

# Physical bases of dental material science

## Polymers, composites

Irén Bárdos-Nagy

The simplified composition of an amalgam alloy is 45 % mercury, 40 % silver and 15 % tin. Calculate the molar percent of the components.

$M_{\text{Hg}} 200,6$ ,  $M_{\text{Ag}} 107,9$ ,  $M_{\text{Sn}} 118,7$

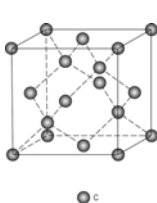
$$c_{v\text{Ag}} = \frac{\frac{40}{107,9}}{\frac{45}{200,6} + \frac{40}{107,9} + \frac{15}{118,7}} \cdot 100 = 51,4\%$$

$$c_{v\text{Hg}} = \frac{\frac{45}{200,6}}{\frac{45}{200,6} + \frac{40}{107,9} + \frac{15}{118,7}} \cdot 100 = 31,1\%$$

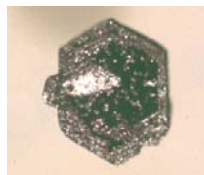
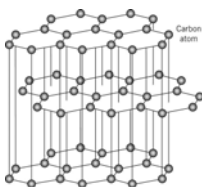
$$c_{v\text{Sn}} = \frac{\frac{15}{118,7}}{\frac{45}{200,6} + \frac{40}{107,9} + \frac{15}{118,7}} \cdot 100 = 17,6\%$$

## Polymers

diamond

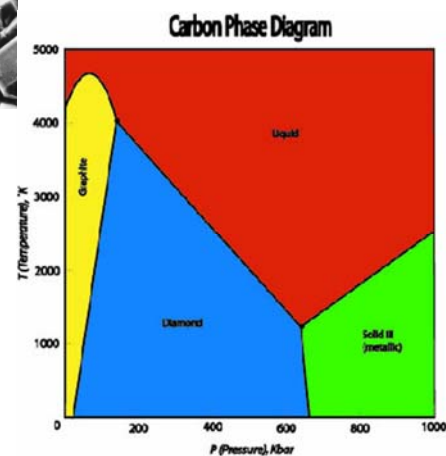


graphite

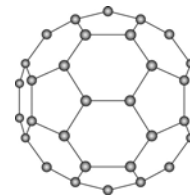


derivate from the Greek roots:

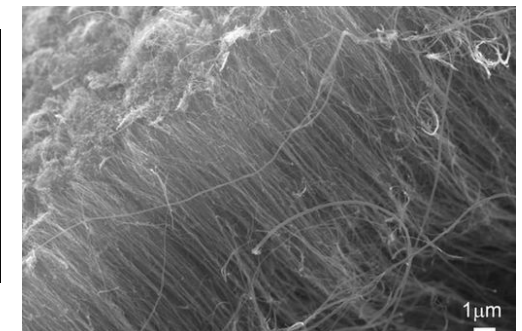
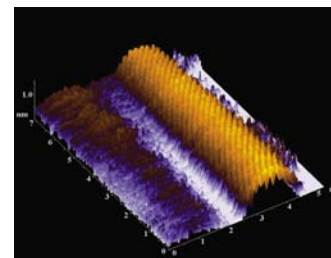
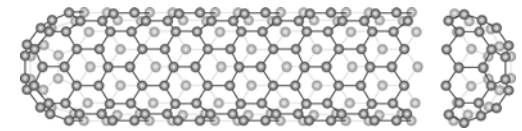
**poly** (many) and **meros** (part)



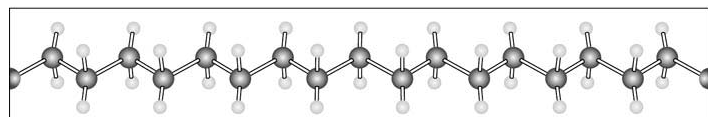
fullerene ( $\text{C}_{60}$ )



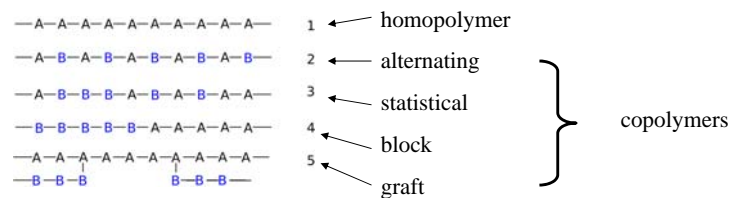
nanotube



example: polyethylene

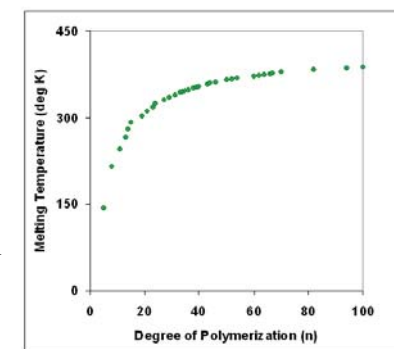


(b)

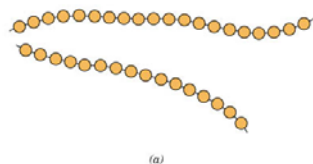


$$DP_n = \frac{\text{Total MW of the polymer}}{\text{MW of the repeating unit}} \equiv X_n = \frac{M_n}{M_0}$$

correlation of molecular weight with physical properties of polymers

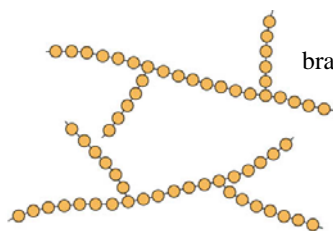


linear



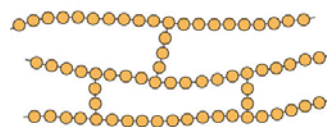
(a)

branched



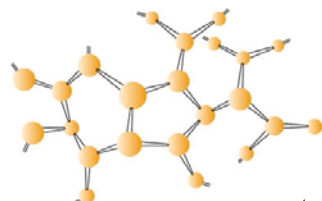
(b)

crosslinked



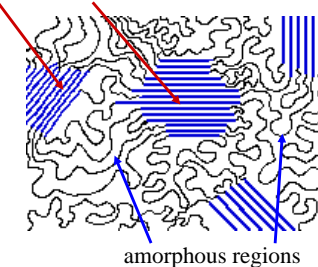
(c)

network

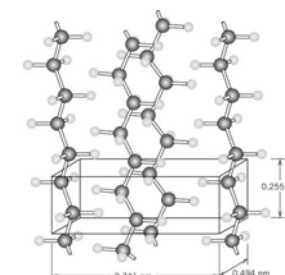


(d)

## crystalline domains



amorphous regions



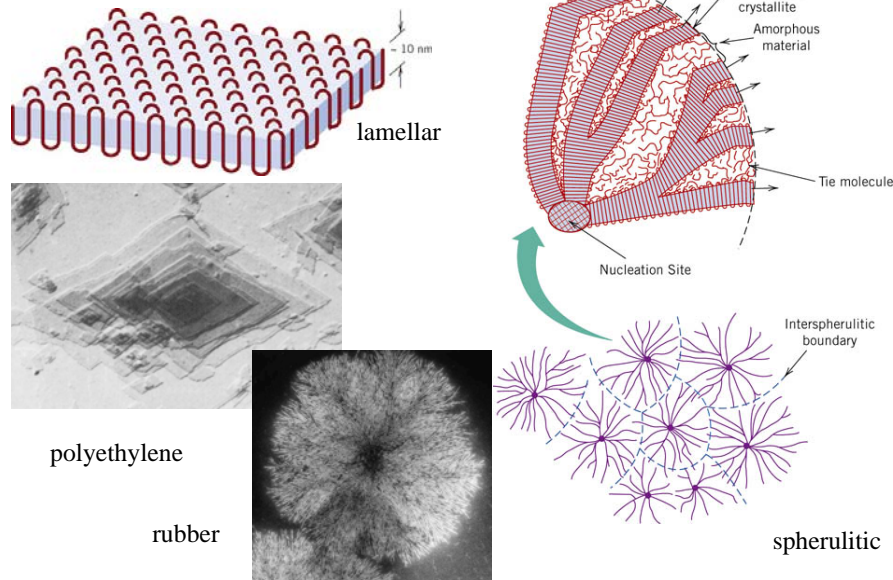
0.255

494 nm

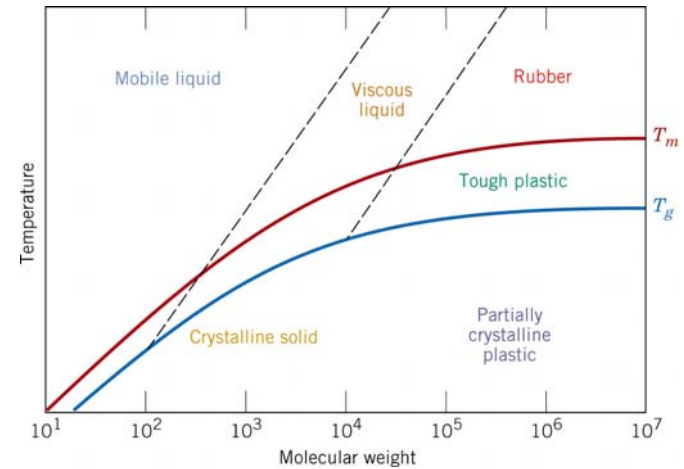
 Springer

factors influencing the degree of crystallinity: temperature, type of the monomer, chain length, chain branching, interchain bonding

Types of structure:



Dependence of melting and glass transition temperatures and polymer properties on molecular weight



**T<sub>m</sub>** is the temperature at which crystalline domains lose their structure, or melt.

As crystallinity increases, so does T<sub>m</sub>.

**T<sub>g</sub>** is the temperature below which amorphous domains lose the structural mobility of the polymer chains and become rigid glasses.

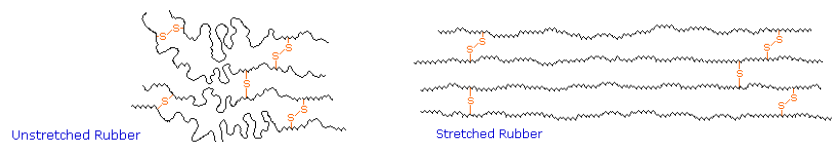
**Thermoplastic polymers (thermoplasts):** **soften reversibly** when heated (harden when cooled)

At elevated T inter-chain bonding is weakened allowing deformation at low stresses. Most thermoplasts are linear polymers and some branched structures.

**Thermosetting polymers (thermosets):** **harden permanently** when heated.

Covalent crosslinks (~ 10 - 50% of mers) formed during heating. Cross-linking hinder bending and rotations. Thermosets are harder, more dimensionally stable, and more brittle than thermoplasts.

**Elastomers:** **a group of amorphous polymers** that have the ability to stretch and then return to their original shape at temperatures above T<sub>g</sub>.

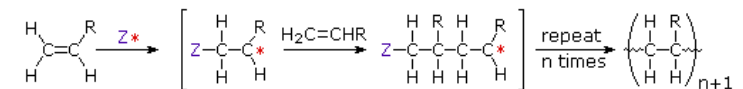


## Synthesis of polymers - polymerization

a./ Addition (chain-reaction or chain-growth) polymerization:

The monomer units are attached one at a time.

Has three distinct stages: initiation, propagation, and termination.

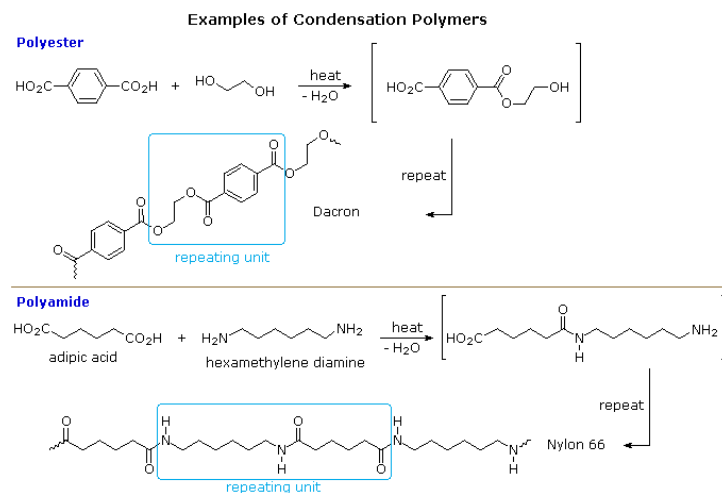


Z\* is an initiating species

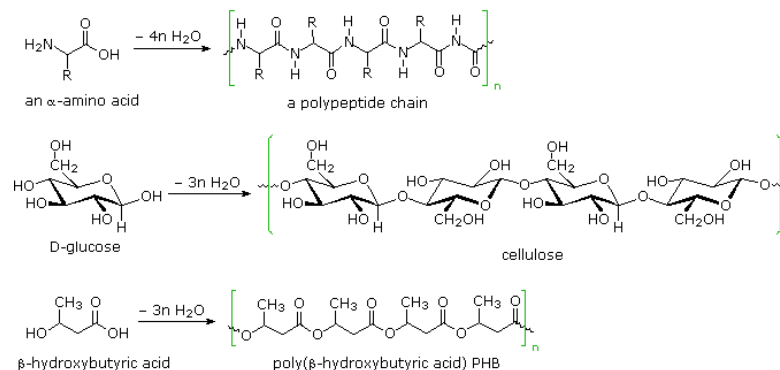
\* may be a radical, a cation or an anion

b./ Condensation (step reaction, step growth) polymerization:

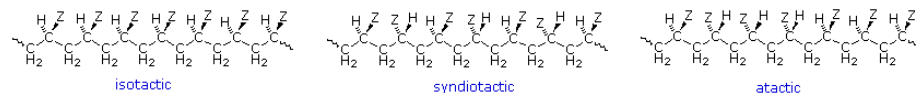
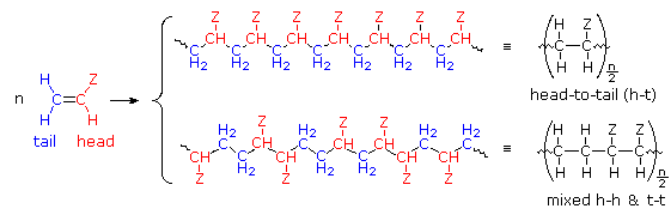
stepwise intermolecular chemical reactions that produce the mer units



#### Some Natural Condensation Polymers



#### Regio and stereoisomerisation in macromolecules

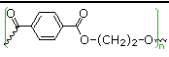
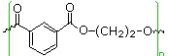
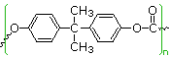

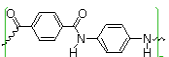
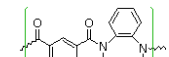
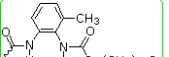
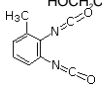


Polymer	T <sub>g</sub> atactic	T <sub>g</sub> isotactic	T <sub>g</sub> syndiotactic
PP	-20 °C	0 °C	-8 °C
PMMA	100 °C	130 °C	120 °C

#### Some examples of common addition polymers

Name(s)	Formula	Monomer	Properties	Uses
<b>Polyethylene</b> low density (LDPE)	$-(\text{CH}_2-\text{CH}_2)_n-$	ethylene $\text{CH}_2=\text{CH}_2$	soft, waxy solid	film wrap, plastic bags
<b>Polyethylene</b> high density (HDPE)	$-(\text{CH}_2-\text{CH}_2)_n-$	ethylene $\text{CH}_2=\text{CH}_2$	rigid, translucent solid	electrical insulation bottles, toys
<b>Polypropylene</b> (PP) different grades	$-(\text{CH}_2-\text{CH}(\text{CH}_3))_n-$	propylene $\text{CH}_2=\text{CHCH}_3$	<u>atactic</u> : soft, elastic solid <u>isotactic</u> : hard, strong solid	similar to LDPE carpet, upholstery
<b>Poly(vinyl chloride)</b> (PVC)	$-(\text{CH}_2-\text{CHCl})_n-$	vinyl chloride $\text{CH}_2=\text{CHCl}$	strong rigid solid	pipes, siding, flooring
<b>Poly(vinylidene chloride)</b> (Saran A)	$-(\text{CH}_2-\text{CCl}_2)_n-$	vinylidene chloride $\text{CH}_2=\text{CCl}_2$	dense, high-melting solid	seat covers, films
<b>Polystyrene</b> (PS)	$-(\text{CH}_2-\text{CH}(\text{C}_6\text{H}_5))_n-$	styrene $\text{CH}_2=\text{CHC}_6\text{H}_5$	hard, rigid, clear solid soluble in organic solvents	toys, cabinets packaging (foamed)

<b>Polyacrylonitrile</b> (PAN, Orlon, Acrilan)	$-(CH_2-CHCN)_n-$	acrylonitrile $CH_2=CHCN$	high-melting solid soluble in organic solvents	rugs, blankets clothing
<b>Polytetrafluoroethylene</b> (PTFE, Teflon)	$-(CF_2-CF_2)_n-$	tetrafluoroethylene $CF_2=CF_2$	resistant, smooth solid	non-stick surfaces electrical insulation
<b>Poly(methyl methacrylate)</b> (PMMA, Lucite, Plexiglas)	$-[CH_2-C(CH_3)(CO_2CH_3)]_n-$	methyl methacrylate $CH_2=C(CH_3)CO_2CH_3$	hard, transparent solid	lighting covers, signs skylights
<b>Poly(vinyl acetate)</b> (PVAc)	$-(CH_2-CHOCOCH_3)_n-$	vinyl acetate $CH_2=CHOCOCH_3$	soft, sticky solid	latex paints, adhesives
<b>cis-Polyisoprene</b> natural rubber	$-[CH_2-CH=C(CH_3)-CH_2]_n-$	isoprene $CH_2=CH-C(CH_3)=CH_2$	soft, sticky solid	requires vulcanization for practical use
<b>Polychloroprene</b> (cis + trans) (Neoprene)	$-[CH_2-CH=CCl-CH_2]_n-$	chloroprene $CH_2=CH-CCl=CH_2$	tough, rubbery solid	synthetic rubber oil resistant

Formula	Type	Components	T <sub>g</sub> °C	T <sub>m</sub> °C
$-[CO(CH_2)_4CO-OCH_2CH_2O]_n-$	polyester	$HO-C-(CH_2)_4-CO_2H$ $HO-CH_2CH_2-OH$	< 0	50
	polyester Dacron Mylar	para $HO_2C-C_6H_4-CO_2H$ $HO-CH_2CH_2-OH$	70	265
	polyester	meta $HO_2C-C_6H_4-CO_2H$ $HO-CH_2CH_2-OH$	50	240
	polycarbonate Lexan	$(HO-C_6H_4)_2C(CH_3)_2$ (Bisphenol A) $X_2C=O$ (X = $OCH_3$ or Cl)	150	267
$-[CO(CH_2)_4CO-NH(CH_2)_6NH]_n-$	polyamide Nylon 66	$HO_2C-(CH_2)_4-CO_2H$ $H_2N-(CH_2)_6-NH_2$	45	265
$-[CO(CH_2)_2NH]_n-$	polyamide Nylon 6 Perlon		53	223
	polyamide Kevlar	para $HO_2C-C_6H_4-CO_2H$ para $H_2N-C_6H_4-NH_2$	---	500
	polyamide Nomex	meta $HO_2C-C_6H_4-CO_2H$ meta $H_2N-C_6H_4-NH_2$	273	390
	polyurethane Spandex	$HOCH_2CH_2OH$ 	52	---

### Physical properties of polymers (summary)

- low rigidity
- good ductility and viscoelasticity
- fragility (mainly the thermosets)
- chemical environment and temperature sensitivity
- low density
- large resistivity against the corrosion
- low resistivity against the heat

strongly depend on:

- molecular mass  
(chain length)
- structure
- degree of crystallinity

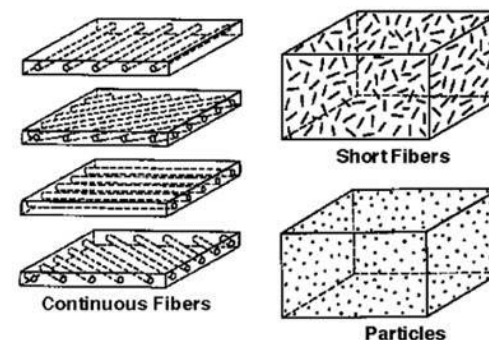
### Dental application of polymers

- impression materials
- bases, liners and varnishes for cavities
- prosthesis



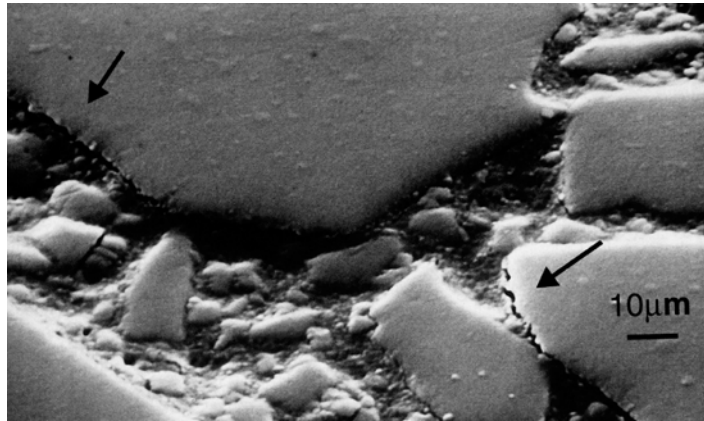
### Composites

Composite materials (or composites) are made from two or more constituent materials with significantly different physical or chemical properties and which remain separate and distinct within the finished structure.(on microscopic and macroscopic scales)





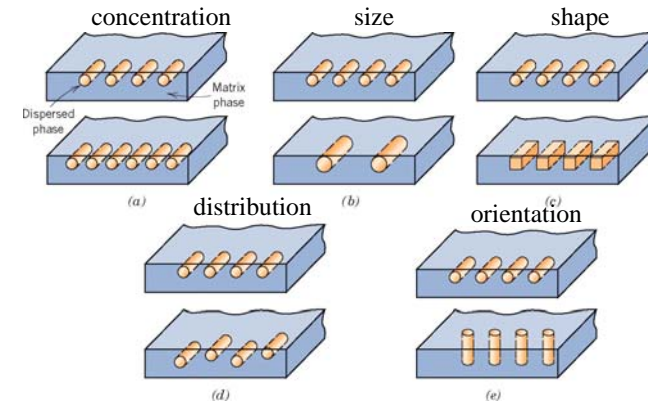
## Bonding of matrix and disperse component



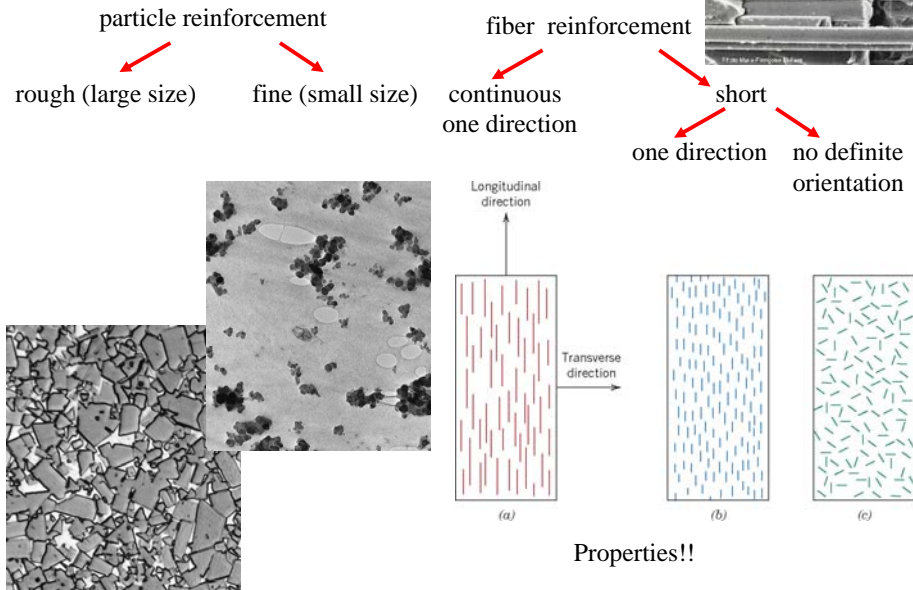
continuous phase (matrix)  
metal, ceramic, polymer

dispersed phase (reinforcement)  
ceramic, glass, metal...

Parameters acting on properties:



## Types of composites



Dental application of composites:

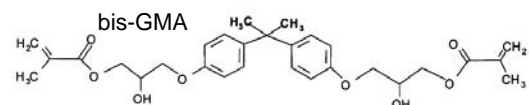
- fillings
- veneers
- restoration
- temporary crowns
- surface shaping and contouring



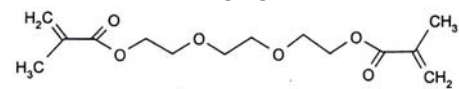
Matrix: polymer (resin)

Reinforcement: ceramic, quartz, glass, polymer,  
+ pigment + UV absorber

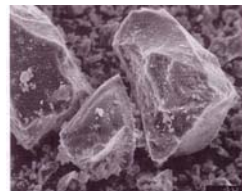
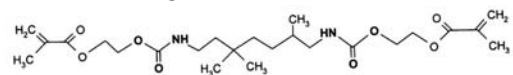
rough grains  
(0,1-100 mm)



TEGDGMA



UDMA



micrograins  
( $\approx 40$  nm)

