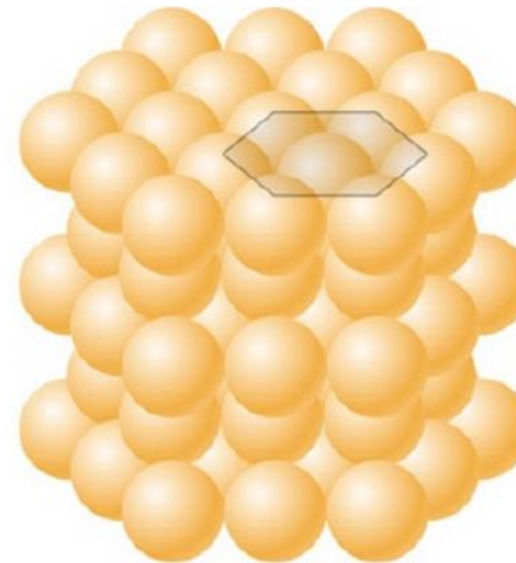


Hexagonal Close Packed Crystal Structure (HCP)

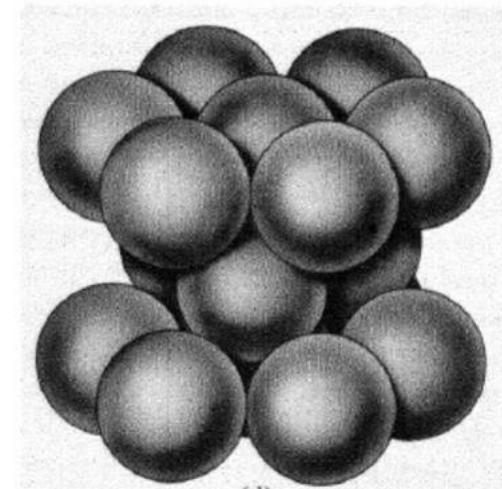
- ▶ Stacking sequence ABABAB
- ▶ 12 corner atoms
- ▶ 2 centre of top and bottom face
- ▶ 3 interior
- ▶ Atomic Packing Factor 0.74
- ▶ Coordination number 12
- ▶ Eg cadmium, magnesium, titanium, zinc



A reduced sphere unit cell



(b)



Question - True or False?

- ▶ Which one of the following statements about unit cells and packing in solids is incorrect?
- ▶ a) In unit cells of solid crystals, every face of the cell must have an opposite face which is equal and parallel to it.
- ▶ b) The faces of unit cells must meet at 90 degrees.
- ▶ c) The coordination number of atoms in a close packed metal is 12.
- ▶ d) The packing efficiency in fcc structures is higher than in bcc structures.
- ▶ e) The packing efficiency in fcc and hcp structures is the same.

Answer

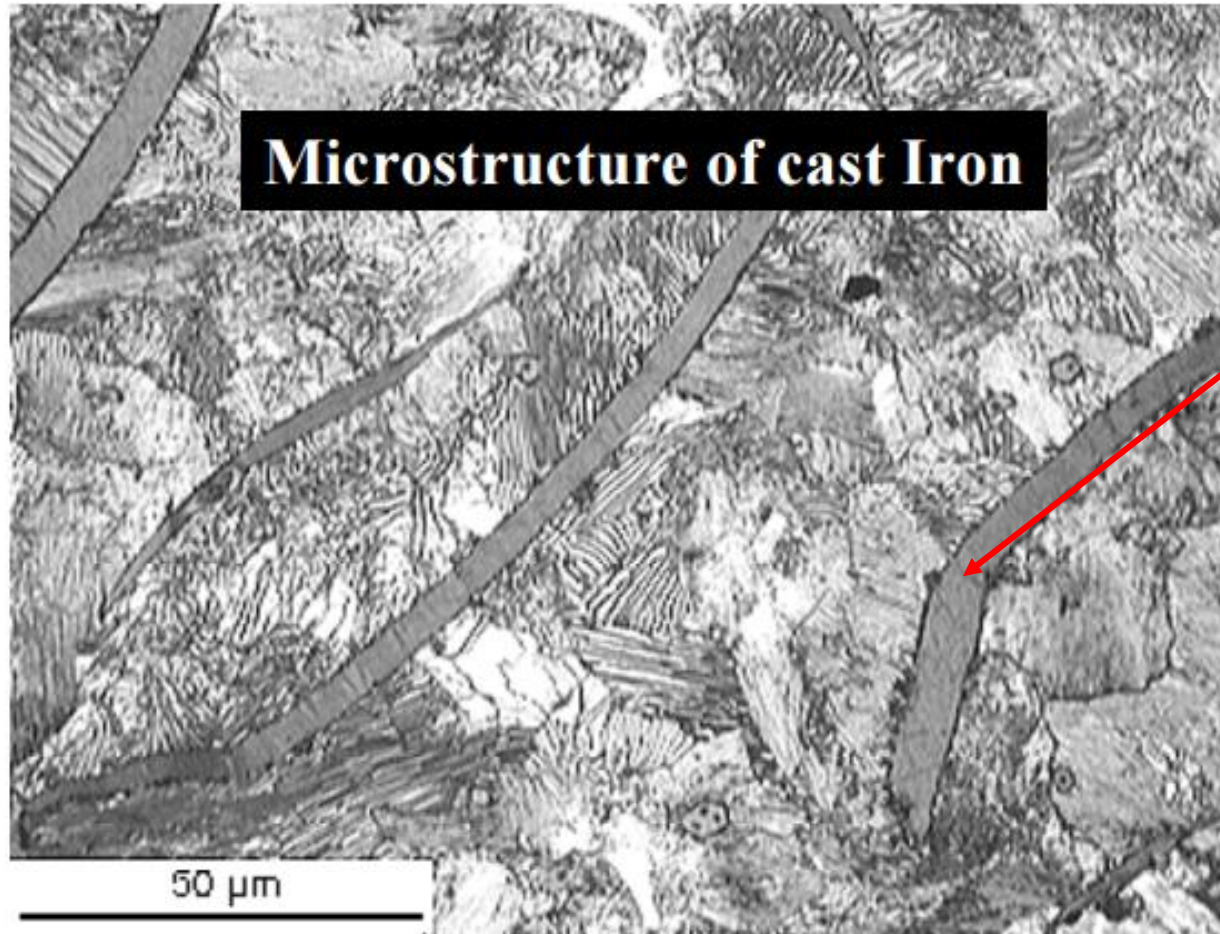
- ▶ Which one of the following statements about unit cells and packing in solids is incorrect?
- ▶ a) In unit cells of solid crystals, every face of the cell must have an opposite face which is equal and parallel to it. True
- ▶ b) The faces of unit cells must meet at 90 degrees. False
- ▶ c) The coordination number of atoms in a close packed metal is 12. True
- ▶ d) The packing efficiency in fcc structures is higher than in bcc structures. True
- ▶ e) The packing efficiency in fcc and hcp structures is the same. True

Structure and Properties -Metals

Introduction to Steel

- ▶ Metals and Alloys have many useful engineering properties and so have widespread applications in Engineering Designs
- ▶ Iron and its alloys (principally steel) account for about 90% of the world's production of metals mainly because of their combination of good strength, toughness and ductility at relatively low cost
- ▶ Alloys based on iron are called ferrous alloys, while those based on other metals are called non-ferrous alloys

Cast Iron



Graphite
flakes

Austenite - an interstitial solid solution of Carbon dissolved in iron FCC,

Average properties of austenite are:

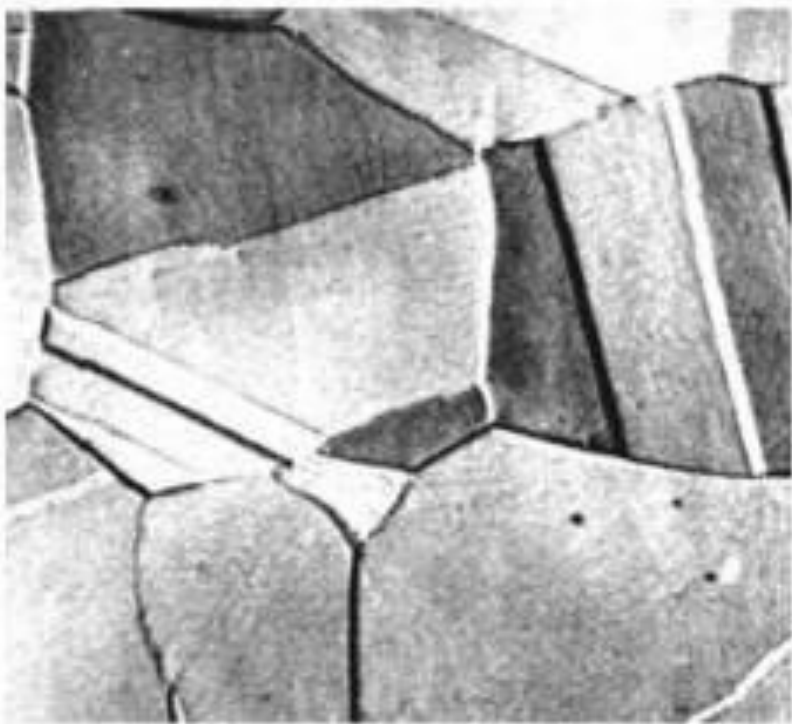
Tensile strength: 150,000 psi

Elongation: 10 % in 2 in. gauge length

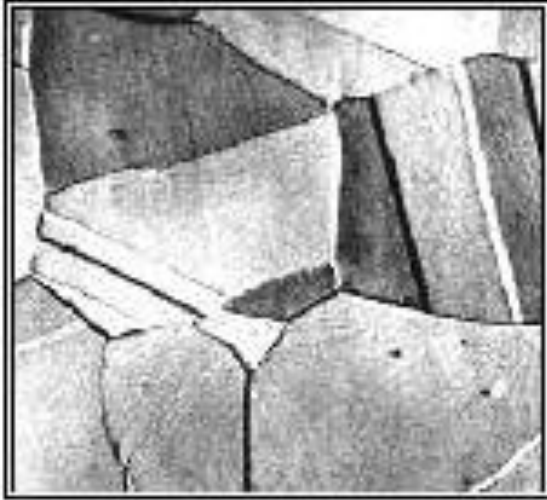
Hardness: Rockwell C 40

Toughness: High

Austenite is normally unstable at room temperature. Under certain conditions it is possible to obtain austenite at room temperature (as in austenite stainless steels). Austenite is non-magnetic.



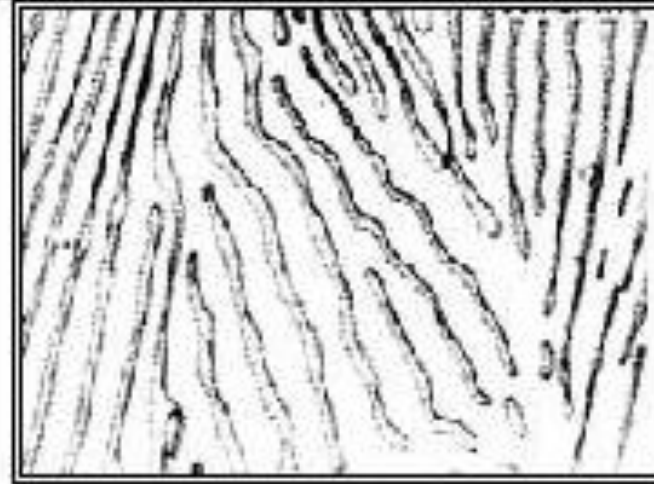
Microstructure of Austenite



Austenite



Ferrite



Pearlite

Figure 3

Different Fe-C system microstructures

Source: Van Vlack 1989

Rockwell Hardness tester

The Rockwell test determines the hardness by measuring the depth of penetration of an indenter under a large load compared to the penetration made by a preload

The equation for Rockwell Hardness is $HR = N - (d/s)$, where d is the depth (from the zero load point), and N and s are scale factors that depend on the scale of the test being used



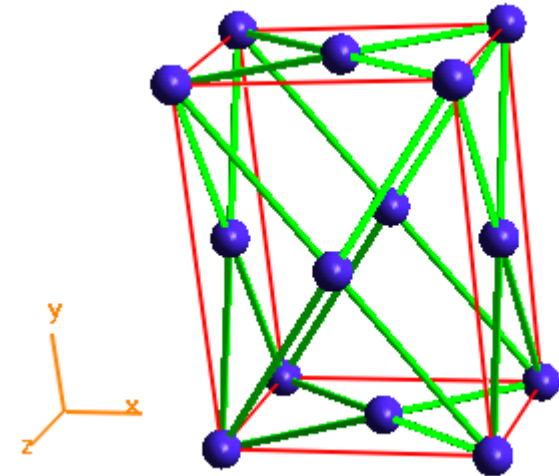
Rockwell Scales

Various Rockwell scales^[11]

Scale	Abbreviation	Load	Indenter	Use	N	s
A	HRA	60 kgf	120° diamond spheroconical [†]	Tungsten carbide	100	0.002mm
B	HRB	100 kgf	1/16-inch-diameter (1.588 mm) steel sphere	Aluminium, brass, and soft steels	130	0.002mm
C	HRC	150 kgf	120° diamond spheroconical	Harder steels >B100	100	0.002mm
D	HRD	100 kgf	120° diamond spheroconical		100	0.002mm
E	HRE	100 kgf	1/8-inch-diameter (3.175 mm) steel sphere		130	0.002mm
F	HRF	60 kgf	1/16-inch-diameter (1.588 mm) steel sphere		130	0.002mm
G	HRG	150 kgf	1/16-inch-diameter (1.588 mm) steel sphere		130	0.002mm
[†] Also called a <i>brale indenter</i>						

Cementite (iron carbide)

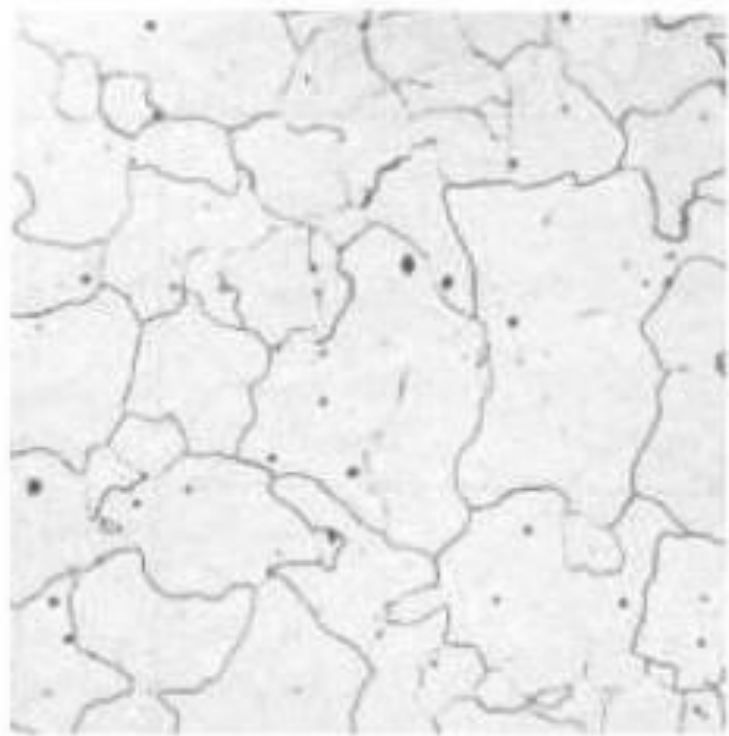
- ▶ Fe_3C
- ▶ 6.67%wt C
- ▶ Hard brittle interstitial compound of low tensile strength (5000psi)
- ▶ High compressive strength
- ▶ The hardest structure on the iron-iron carbide diagram
- ▶ Orthorhombic -three unequal axes at right angles.



Ledeburite

- ▶ It is the eutectic mixture of austenite and cementite.
- ▶ It contains 4.3 percent carbon
- ▶ It exists when the carbon content is greater than 2%, which represents the dividing line on the equilibrium diagram between steel and cast iron.

Ferrite - interstitial solid solution of C in iron. BCC max solubility 0.025% C
softest structure on the iron-iron carbide diagram

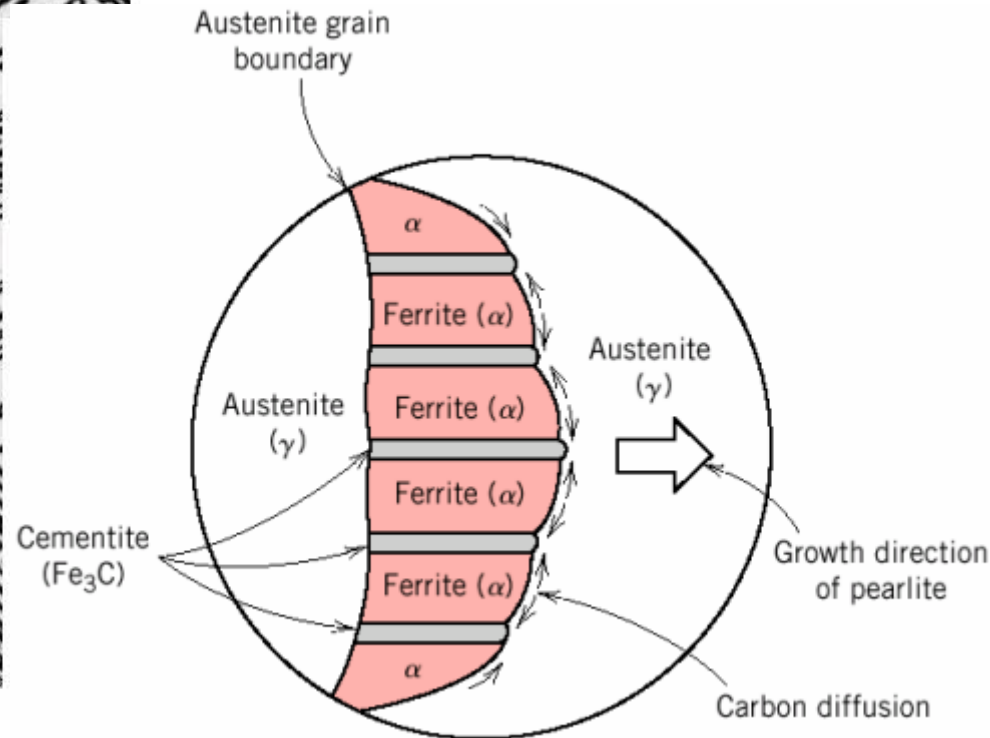
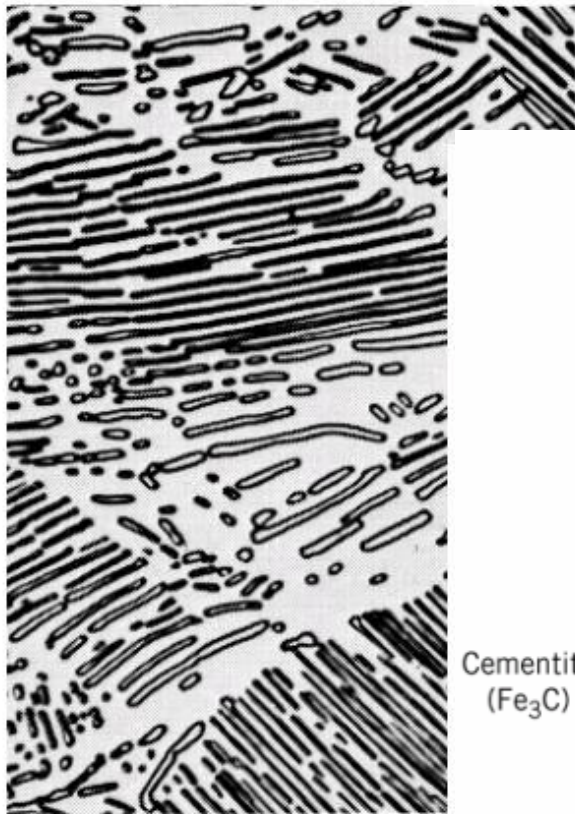


Microstructure of Ferrite

Tensile Strength: 40,000 psi
Elongation: 40 % in 2 in. gage length
Hardness: Less than Rockwell C 0 or less than Rockwell B 90
Toughness: Low

Steel - Pearlite is a slowly cooled 0.76 wt%C alloy, lamellar or layered α -ferrite (0.022 wt%C) and cementite (6.7 wt%C) Fe_3C as C atoms redistribute by atomic diffusion

Dark areas of Fe_3C
Light phase α -ferrite

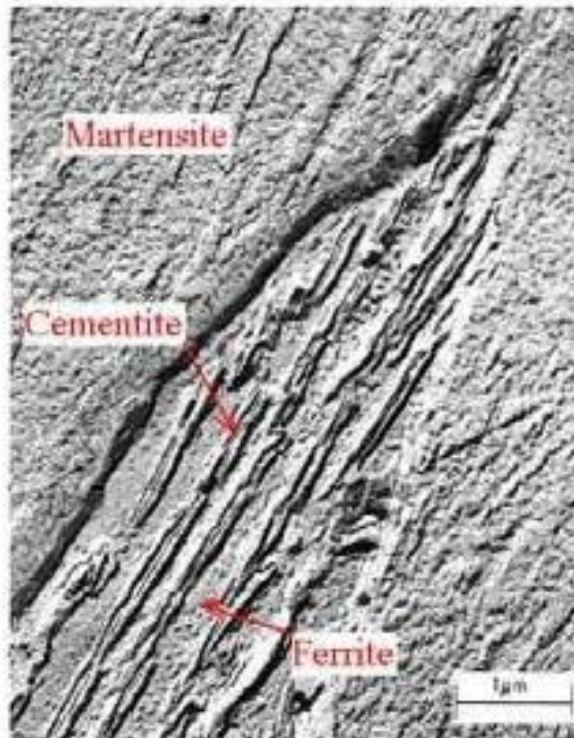


Pearlite properties in between soft, ductile ferrite and hard brittle cementite.

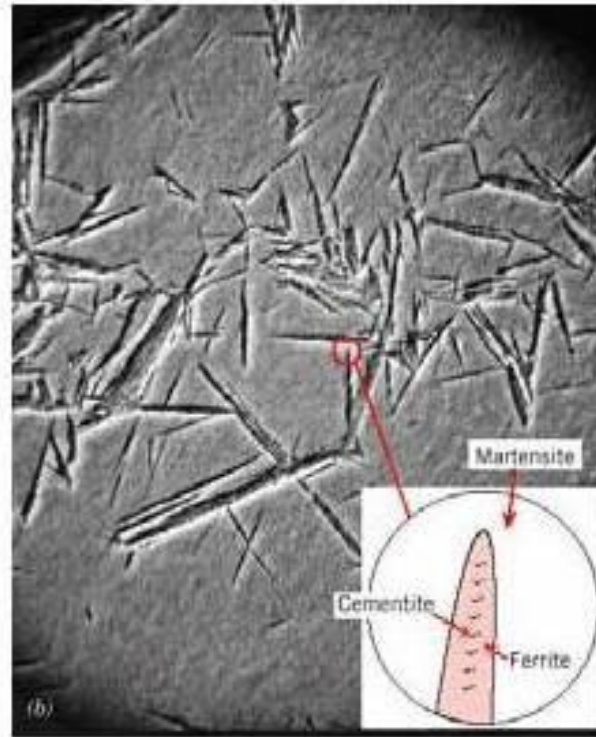
Tensile Strength: 120,000 psi
Elongation: 20 % in 2 in gauge length
Hardness: Rockwell C 20 or BHN 250-300

Pearlite needs fixed amounts of cementite and ferrite.

Bainite



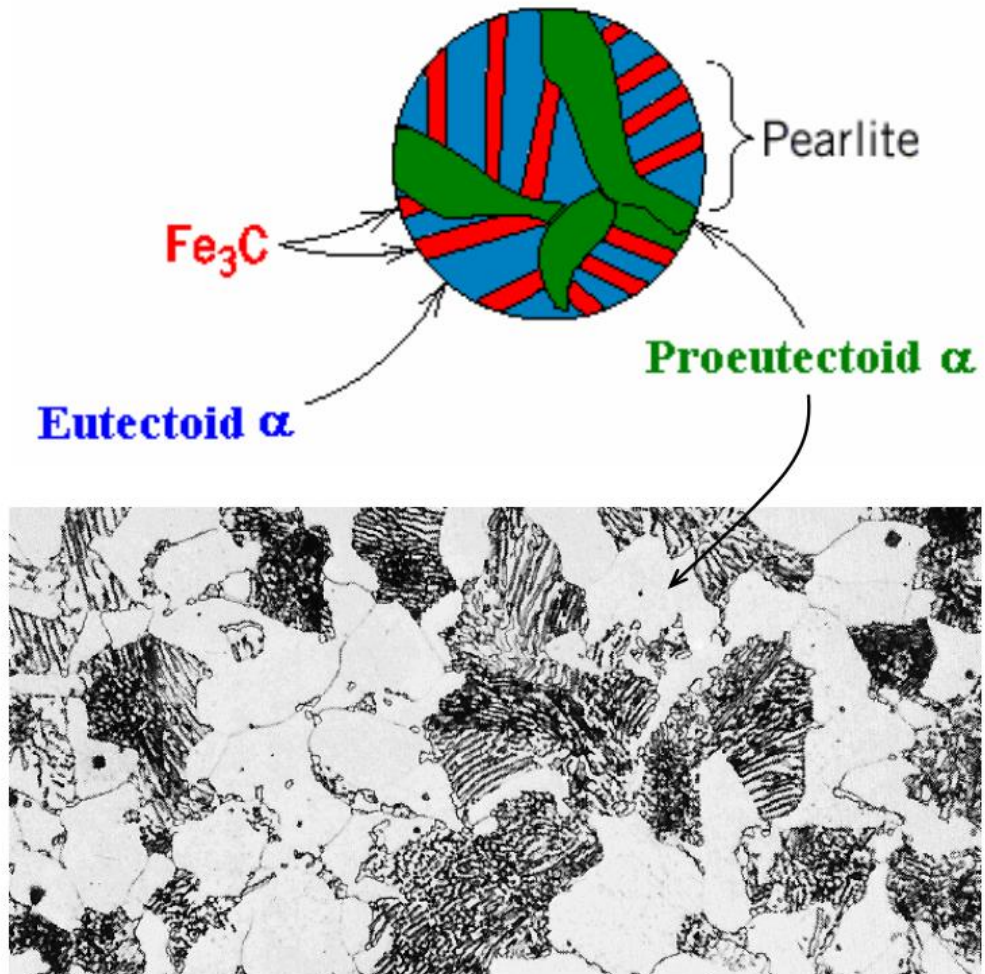
Upper Bainite
Microstructure of Upper Bainite and Lower Bainite



Lower Bainite

Hypoeutectoid steel

p

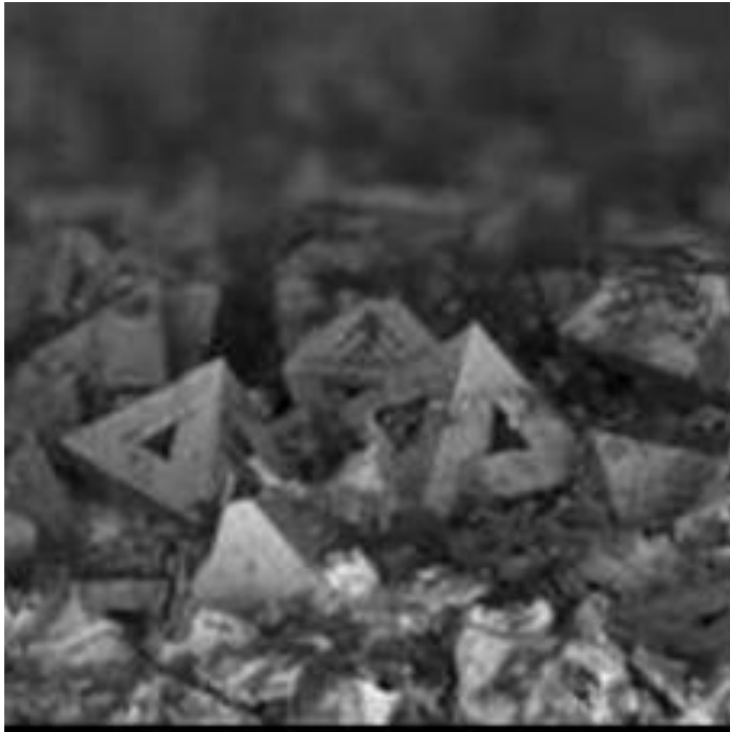


Metalloids



- Have some characteristics of metals, some of nonmetals.
- For instance, silicon looks shiny, but is brittle and fairly poor conductor.

Germanium - a grey-white metalloid.
Crystalline and brittle
An important semiconductor

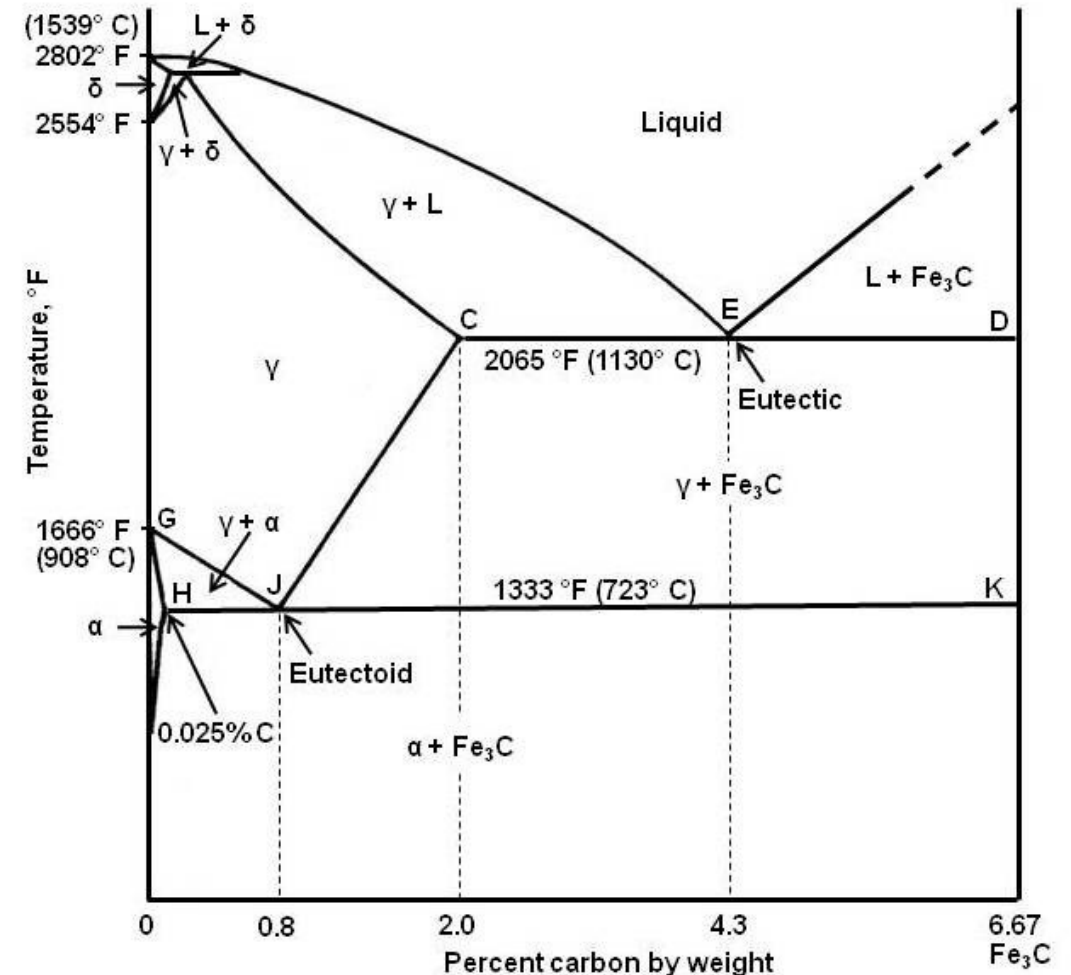


The Iron-Iron Carbide Equilibrium Diagram

Iron is an allotropic material. The temperature at which the allotropic changes take place in iron is influenced by alloying elements, the most important of which is carbon

The part of iron-carbon alloy system diagram between pure iron and an interstitial compound, iron carbide (Fe_3C), containing 6.67 percent carbon by weight is called iron-iron carbide equilibrium diagram

it is not a true equilibrium diagram, since equilibrium implies no change of phase with time. In fact, the compound iron carbide decomposes into iron and carbon (graphite). This decomposition takes a very long time at room temperature, it takes several years to form graphite. The iron carbide is called metastable phase. Therefore, iron-iron carbide diagram even though technically represents metastable conditions, can be considered as representing equilibrium changes, under conditions of relatively slow heating and cooling.



The iron-iron carbide equilibrium diagram labeled in general terms

In the iron-iron carbide diagram, upper and lower critical temperature lines are shown as single lines under equilibrium conditions and labelled A_{e3} and A_{e1} etc. They are labelled differently because when they are determined, they don't occur at the same temperature.

The critical line on heating is always higher than the critical line on cooling. To distinguish them, the critical lines on heating are called A_c (c from chauffage which means heating in French)

The critical line on cooling is called A_r (r from refroidissement meaning cooling in French)

Eg Upper critical line of hypoeutectoid steel on heating would be A_{c3} and the same line on cooling would be A_{r3}

The rate of heating and cooling definitely has an effect on the temperature gap between these two lines. The slower the rate of heating and cooling the nearer the two lines are to each other so with infinitely slow heating and cooling they would probably occur at exactly the same temperature

The Rolling Process

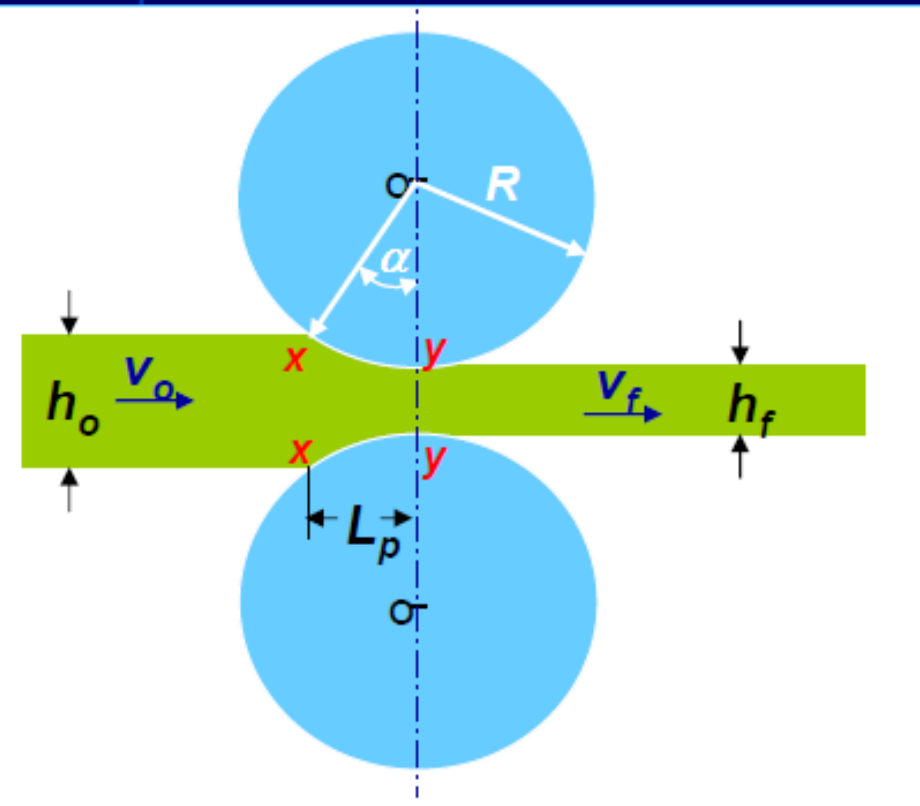
In the basic rolling process metal is passed between two rolls that rotate in opposite directions, the gap between the rolls being somewhat less than the thickness of the material.

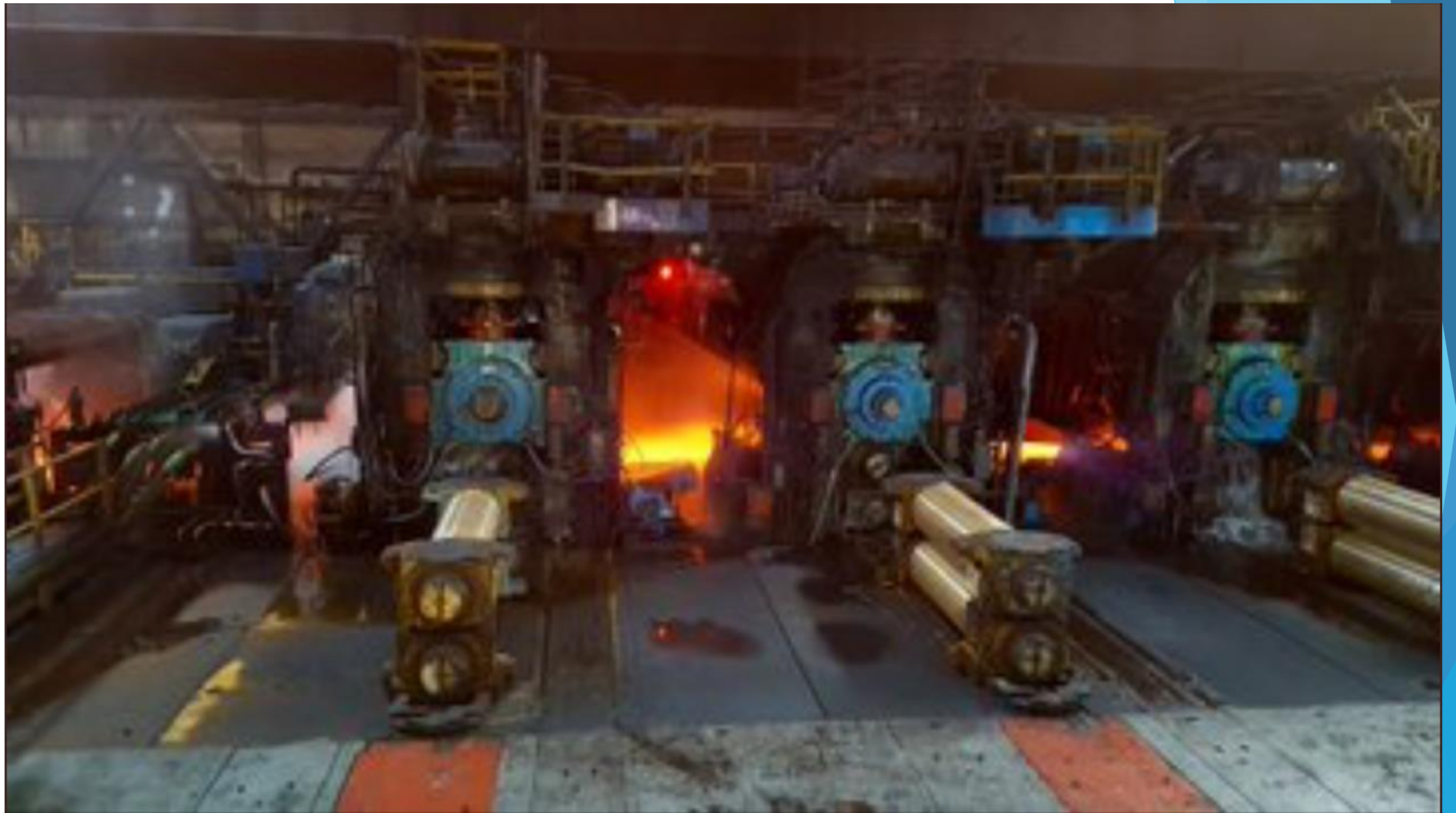
Because the rolls rotate faster than the speed of the incoming metal, friction along the contact interface acts to propel the metal forward.

The metal is then squeezed and elongates to compensate for the decrease in thickness.

The amount of deformation that can be achieved in a single pass between one pair of rolls depends on the friction conditions.

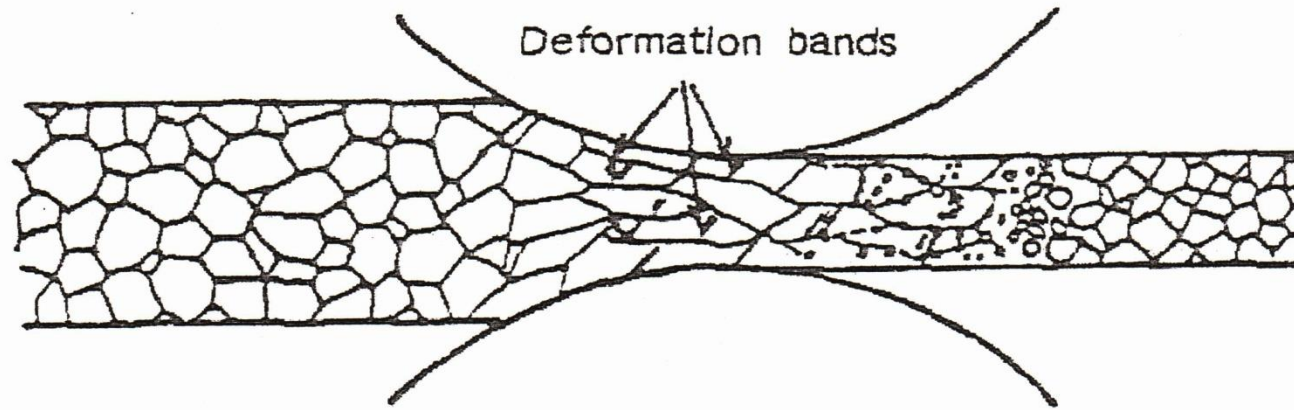
- If too much thickness reduction is demanded the rolls cannot advance the material, and simply skid over its surface.
- If too little deformation is given, the operation will be successful, but more passes will be needed to produce a given part which will increase the cost of production.





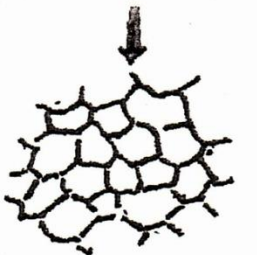
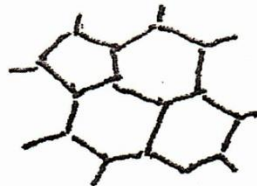
Conventional hot rolling of plain carbon steel

Finishing mill



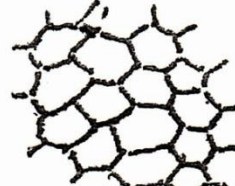
ROT and coiling

FT well above A_3
Coarse γ



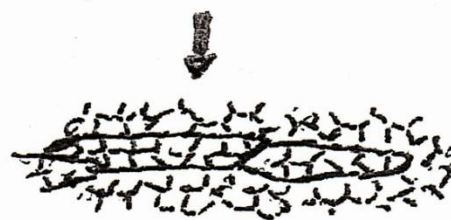
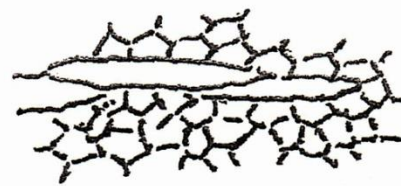
Coarse α

FT just above A_3
Fine γ



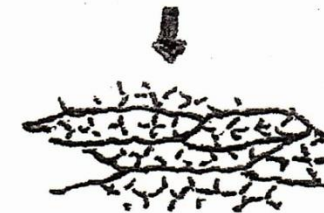
Fine α

Partly recrystallized
partly deformed γ



Mixed α grain size

Deformed γ



α grains in bands

Properties and grain structure

- ▶ https://www.youtube.com/watch?v=uG35D_euM-0

Primary Bonds

- ▶ Strong bonds
- ▶ Direct interaction of electrons between two atoms by transfer or sharing
- ▶ The more electrons per atom that take place in this process, the higher the bond “order” (e.g., single, double, or triple bond)
- ▶ four general categories of primary bonds: ionic, covalent, polar covalent, and metallic.

Ionic Bonds - heteropolar

- ▶ results when electrons are transferred from the more electropositive atom to the more electronegative atom, as in sodium chloride, NaCl.
- ▶ Ionic bonds usually result when the electronegativity difference between two atoms in a diatomic molecule is greater than about 2.0.
- ▶ Because of the large discrepancy in electronegativities, one atom will generally gain an electron, while the other atom in a diatomic molecule will lose an electron.

Covalent bonds - homopolar

- ▶ Weaker bond
- ▶ Electrons shared between two atoms - O_2 , H_2

Polar Covalent

- ▶ Polar covalent bonds are a particular type of covalent bond for example in water.
- ▶ In a polar covalent bond, the electrons shared by the atoms spend a greater amount of time, on the average, closer to the Oxygen nucleus than the Hydrogen nucleus. This is because of the geometry of the molecule and the great electronegativity difference between the Hydrogen atom and the Oxygen atom.
- ▶ The result of this pattern of unequal electron association is a charge separation in the molecule, where one part of the molecule, the Oxygen, has a partial negative charge and the Hydrogens have a partial positive charge.

Metallic

- ▶ Metallic bonds eg in copper or sodium were discovered by Lorentz
- ▶ the bonding electrons are “decentralized” and are shared by the core of positive nuclei.
- ▶ Metallic bonds occur when elements of low electronegativity (usually found in the lower left region of the periodic table) bond with each other to form a class of materials we call metals.
- ▶ an assembly of positively charged ion cores surrounded by free electrons or an “electron gas.” - Lorentz

Secondary bonds

- ▶ Weak bonds
- ▶ Indirect interaction of electrons in adjacent atoms or molecules
- ▶ Three types:
- ▶ Hydrogen bonding
- ▶ Dipole-dipole interactions
- ▶ Van der Waals forces (Dutch physicist)

Hydrogen bonds

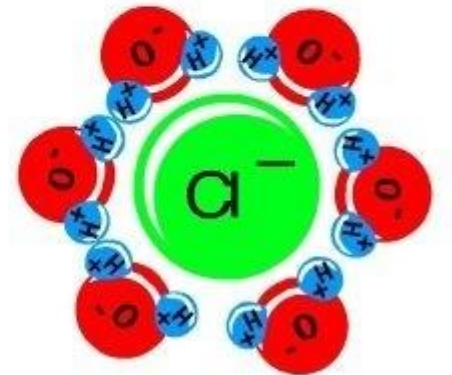
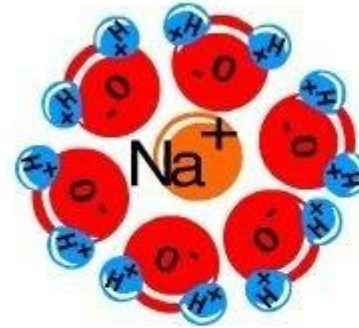
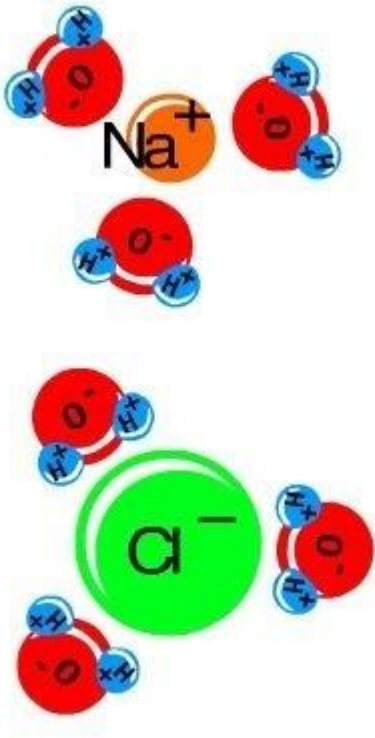
- ▶ Attraction between hydrogen in a highly polar molecule and the electronegative atom in another polar molecule. Eg in water H_2O
- ▶ In the water molecule, oxygen draws much of the electron density around it, creating positively charged centres at the two hydrogen atoms. These positively charged hydrogen atoms can interact with the negative centre around the oxygen in adjacent water molecules.
- ▶ Same strength as Van der Waals
- ▶ Affects boiling and melting point
- ▶ Causes ice to be less dense than water (most substances more dense as solid than as liquid)

Van der Waals forces

- ▶ Due to momentary electric dipoles (regions of positive and negative charges)
- ▶ These occur due to variations in charge density
- ▶ Common bond
- ▶ Very weak
- ▶ Found in inert gases where other bonds don't exist

Dipole-dipole interaction

- ▶ On addition to water the Na^+ section of NaCl is attracted to the oxygen side of the water molecules, while the Cl^- side is attracted to the hydrogen's side of the water molecule. This causes the sodium chloride to split in water, and the NaCl dissolves into separate Na^+ and Cl^- atoms. A hydration shell is formed around them which prevents Na^+ and Cl^- forming ionic bonds.



Dipole-dipole interaction

- ▶ Some molecules have permanent charge separations or dipoles
- ▶ The interaction of a positive dipole with a negative dipole
- ▶ Eg NaCl in water is split due to very strong dipole -dipole interactions splitting the molecule
- ▶ On addition to water the Na^+ section of NaCl is attracted to the oxygen side of the water molecules, while the Cl^- side is attracted to the hydrogens' side of the water molecule. This causes the sodium chloride to split in water, and the NaCl dissolves into separate Na^+ and Cl^- atoms. A hydration shell is formed around them which prevents Na^+ and Cl^- forming ionic bonds.

Table 1.5 Examples of Substances with Different Types of Interatomic Bonding

Type of Bond	Substance	Bond Energy, kJ/mol	Melting Point, (°C)	Characteristics
Ionic	CaCl	651	646	Low electrical conductivity, transparent, brittle, high melting point
	NaCl	768	801	
	LiF	1008	870	
	CuF ₂	2591	1360	
	Al ₂ O ₃	15,192	3500	
Covalent	Ge	315	958	Low electrical conductivity, very hard, very high melting point
	GaAs	~315	1238	
	Si	353	1420	
	SiC	1188	2600	
	Diamond	714	3550	
Metallic	Na	109	97.5	High electrical and thermal conductivity, easily deformable, opaque
	Al	311	660	
	Cu	340	1083	
	Fe	407	1535	
	W	844	3370	
van der Waals	Ne	2.5	−248.7	Weak binding, low melting and boiling points, very compressible
	Ar	7.6	−189.4	
	CH ₄	10	−184	
	Kr	12	−157	
	Cl ₂	31	−103	
Hydrogen bonding	HF	29	−92	Higher melting point than van der Waals bonding, tendency to form groups of many molecules
	H ₂ O	50	0	