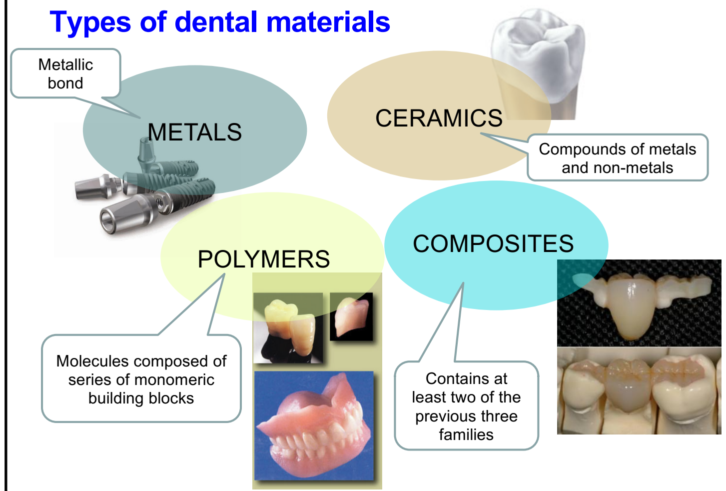
Physical Bases of Dental Material science 5.

Polymers, composites.

E-book Chapters: 12-13

Homework: Chapter 3.: 21, 24, 25, 27

Types of dental materials



Polymers

Macromolecule, that is a long chain of monomers

Properties:

- low density
- liquid or solid at room temperature
- low/medium stiffness and hardness, but easily malleable
- viscoelasticity
- relatively bad heat and corrosion resistance
- relatively bad electric and heat conduction
- diverse optical properties

Structure:

- covalent bonds between monomers in the chain, but usually weaker secondary bonds between chains
- semi-crystalline or amorphous

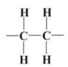
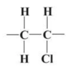
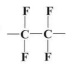
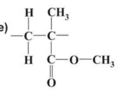
synthesis:

- addition
- condensation

Applications:

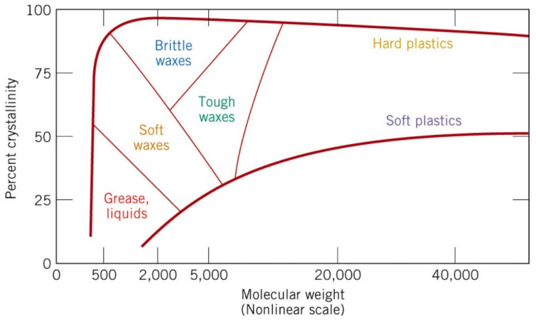
- denture
- temporary filling
- impression materials

Monomer

name of the polymer	structure of the monomer	industrial application	dental application
polyethylene (PE)			
polyvinylchloride (PVC)			
polytetrafluoroethylene (PTFE, Teflon)			
Poly(methyl methacrylate) (PMMA, acrylic glass)			

- **homopolymer:** one kind of monomer only
- **heteropolymer (copolymer):** two or more kinds of monomers

The length (molar mass) of polymer molecules and percent of crystallinity determines the physical properties:



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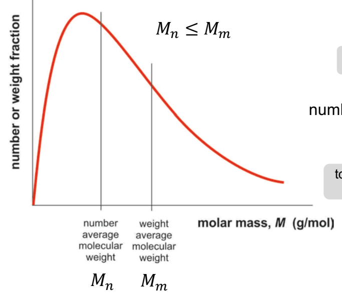
Polymer composition

Statistics!



...of molecules with given molecular weight

number... number ratio: $\frac{n_i}{n}$ — total number of molecules

mass... mass ratio: $\frac{m_i}{m}$ — total mass of molecules

number average molecular weight (M_n):

$$M_n = \frac{n_1 M_1 + n_2 M_2 + \cdots + n_i M_i + \cdots + n_k M_k}{n_1 + n_2 + \cdots + n_i + \cdots + n_k} = \frac{\sum_{i=1}^{k} n_i M_i}{\sum_{i=1}^{k} n_i} .$$

weight average molecular weight (M_m):

$$M_m = \frac{m_1 M_1 + m_2 M_2 + \cdots + m_i M_i + \cdots + m_k M_k}{m_1 + m_2 + \cdots + m_i + \cdots + m_k} = \frac{\sum_{i=1}^{k} m_i M_i}{\sum_{i=1}^{k} m_i} .$$

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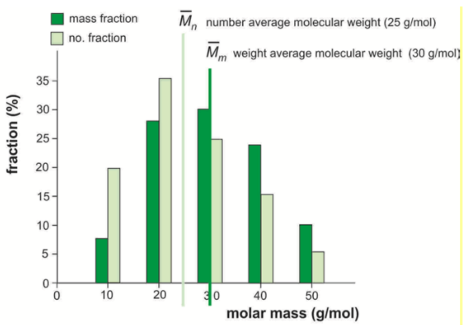
An example:

molar mass, M_i (g/mol)	n_i	no. fraction n_i/n (proportion)	$m_i = n_i \cdot M_i$ (g/mol)*	mass fraction m_i/m
$M_1 = 10$	$n_1 = 4$	4/20 = 0.20 = 20%	$m_1 = 4 \cdot 10 = 40$	40/500 = 0.08 = 8%
$M_2 = 20$	$n_2 = 7$	7/20 = 0.35 = 35%	$m_2 = 7 \cdot 20 = 140$	140/500 = 0.28 = 28%
$M_3 = 30$	$n_3 = 5$	5/20 = 0.25 = 25%	$m_3 = 5 \cdot 30 = 150$	150/500 = 0.30 = 30%
$M_4 = 40$	$n_4 = 3$	3/20 = 0.15 = 15%	$m_4 = 3 \cdot 40 = 120$	120/500 = 0.24 = 24%
$M_5 = 50$	$n_5 = 1$	1/20 = 0.05 = 5%	$m_5 = 1 \cdot 50 = 50$	50/500 = 0.10 = 10%
total	$n = 20$	1 = 100%	$m = 500$	1 = 100%

$$M_n = \frac{\sum_{i=1}^{k} n_i M_i}{\sum_{i=1}^{k} n_i}$$

$$M_m = \frac{\sum_{i=1}^{k} m_i M_i}{\sum_{i=1}^{k} m_i}$$



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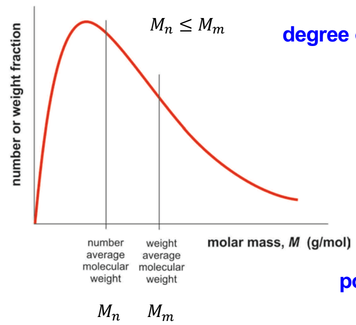

degree of polymerization: $\frac{M_n}{M_{\text{monomer}}}$

average length of polymer molecules

polydispersity index: $\frac{M_m}{M_n}$

diversity of polymer molecules

= 1: monodisperse
1< : polydisperse

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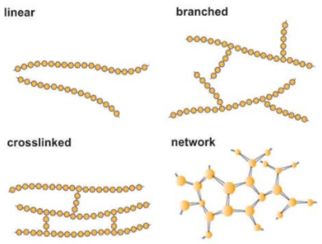
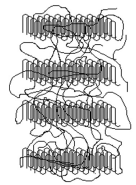
Structure of polymers



- thermoplastics
- elastomers

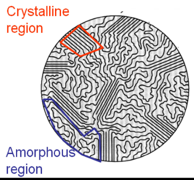
semi-crystalline



Degree of crystallinity (x):

amorphous $x = \frac{m_{crystalline}}{m_{total}} (\cdot 100\%)$ crystalline

0% → 100%



Composites

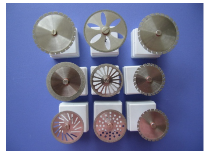
Materials of multiple, chemically different components with distinct phase boundaries

Properties:

- low density
- solid at room temperature
- combines the benefits of each of the phases
- strong, elastic and tough
- diverse optical properties

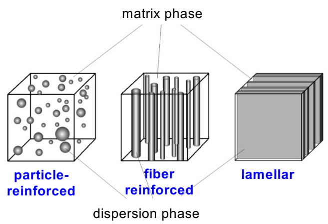
Applications:

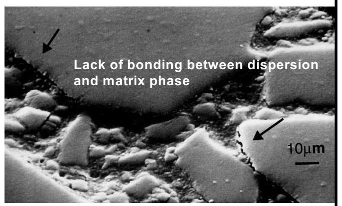
- filling
- dental tools



Structure of composites

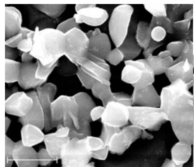
Two-phase composite: **Matrix phase** **(polymer, metal, ceramics)**
+
dispersion phase **(ceramics, metal, ...)**
+
couplin agent! **(silanes)**

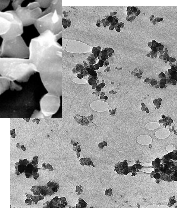




Hybrid composites: multiple dispersion phases

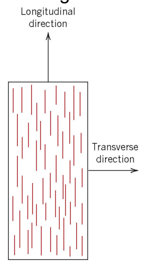
particle-reinforced → large particles, fine particles

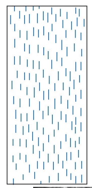


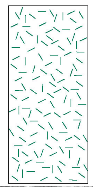


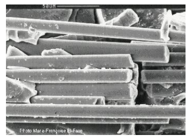
fiber-reinforced → long unidirectional, short fiber

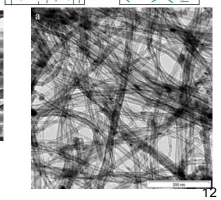
short fiber → unidirectional, randomly oriented



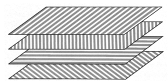








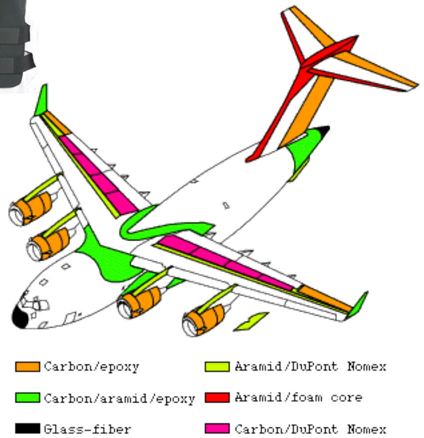
Structural compsites



Applications







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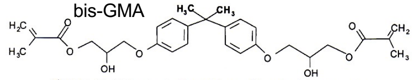
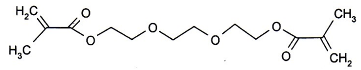
Dental composites

matrix: polymer (dimethacrylate)
dispersion material: glass (silica), ceramic crystal (i.e. quartz), polymer, (photoinitiator), ... + pigment, + UV absorbent

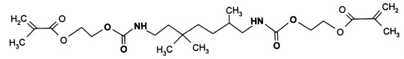
bis-GMA



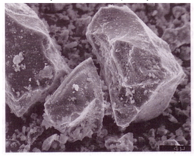
TEGDGMA



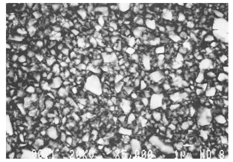
UDMA



large-grained (0,1-100 μm)



micrograined (≈ 40 nm)



shrinkage during polymerization may cause secondary caries

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DEFINITIONS

a) Frenkel defect ***(d)***

a) Eutectic alloy

a) Thixotropic fluid ***(g)***

a) Surface tension ***(f)***

a) Degree of crystallinity

a) Cohesion

CALCULATIONS

The vacancy formation energy in aluminium is 0.66 eV. What is the percentage of vacancies in the metal lattice at a temperature of 500 °C? (10p)

The mass percent of gold is 59.1% in a gold-copper alloy.
a) Calculate the molar percent of the metals! (M_{Au}=197 g/mol, M_{Cu}= 63.9 g/mol) (5p)

b) Calculate the mean density of the alloy! (ρ_{Cu}= 8.96 g/cm^3, ρ_{Au}= 19.3 g/cm^3) (5p)

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Alloying ratios:

- mass% $c_{m,1} = \frac{m_1}{m_1 + m_2} (\cdot 100\%)$
- mole% $c_{v,1} = \frac{\nu_1}{\nu_1 + \nu_2} (\cdot 100\%)$ → properties!

(i.e. Ni-Cr-Mo-Be alloy: Be 1,8 mass% ↔ 11 mole%)

Conversion:

$$c_{v,1} = \frac{c_{m,1} \cdot M_2}{c_{m,1} \cdot M_2 + c_{m,2} \cdot M_1} (\cdot 100\%) \qquad c_{m,1} = \frac{c_{v,1} \cdot M_1}{c_{v,1} \cdot M_1 + c_{v,2} \cdot M_2} (\cdot 100\%)$$

Mean density: $\bar{\rho} = \frac{\rho_1 \cdot \rho_2}{c_{m,1} \cdot \rho_2 + c_{m,2} \cdot \rho_1}$

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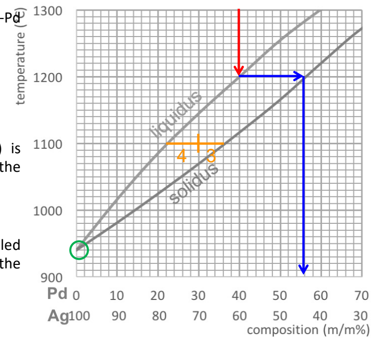
5. The figure shows the phase diagram of Ag-Pd alloy. Answer the questions!



a) What is the melting point of silver? (2p)

940 ºC

b) A 40% Pd — 60% Ag melted alloy (m/m) is cooled from 1300 °C. At which temperature will the first solid grains appear? (2p)

1200 ºC

c) A 40% Pd — 60% Ag melted alloy (m/m) is cooled from 1300 °C. Determine the mass % of Pd in the solid grains that appear first! (3p)

56%

d) A 30% Pd — 70% Ag alloy has a temperature of 1100 °C. Determine how many percent of the total mass is in liquid and in solid phases! (3p)

l=3/7=43%
s=5/7=57%