### **Textile Chemistry**





Jakub Wiener



### Classification of polymers



 inorganic - e.g. diamond, graphite, various carbides, silica (SiO2)x

organic - natural ( = biopolymers )

- synthetic

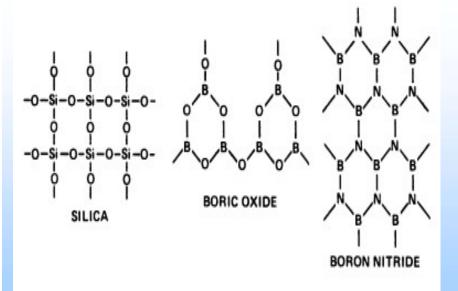
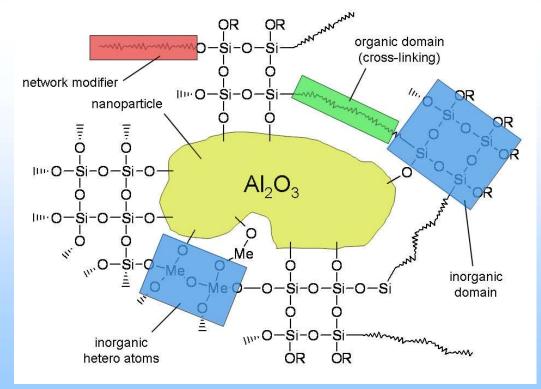


Figure 1.— Some inorganic polymers.



#### **Hybrid (organic-inorganic polymers)**



### **Silicones**



If the bonds between the atoms in the macromolecule chain are strong, the energy of these chemical bonds will be high and the polymer will be stable.

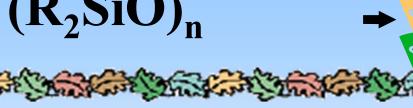
Chemical bond energies - if they are high, the bonds between the atoms in the macromolecule chain are strong and the polymer is stable.

(e.g. in silicones, the Si-O bond energy is much higher than the C-C bond energy in carbon polymers)

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Si-O (444.1 kJ/mol) > C-C (347.8 kJ/mol)

## Silicones (R<sub>2</sub>SiO)<sub>n</sub>



contain siloxane bonds - O - Si -

 $\begin{bmatrix}
CH_3 \\
\\
O - Si \\
\\
CH_3
\end{bmatrix}_n$ 

**Inorganic-organic polymers** 

The long-term heat resistance of silicone rubbers ranges from -60 to +180 °C (special types -100 to +260 °C, short-term up to +320 °C).

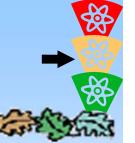
Inert to living organisms. Other properties include relative fire resistance, good electrical insulation properties, long-term resistance to UV radiation and weather conditions, water repellency (hydrophobicity) and vapour permeability

Production: They are prepared by hydrolysis of alkyl or arylchlorosilanes

These are prepared by direct synthesis of alkyl or aryl chlorides and elemental °C (Cu catalysis, 400°C)







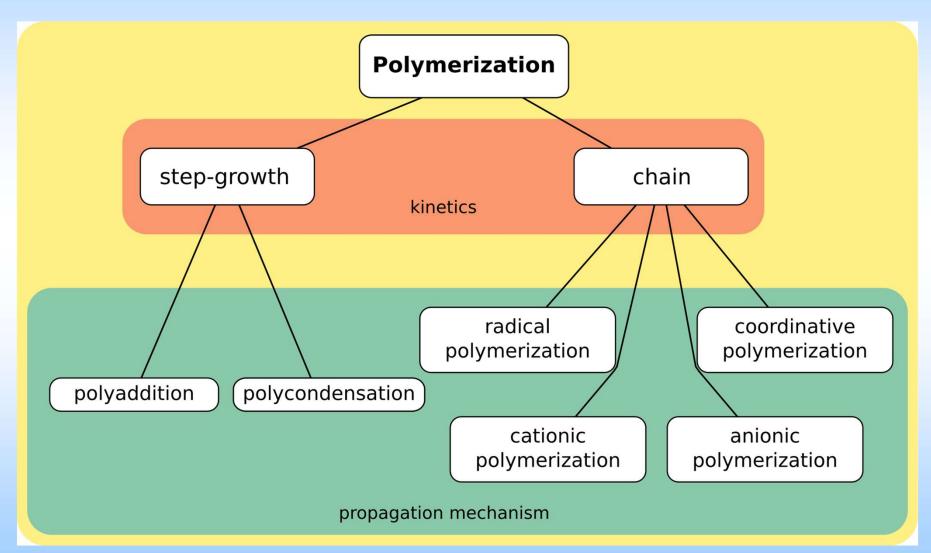
Silicones - They tolerate high temperatures well, are chemically less reactive, and are hydrophobic.

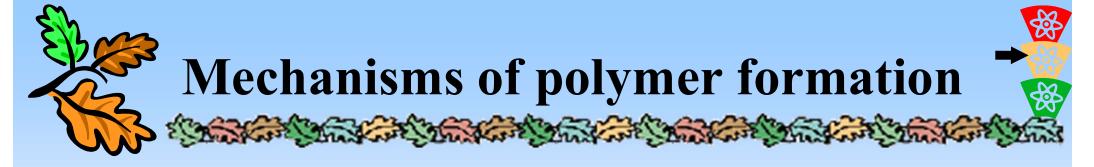
#### **Use of silicones:**

- as lubricants for heat-stressed machine parts
- plasticizers
- as hydrophobicity agents (water repellent)



## Mechanisms of polymer formation

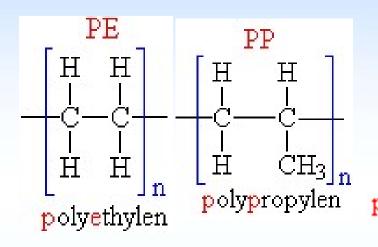


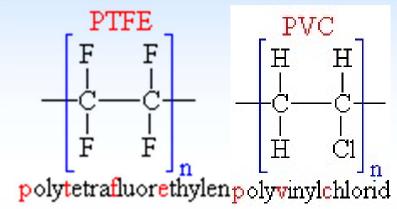


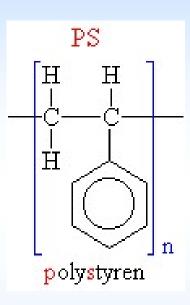
- Chain Polymerization: double bond required in the starting monomer A-A-A-A..
- Polycondensation: a small molecule is released during synthesis (e.g. water, methanol...) ..A-B-A-
- **A** + **B** ► macromolecule + e.g. water
- Polyaddition: monomers have reactive groups, no low molecular weight substance is released ..A-B-A-B-A
- A + B ➤ macromolecule













## Polyethylene



abbreviation: PE

HDPE (High Density PE)
LDPE (low density PE)





- properties: white, semi-transparent, flexible and tough to the touch;

has excellent electrical insulating properties; thermoplastic substance that can be moulded into desired products,

- applications: food packaging, foil, crockery, toys, chemical bottles, hoses, electrical cable insulation, in the medical sector for the manufacture of artificial blood vessels, etc,
- monomer: ethene (ethylene).

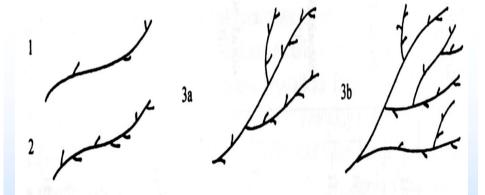
$$-\left\{ -CH_{2}-CH_{2}\right\} _{n}$$



## Polyethylene



Zkratka	Hustota (g/cm <sup>3</sup> )
ULDPE (Ultra-Low Density)	0,888-0,915
LDPE (Low Density)	0,910–0,955
LLDPE (Linear Low Density)	0,918–0,955
MDPE (Medium Density)	0,925–0,940
HDPE (High Density)	0,941–0,954
HMW-HDPE (High Molecular Weight HDPE)	0,944–0,954 MH = 200 000–500 000
UHMW-HDPE (Ultra-High Molecular Weight HDPE	0,955–0,957 MH = 3 000 000–6 000 000



Obr. 2.1. Struktura makromolekul různých typů PE: 1 – HDPE, 2 – LLDPE (krátké větvení), 3 – LDPE (dlouhé a krátké větvení, a – trubkový reaktor, b – autokláv)



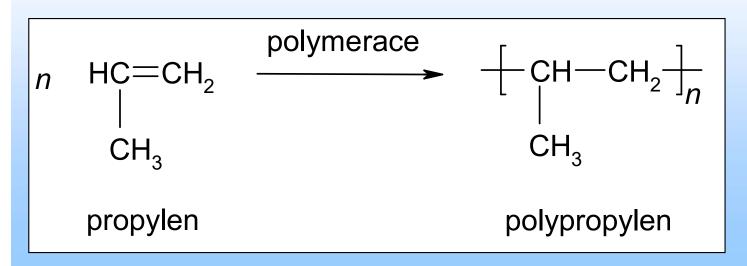




## Polypropylene



- properties: similar to PE, but stronger; resistant to temperatures up to 160°C,
- use: packaging material, utensils, insulation of electrical cables, in the medical sector for the production of syringes and items that can be sterilised (free of germs) at temperatures above 60°C, for the production of fibres, ropes
- monomer: propene (propylene)



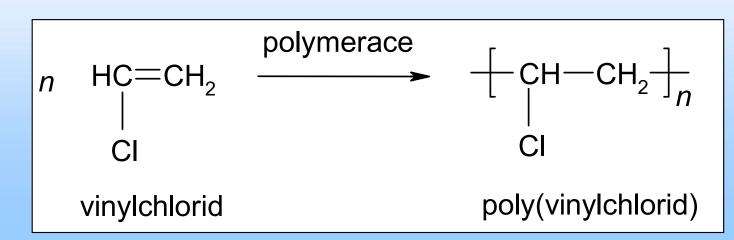




## Polyvinylchloride

- abbreviation: PVC,
- properties: thermoplastic substance that can be well thermoformed (softens at 80°C); resistant to acids and hydroxides, use:
- non-plasticized PVC is used for the production of water pipes, rods or plates;
- softened PVC for the production of plastic, foils, jackets raincoats, toys, films, tablecloths, bottles, artificial fur, etc, monomer: vinyl chloride.







### Polystyrene

- PS,
- Properties: hard, strong but brittle; acid and alkali resistant, thermoplastic, soluble in organic solvents (aldehydes, ketones, gasoline), acoustic and low-temperature insulator,

use: for the production of consumer goods, packaging, combs, bowls, spoons, yoghurt cups; foam PS as thermal or insulating material in the construction and refrigeration industry, etc,

- monomer: styrene (vinylbenzene).





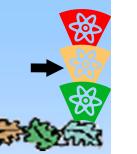
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- abbreviation: PTFE,
- trade name: Teflon,
- Properties: non-flammable, non-toxic thermoplastic, chemically very resistant (can withstand even hot Arctic Charcoal),
- use: special laboratory equipment, bone substitutes in surgery, kitchen utensils, etc,
- monomer: tetrafluoroethylene (tetrafluoroethylene).

$$-\left\{ -CF_{2} - CF_{2} \right\}_{n}$$



### **Elastomers**



CH<sub>3</sub>



#### Natural rubber

latex milk from rubber tree

$$\begin{bmatrix} CH_3 & H \\ & | & \\ -CH_2 - C = C - CH_2 \end{bmatrix}_n$$

structural unit of natural rubber

#### Natural rubber

$$\begin{array}{c|c}
 & CH_3 & H \\
 & | & | \\
 & CH_2 - C = C - CH_2 \\
 & & n
\end{array}$$

**Vulcanisation** of rubber

Elastomere



#### **Elastomers**

polyreakce

## Polybutadiene rubber BR, Buna

#### Polybutadiene styrene rubber

#### SBR, Kralex, Buna S

$$H_2C = CH - CH = CH_2 + n H_2C = CH$$

buta-1,3-dien

styren

monomer monomer

#### strukturní jednotka

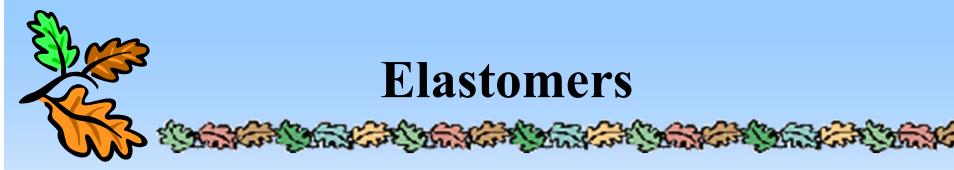
stavební jednotka

stavební jednotka

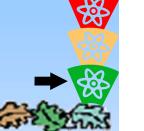
$$- CH_2 - CH = CH - CH_2 - CH_2 - CH_n$$

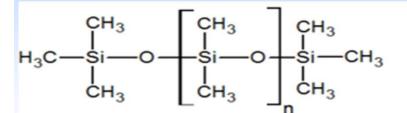
butadien-styrenový kaucuk

kopolymer



#### **Elastomers**





 $\frac{\text{POOR} \longrightarrow 2\text{RO}^{\bullet}}{\text{Vulcanisation}^{\text{H}_{3}\text{C}} - \bigvee_{\text{Si} \longrightarrow 0}^{\text{CH}_{3}} - \bigvee_{\text{CH}_{3}}^{\text{CH}_{3}} - \bigvee_{\text{CH}_{3}}^{\text{CH}_{3}}$ 

+2ROH

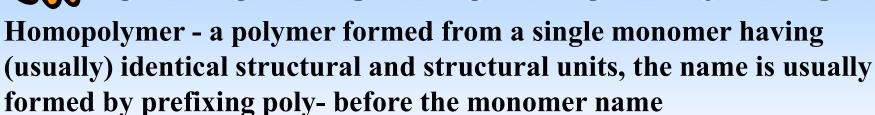
$$H_3C$$
  $\xrightarrow{CH_3}$   $\xrightarrow{CH_3}$   $\xrightarrow{CH_3}$   $\xrightarrow{CH_3}$   $\xrightarrow{CH_3}$   $\xrightarrow{CH_3}$   $\xrightarrow{CH_3}$   $\xrightarrow{CH_3}$  using peroxide

#### Benzoilperoxid



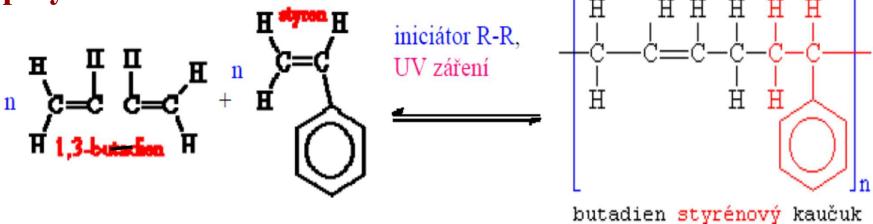


## **Copolymers**



Copolymers - polymers purposefully prepared from 2 or more monomers, the order of the units is not as important as DNA, but determines the properties of the resulting

polymer



## 

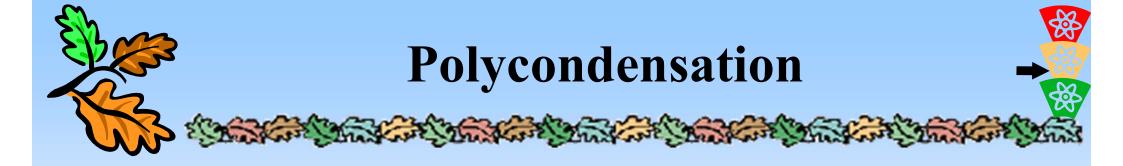
$$-A-B-A-B-A-B-A-B-A-B-$$
 2

$$-A-B-B-B-A-B-A-B-A-A-$$

$$-B-B-B-B-B-A-A-A-A-A-A$$

#### Different types of polymers:

- 1) homopolymer 2) alternating copolymer 3) random copolymer
- 4) block copolymer 5) graft copolymer.



Reaction of 2 different (or identical monomers) - at least two functional groups on each monomer

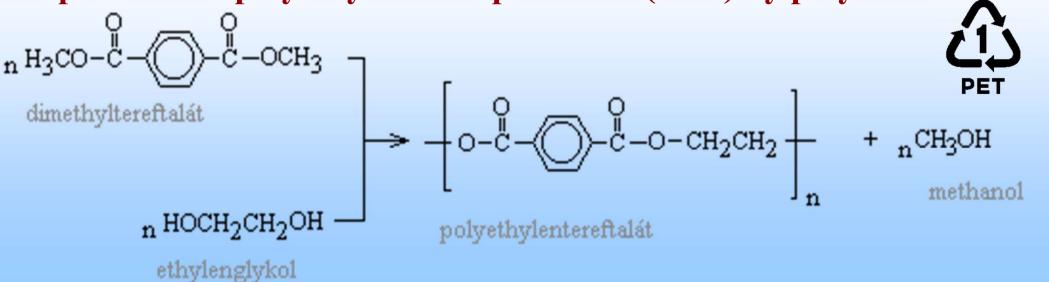
Reaction of functional groups brings molecules together - macromolecule is formed, simultaneously low molecular weight product is released (e.g. water, methanol...)

This is how polyamides and polyesters are formed



## **Polycondensation**

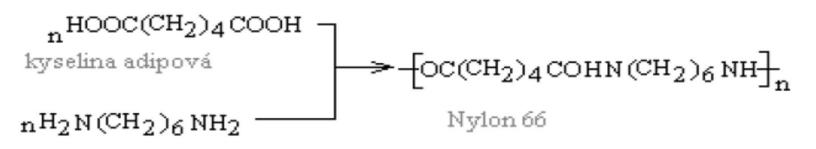
Preparation of polyethylene terephthalate (PET) by polycondensation





## Polycondensation

Polyamide 6.6 is formed by the reaction of adipic acid and hexamethylene diamine (The by-product of the reaction is water)



+ H<sub>2</sub>O

hexamethylendiamin

$$\begin{array}{c} H \\ N - (CH_2)_6 - N \\ H \end{array} + H - \underline{0} - C - (CH_2)_4 - \underline{0} - H \\ Polykondensation \\ 2H_2 0 \end{array} + \underbrace{\begin{array}{c} H \\ N - (CH_2)_6 - N - C - (CH_2)_4 - C \\ 0 - N - (CH_2)_5 -$$

Polyamides - prepared by polycondensation of diamines with dicarboxylic acids or polymerization of cyclic amides,

- polyamide macromolecules contain a peptide bond (-CO-NH-), which repeats regularly in the macromolecule chain.



# Polycondensation



#### How polyamide 6 is formed from εcaprolactam

ε-Caprolactam



#### Paul Schlack 1938 (Perlon), Otto Wichterle 1940 (Silon)

ε-Aminocapronsäure

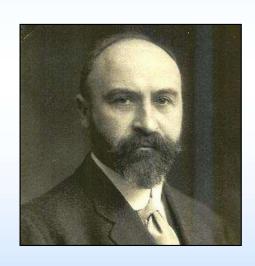
Polyamid 6 (Perlon)



# 



#### Leo Hendrik Baekeland (1863-1944)



- in 1907 he prepared the first phenoplast
- by polycondensation of phenol with formaldehyde,
- which can take place in both acidic and basic environments,
- in acidic environments, a linear
- polycondensate (Novolak),
- in alkaline media, a polycondensate is formed
- with a densely cross-linked structure (Bakelite).



# 

Polyaddition (or addition polymerisation) is a polymerization reaction that forms polymers via individual independent addition reactions. Polyaddition occurs as a reaction between functional groups on molecules with low degrees of polymerization, such as dimers, trimers and oligomers, to form species of higher molar mass. A typical polyaddition is the formation of a polyurethane.

n O=C=N-(CH<sub>2</sub>)<sub>6</sub>-N=C=O + n HO-(CH<sub>2</sub>)<sub>4</sub>-OH
$$O=C=N-(CH_2)_6-N$$

$$O=C=N-(CH_2)_6-N$$

$$O=C=N-(CH_2)_6-N$$

$$O=C=N-(CH_2)_6-N$$

$$O=C=N-(CH_2)_6-N$$

$$O=C=N-(CH_2)_6-N$$

$$O=C=N-(CH_2)_6-N$$

$$O=C=N-(CH_2)_6-N$$

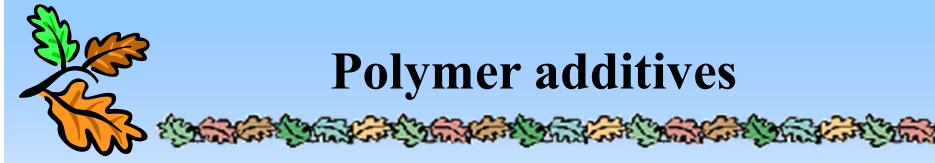
$$O=C=N-(CH_2)_6-N$$

$$O=C=N$$

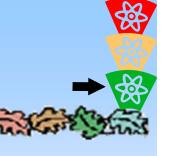
$$O=C$$

$$O$$

**Polyurethane = elastane, lycra ... elastic fibres** 



## Polymer additives



For utility:

Lubricants (slip resistance)

**Emollients** 

**Antistatic** 

blowing agents (foams)

Fillers and binders

**Pigments** 

**PCM** 

For durability: **Antioxidants** 

Heat stabilizers

**UV** stabilisers

Flame retardants



Influenced by particle size and effect required

Non-flammability: high doses

UV protection: low doses

Mechanical properties:

Large particles: approx. 10%

Nanoparticles: approx. 1 %



### Polymer additives - pigments



Application via "Masterbatch"

(= pigment concentrate in polymer)



Pigment size: approx. **1micrometer** 

Organic and inorganic

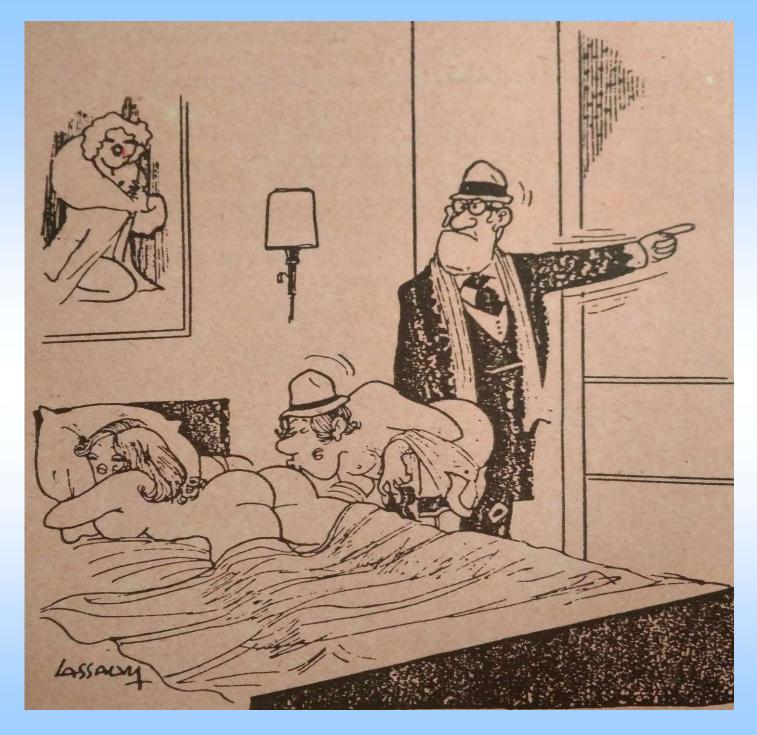
Can also be used for fibre production, but it is an inflexible technology



- Chemical fibres: glossy, transparent ... = different from cotton and wool
- Need to increase light scattering using tiny undyed particles in the fibre mass with high refractive index and stability
- Reality: only using TiO2 (titanium dioxide, approx. 0.5 micrometer)
- Delustrad fibres contain about 1% TiO2 (they are then matt, opaque, not shiny...)



- Fibres (approx. 95%)
- Binders (nonwovens, coatings, pigment printing...)
- Thickeners (printing...)
- Layers (finishing...)
- Composites



Thank you for your attention!