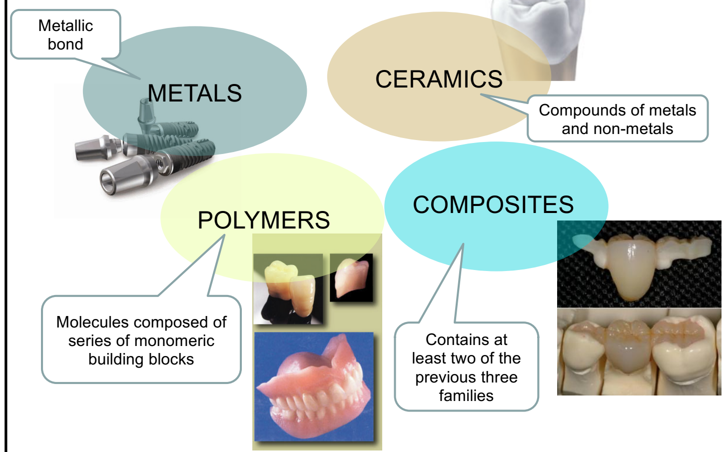
Physical Foundations of Dental Materials Science 5.

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

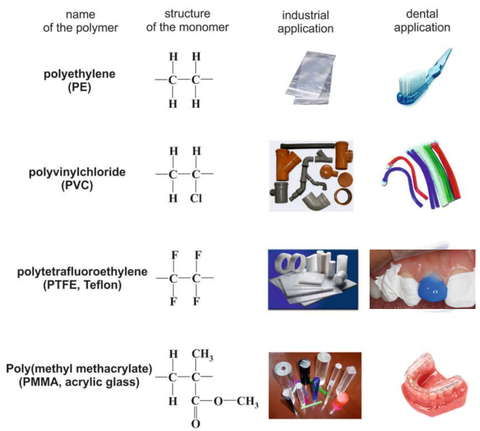
synthesis:

- addition
- condensation

Applications:

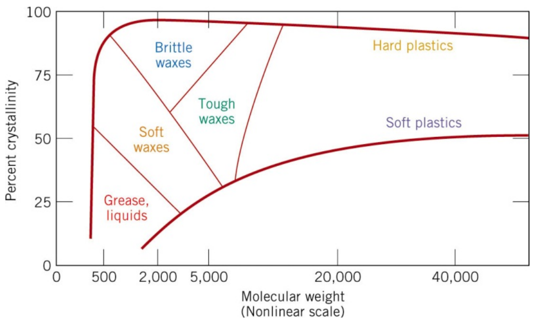
- denture
- filling
- impression materials (siloxane

Monomer



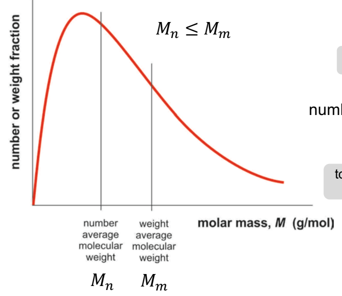
- **homopolymer:** one kind of monomer only
- **heteropolymer (copolymer):** two or more kinds of monomers

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



Polymer composition

Statistics!



number... ...of molecules with given molecular weight mass...

number ratio: $\frac{n_i}{n}$ mass ratio: $\frac{m_i}{m}$

total number of molecules total mass of molecules

number average molecular weight (M_n):

$$M_n = \frac{n_1M_1 + n_2M_2 + \cdots + n_iM_i + \cdots + n_kM_k}{n_1 + n_2 + \cdots + n_i + \cdots + n_k} = \frac{\sum_{i=1}^{k} n_iM_i}{\sum_{i=1}^{k} n_i} .$$

weight average molecular weight (M_m):

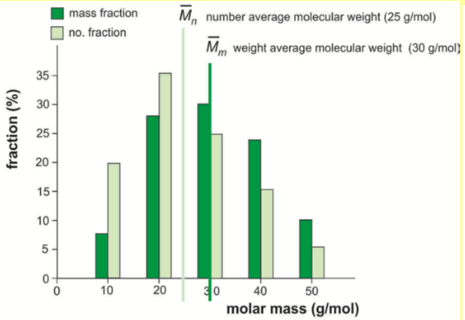
$$M_m = \frac{m_1M_1 + m_2M_2 + \cdots + m_iM_i + \cdots + m_kM_k}{m_1 + m_2 + \cdots + m_i + \cdots + m_k} = \frac{\sum_{i=1}^{k} m_iM_i}{\sum_{i=1}^{k} m_i} .$$

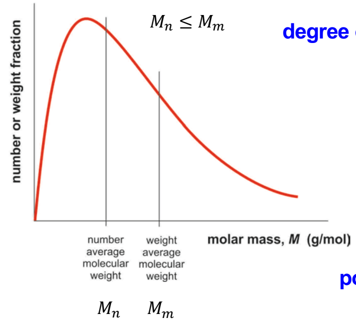
An example:

molar mass, M_i (g/mol)	n_i	number ratio n_i/n	$m_i = n_i \cdot M_i$ (g/mol)*	mass ratio m_i/m
M_1 = 10	n_1 = 4	4/20 = 0.20 = 20%	m_1 = 4·10 = 40	40/500 = 0.08 = 8%
M_2 = 20	n_2 = 7	7/20 = 0.35 = 35%	m_2 = 7·20 = 140	140/500 = 0.28 = 28%
M_3 = 30	n_3 = 5	5/20 = 0.25 = 25%	m_3 = 5·30 = 150	150/500 = 0.30 = 30%
M_4 = 40	n_4 = 3	3/20 = 0.15 = 15%	m_4 = 3·40 = 120	120/500 = 0.24 = 24%
M_5 = 50	n_5 = 1	1/20 = 0.05 = 5%	m_5 = 1·50 = 50	50/500 = 0.10 = 10%
total	*n* = 20	1 = 100%	*m* = 500	1 = 100%

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

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





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

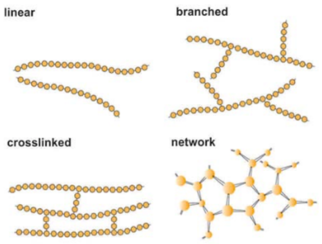
average length of polymer molecules

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

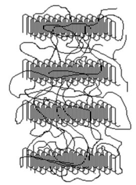
diversity of polymer molecules

= 1: monodisperse
1< : polydisperse

Structure of polymers



semi-crystalline

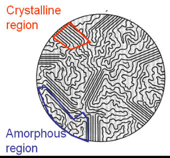


Degree of crystallinity (x):

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

0% → 100%

- thermoplastics: *Acrylic (PMMA), Nylon, polyethylene, PVC, teflon...*
- thermosets: vulcanized rubber, bakelite, epoxy...
  - elastomers: great elasticity



9

9

Composites

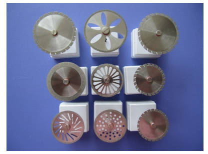
Materials of multiple, chemically different components with distinct phase boundaries

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



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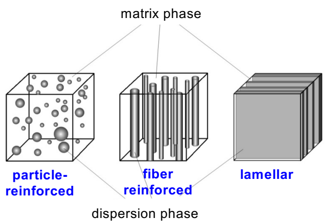
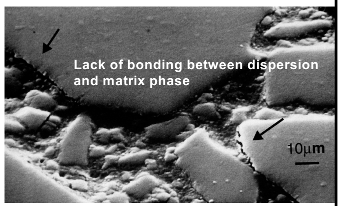
10

Structure of composites

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

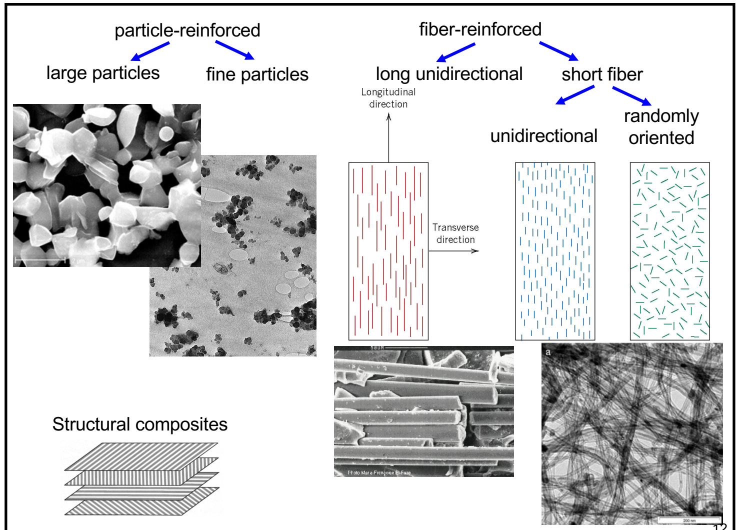




Hybrid composites: multiple dispersion phases

11

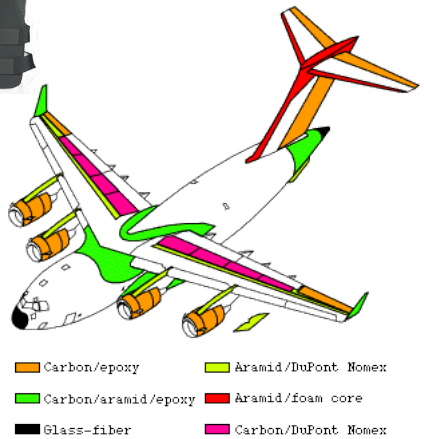
11



12

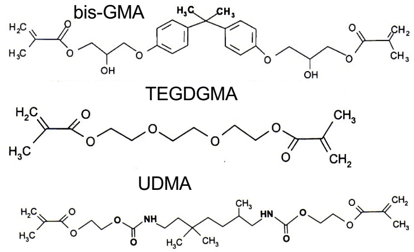
12

Applications

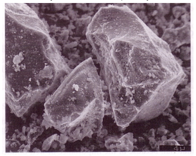


Dental composites

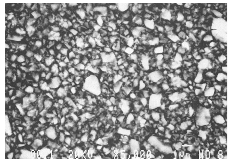
matrix: polymer (dimethacrylate)
dispersion material: glass (silica), ceramic crystal (i.e. quartz), polymer, + pigment, + UV absorbent (photo initiator), ...



large-grained (0,1-100 μm)



micrograined (≈ 40 nm)



shrinkage during polymerization may cause secondary caries

DEFINITIONS

Frenkel defect *(d)*

Eutectic alloy

Thixotropic fluid *(g)*

Surface tension *(f)*

Degree of crystallinity

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)

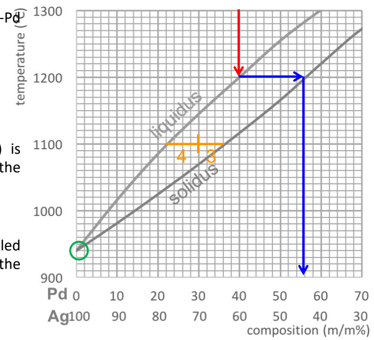
The mass percent of gold is 59.1% in a gold-copper alloy.
a) Calculate the molar percent of the metals! (M_{Au}=197 g/mol, M_{Cu}= 63.9 g/mol) (5p)

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

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

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

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



a) What is the melting point of silver? (2p)
940 °C

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 °C

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%