



## Physical Bases of Dental Material science

### 5.

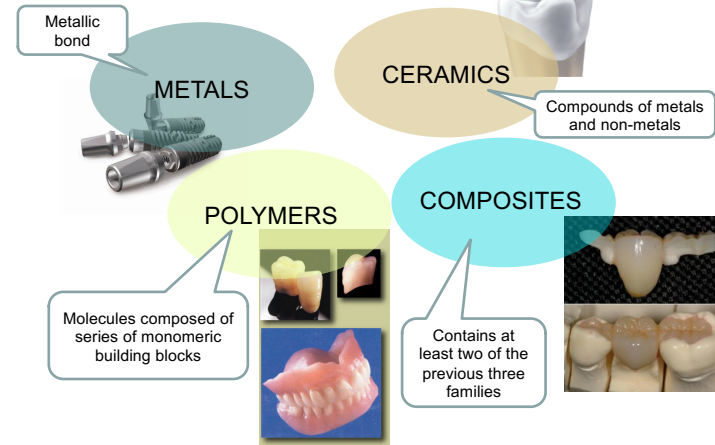
Polymers, composites.

E-book  
Chapters:  
12-13

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

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## Types of dental materials



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## 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



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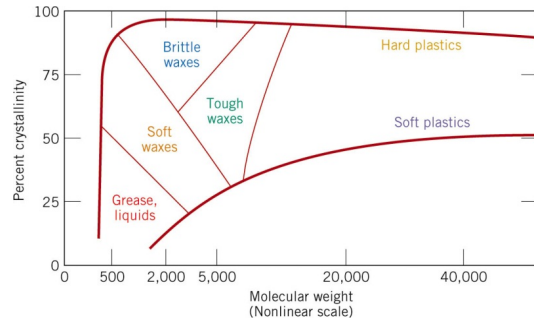
## Monomer

name of the polymer	structure of the monomer	industrial application	dental application
polyethylene (PE)	$\begin{array}{c} \text{H} & \text{H} \\   &   \\ -\text{C}- & -\text{C}- \\   &   \\ \text{H} & \text{H} \end{array}$		
polyvinylchloride (PVC)	$\begin{array}{c} \text{H} & \text{H} \\   &   \\ -\text{C}- & -\text{C}- \\   &   \\ \text{H} & \text{Cl} \end{array}$		
polytetrafluoroethylene (PTFE, Teflon)	$\begin{array}{c} \text{F} & \text{F} \\   &   \\ -\text{C}- & -\text{C}- \\   &   \\ \text{F} & \text{F} \end{array}$		
Poly(methyl methacrylate) (PMMA, acrylic glass)	$\begin{array}{c} \text{H} & \text{CH}_3 \\   &   \\ -\text{C}- & -\text{C}- \\   &   \\ \text{H} & \text{O}-\text{CH}_3 \\ & \text{O} \end{array}$		

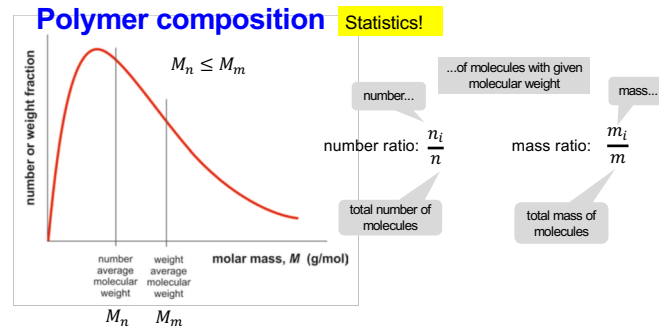
- **homopolymer:** one kind of monomer only
- **heteropolymer (copolymer):** two or more kinds of monomers

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



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number average molecular weight ( $M_n$ ):

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

weight average molecular weight ( $M_m$ ):

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

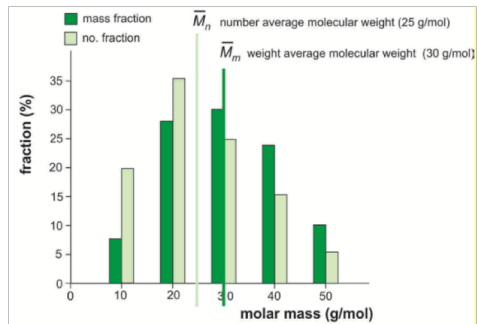
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An example:

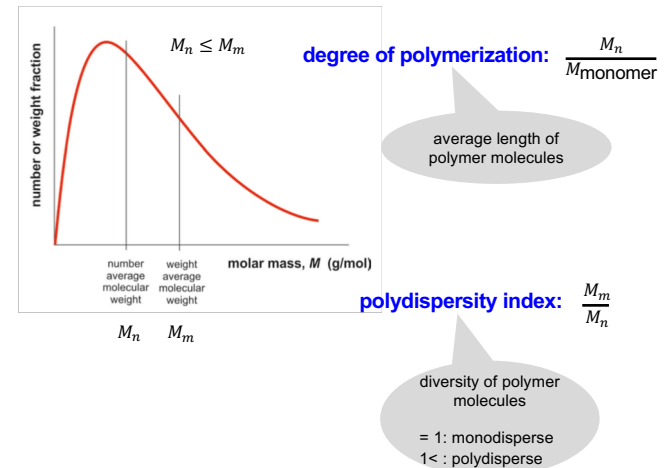
molar mass, $M_i$ (g/mol)	$n_i$	no. fraction $n_i/n$ (proportion)	$m_i = n_i \cdot M_i$ (g/mol)*	mass fraction $m_i/m$
$M_1 = 10$	$n_1 = 4$	$4/20 = 0.20 = 20\%$	$m_1 = 4 \cdot 10 = 40$	$40/500 = 0.08 = 8\%$
$M_2 = 20$	$n_2 = 7$	$7/20 = 0.35 = 35\%$	$m_2 = 7 \cdot 20 = 140$	$140/500 = 0.28 = 28\%$
$M_3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

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

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

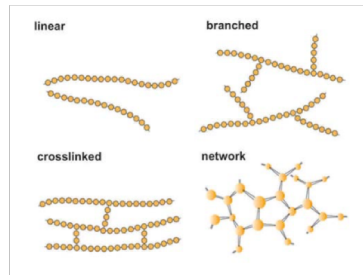


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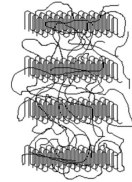
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## Structure of polymers



- thermoplastics
- duroplasts
- elastomers

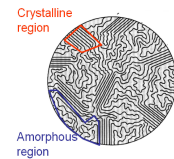
## semi-crystalline



## Degree of crystallinity (x):

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

0% 
0%
100%



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## 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:

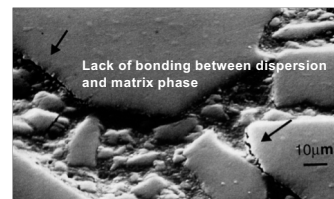
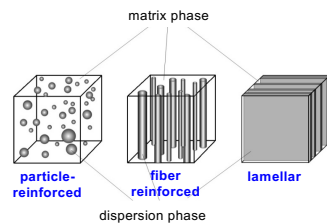
- filling
- dental tools



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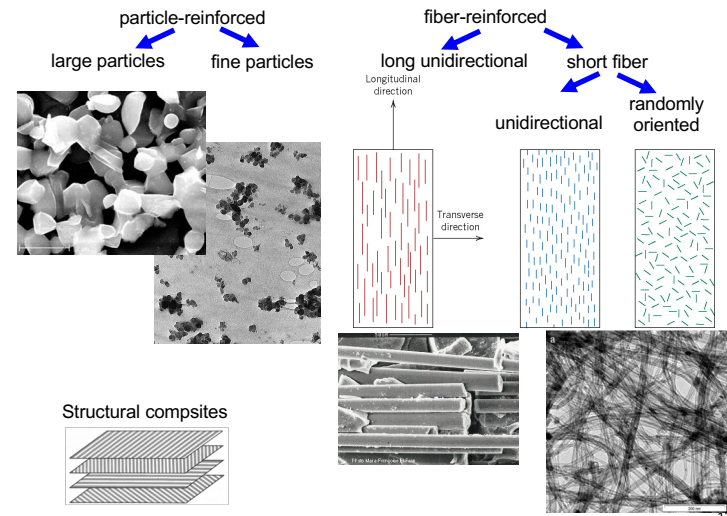
## Structure of composites

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



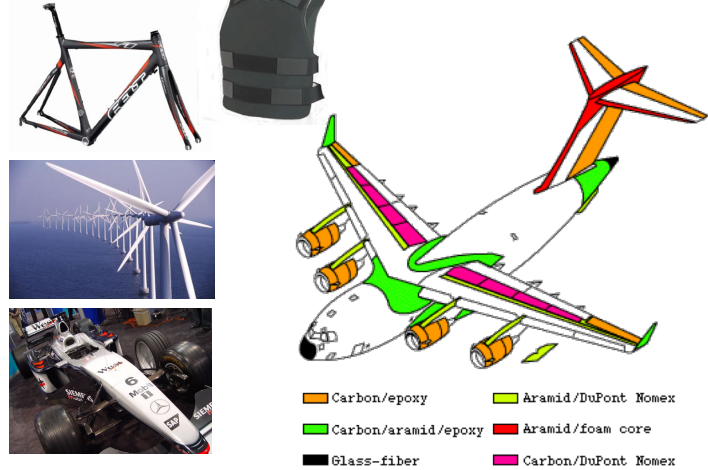
**Hybrid composites:** multiple dispersion phases

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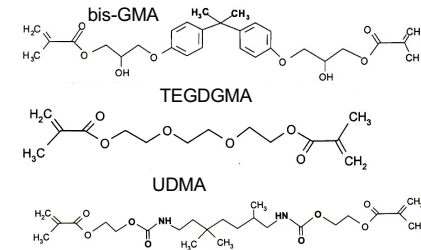
## Applications



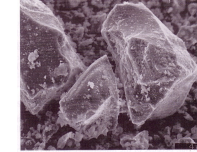
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## Dental composites

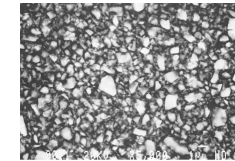
**matrix:** polymer (dimethacrylate)  
**dispersion material:** glass (silica), ceramic crystal (i.e. quartz), polymer, + pigment, + UV absorbent (photoinitiator), ...



large-grained  
(0,1-100 μm)



micrograined  
(≈ 40 nm)



shrinkage during polymerization  
may cause secondary caries

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## 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! ( $M_{Au}=197 \text{ g/mol}$ ,  $M_{Cu}=63.9 \text{ g/mol}$ ) (5p)

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

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## Alloying ratios:

- mass%**  $c_{m,1} = \frac{m_1}{m_1 + m_2} (\cdot 100\%)$
- mole%**  $c_{v,1} = \frac{V_1}{V_1 + V_2} (\cdot 100\%) \rightarrow \text{properties!}$   
 (i.e. Ni-Cr-Mo-Be alloy: Be 1,8 mass%  $\leftrightarrow$  11 mole%)

Conversion:

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

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 °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)

$l=3/7=43\%$

$s=5/7=57\%$

