Microstructure Mechanics
Polymers: Structure and Properties

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Class 2013
Zeitalter tragen die Namen von Materialien.
Technology Status A380 – Material Distribution (courtesy Airbus)

- 62% Aluminum
- 20% Composite
- 10% Titanium / Steel
- 4% Glare
- 2% Surface protections
- 2% Miscellaneous

Fly
GLARE: "Glass Laminate Aluminium Reinforced Epoxy“

several thin layers of metal (usually aluminium) interspersed with layers of glass-fibre "pre-preg", bonded together with a matrix such as epoxy.

Uni-directional pre-preg layers may be aligned in different directions to suit the predicted stress conditions.

Next generation: CFK
Technology Status A380 – Material Distribution (courtesy Airbus)

A380 / A350

Status: A380 – Advanced
Advanced Metal-Technologies in Fuselage and Wing

Status: Composite Wing
Advanced Metal-Technologies in Fuselage

Status: Full Composite
Car Body Structure.
High Strength Steel.
BMW 1 Series.

New materials automotive (courtesy BMW)
Car Body Structure.
Aluminium Front End / Steel passenger Cab. BMW 5 Series.
Car Body Shell.
Materials for the BMW 6 Series.
Weight savings compared to Steel

- Aluminium Bonnet: -10 kg
- Sheet moulded Compound Deck Lid (SMC): -2 kg
- Thermoplast Fenders (PPE+PA): -4 kg
- Aluminium Doors: -10 kg
Car Body Shell.
Sheet Moulded Compound (SMC).
Deck Lid BMW 6 Series.

- Lightweight design
- Complex shape
- Integrated antennas
  AM, FM, Diversity,
  TV, Tel, GPS,
  SDARS, digital Tuner
Car Body Shell.
Aluminium and Thermoplastic.

- BMW 5 Series (Aluminium)
- BMW 6 Series (Thermoplastics)
Neutral Fiber: Center line remains unchanged during bending

Material is under tensile stress above the neutral fiber

Material is compressed below the neutral fiber

“Neutral Fiber”: Center line remains unchanged during bending
### Beam Bending Stiffness

<table>
<thead>
<tr>
<th>Formula</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta h = \frac{4 \cdot F \cdot l^3}{E \cdot b \cdot a^3} )</td>
<td>1 m</td>
<td>supported on one end</td>
</tr>
<tr>
<td>( \Delta h = \frac{F \cdot l^3}{4 \cdot E \cdot b \cdot a^3} )</td>
<td>1 m</td>
<td>supported on both ends</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta h )</td>
<td>1 m</td>
<td>displacement</td>
</tr>
<tr>
<td>( F )</td>
<td>1 N</td>
<td>load</td>
</tr>
<tr>
<td>( a )</td>
<td>1 m</td>
<td>beam thickness</td>
</tr>
<tr>
<td>( l )</td>
<td>1 m</td>
<td>beam length</td>
</tr>
<tr>
<td>( b )</td>
<td>1 m</td>
<td>beam width</td>
</tr>
<tr>
<td>( E )</td>
<td>1 N/m²</td>
<td>Elastic modulus</td>
</tr>
</tbody>
</table>

**Beam thickness a:** 3rd power against displacement, modulus acts only linear
Construction stiffness: how design parts with light-weight materials

1) Intrinsic elastic stiffness of the material (elastic modulus)

2) Dimension of the structure that is made of the material (third order increase of structure stiffness with cross section)

\[
\Delta h = \frac{4 \cdot F \cdot l^3}{E \cdot b \cdot a^3}
\]
Construction stiffness: how design parts with light-weight materials

1) Intrinsic elastic stiffness of the material (elastic modulus)

2) Dimension of the structure that is made of the material (third order increase of structure stiffness with cross section)

\[ \Delta h = \frac{4 \cdot F \cdot l^3}{E \cdot b \cdot a^3} \]

same force
same mass of beam
same material
Construction stiffness: how design parts with light-weight materials

1) Intrinsic elastic stiffness of the material (elastic modulus)

2) Dimension of the structure that is made of the material (third order increase of structure stiffness with cross section)
- **Structures**
Soft Matter Theory: Comprehensive Understanding of Physical and Chemical Properties

Analytic Theory

Finite Elements, Macrosc. Theory

Local Chemical Properties ↔ Scaling Behavior of Nanostructures
Energy Dominance ↔ Entropy Dominance of Properties
Polymers: Introduction

- **Polymers** – materials consisting of *polymer molecules* that consist of repeated chemical units ('mers') joined together, like beads on a string. Some polymer molecules contain hundreds or thousands of monomers and are often called *macromolecules*.

- Polymers may be **natural**, such as leather, rubber, cellulose or DNA, or **synthetic**, such as nylon or polyethylene.
• Macromolecule that is formed by linking of repeating units through covalent bonds in the main backbone

• Properties are determined by
  – molecular weight
  – length
  – backbone structure
  – side chains
  – crystallinity

• Resulting macromolecules have huge molecular weights
Types of polymers

Methane, CH$_4$

Ethane, C$_2$H$_6$

Propane, C$_3$H$_8$
Types of polymers

- Polymer molecules can be very large (macromolecules)
- Most polymers consist of long and flexible chains with a string of C atoms as a backbone
- Side-bonding of C atoms to H atoms or radicals
- Double bonds are possible in both chain and side bonds
- Repeat unit in a polymer chain (“unit cell”) is a mer
- Small molecules from which polymer is synthesized is monomer. A single mer is sometimes also called a monomer.
### Types of polymers

<table>
<thead>
<tr>
<th>Structure</th>
<th>Source-Based Name</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R = -H$</td>
<td>Polyethylene</td>
<td>Plastic</td>
</tr>
<tr>
<td>$R = -\text{CH}_3$</td>
<td>Polypropylene</td>
<td>Rope</td>
</tr>
<tr>
<td>$R = -\text{Cl}$</td>
<td>Poly(vinyl chloride)</td>
<td>&quot;Vinyl&quot;</td>
</tr>
<tr>
<td>$X = -H, R = -\text{C}_2\text{H}_5$</td>
<td>Poly(ethyl acrylate)</td>
<td>Latex paints</td>
</tr>
<tr>
<td>$X = -\text{CH}_3, R = -\text{CH}_3$</td>
<td>Poly(methyl methacrylate)</td>
<td>Plastic</td>
</tr>
<tr>
<td>$R = -H$</td>
<td>Polybutadiene</td>
<td>Tires</td>
</tr>
<tr>
<td>$R = -\text{CH}_3$</td>
<td>Polyisoprene</td>
<td>Tires</td>
</tr>
<tr>
<td>$X = -\text{F}, R = -\text{F}$</td>
<td>Polytetrafluoroethylene</td>
<td>Teflon®</td>
</tr>
</tbody>
</table>
Types of polymers

hydrogen atoms in polyethylene are replaced by fluorine:
**polytetrafluoroethylene**
PTFE – Teflon

every fourth hydrogen atom in polyethylene is replaced with chlorine:
**poly(vinyl chloride)** PVC

every fourth hydrogen atom in polyethylene is replaced with methyl group (CH₃):
**polypropylene** PP
Polymer structure

Molecular shape (conformation)

- The angle between the singly bonded carbon atoms is \( \sim 109^\circ \) – carbon atoms form a zigzag pattern in a polymer molecule.

- Moreover, while maintaining the 109° angle between bonds polymer chains can rotate around single C-C bonds (double and triple bonds are very rigid).

- Random kinks and coils lead to entanglement, like in the spaghetti structure:
1 **Linear polymers**: Van der Waals bonding between chains. Examples: polyethylene, nylon.
2 Branched polymers: Chain packing efficiency is reduced compared to linear polymers - lower density
3 Cross-linked polymers: Chains are connected by covalent bonds. Often achieved by adding atoms or molecules that form covalent links between chains. Many rubbers have this structure.
4 Network polymers: 3D networks made from trifunctional mers. Examples: epoxies, phenol-formaldehyde
Atomic arrangement in polymer crystals is more complex than in metals or ceramics (unit cells are typically large and complex).
Polymer molecules are often partially crystalline (semi-crystalline), with crystalline regions dispersed within amorphous material.
Structure, scales, partially crystalline polymers
Structure, scales, partially crystalline polymers
The crystalline unit cell for PET ($a = 4.56 \, \text{Å}$, $b = 5.94 \, \text{Å}$, $c = 10.75 \, \text{Å}; \, \alpha = 98.5^\circ$, $\beta = 118^\circ$, $\gamma = 112^\circ$),

M Durell (2002)
Polymer structure: spherulite growth

Polymer structure: spherulite growth

Thin crystalline platelets grown from solution - chains fold back and forth: chain-folded model

The average chain length can be much greater than the thickness of the crystallite
**Spherulites:** Aggregates of lamellar crystallites ~ 10 nm thick, separated by amorphous material. Aggregates are formed upon solidification from a melted state and are approximately spherical in shape.
Polymer structure: spherulite growth

Fig. 2 AFM contact mode images. Cellulose molecules in micro-fibril crystal: (a) topographic image; and (b) error-signal image. Polybutene-1 molecules: (c) topographic image; and (d) simulated AFM image based on crystallographic data.

M. Miles, M. Antognozzi, H. Haschke, J. Hobbs, A. Humphris, I. McMaster
H.H. Wills Physics Laboratory, University of Bristol, Materials Today, Feb. 2003
Polymer structure: spherulite growth

Bamford, Nature 173 (1954) p. 27;  Astbury, Endeavor 1(1942) p. 70

1 millimeter square, OM
Polymer structure: PET: XRD

Polyethylene-Terephthalate (PET), Cr-Kα1, 40KV 40mA

(hkl) 2theta

(Cr)  

(001) 15.12
(0-11) 24.52
(010) 26.2
(-111) 31.92
(101) 32.2
(-110) 33.8
(011) 35.36
(100) 38.64
(111) 41.94
(101) 49.68
(11-1) 50.36
(110) 58.28
(111) 69.84
Polymer structure: deformation
Durability of polymer composites

Polymer composites change with time and most significant factors are

• Elevated temperatures
• Fire
• Moisture
• Adverse chemical environments
• Natural weathering when exposed to sun’s ultra-violet radiation
# Polymer composites: mechanical properties

<table>
<thead>
<tr>
<th>MATERIAL</th>
<th>Relative density</th>
<th>Diameter thickness ratio (microns)</th>
<th>Length (mm)</th>
<th>E (GPa)</th>
<th>Tens. Str. (MPa)</th>
<th>Failure strain (%)</th>
<th>Volume in composite (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortar matrix</td>
<td>1.8-2.0</td>
<td>300-5000</td>
<td>-</td>
<td>10-30</td>
<td>1-10</td>
<td>0.01-0.05</td>
<td>85-97</td>
</tr>
<tr>
<td>Concrete matrix</td>
<td>1.8-2.4</td>
<td>10000-20000</td>
<td>-</td>
<td>20-40</td>
<td>1-4</td>
<td>0.01-0.02</td>
<td>97-99.5</td>
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<tr>
<td>Asbestos</td>
<td>2.55</td>
<td>0.02-30</td>
<td>5-40</td>
<td>164</td>
<td>200-1800</td>
<td>2.3</td>
<td>5-15</td>
</tr>
<tr>
<td>Carbon</td>
<td>1.16-1.95</td>
<td>7-18</td>
<td>3-cont.</td>
<td>30-390</td>
<td>600-2700</td>
<td>0.5-2.4</td>
<td>3-5</td>
</tr>
<tr>
<td>Glass</td>
<td>2.7</td>
<td>12.5</td>
<td>10-50</td>
<td>70</td>
<td>600-2500</td>
<td>3.6</td>
<td>3-7</td>
</tr>
<tr>
<td>Polyethylene</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HDPE filament</td>
<td>0.96</td>
<td>900</td>
<td>3-5</td>
<td>5</td>
<td>200</td>
<td>-</td>
<td>2-4</td>
</tr>
<tr>
<td>High modulus</td>
<td>0.96</td>
<td>20-50</td>
<td>Cont.</td>
<td>10-30</td>
<td>&gt; 400</td>
<td>&gt; 4</td>
<td>5-10</td>
</tr>
<tr>
<td>Polypropylene</td>
<td>0.91</td>
<td>20-100</td>
<td>5-20</td>
<td>4</td>
<td>-</td>
<td>-</td>
<td>0.1-0.2</td>
</tr>
<tr>
<td>(Monofilament)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Polyvinyl alcohol</td>
<td>1-3</td>
<td>3-8</td>
<td>2-6</td>
<td>12-40</td>
<td>700-1500</td>
<td>-</td>
<td>2-3</td>
</tr>
<tr>
<td>(PVA)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Steel</td>
<td>7.86</td>
<td>100-600</td>
<td>10-60</td>
<td>200</td>
<td>700-2000</td>
<td>3.5</td>
<td>0.3-2.0</td>
</tr>
</tbody>
</table>

Performance is controlled by:
- vol. fraction of fibers
- properties of fibers and matrix
- bond between the two