Microstructure Mechanics

Polymers: Structure and Properties

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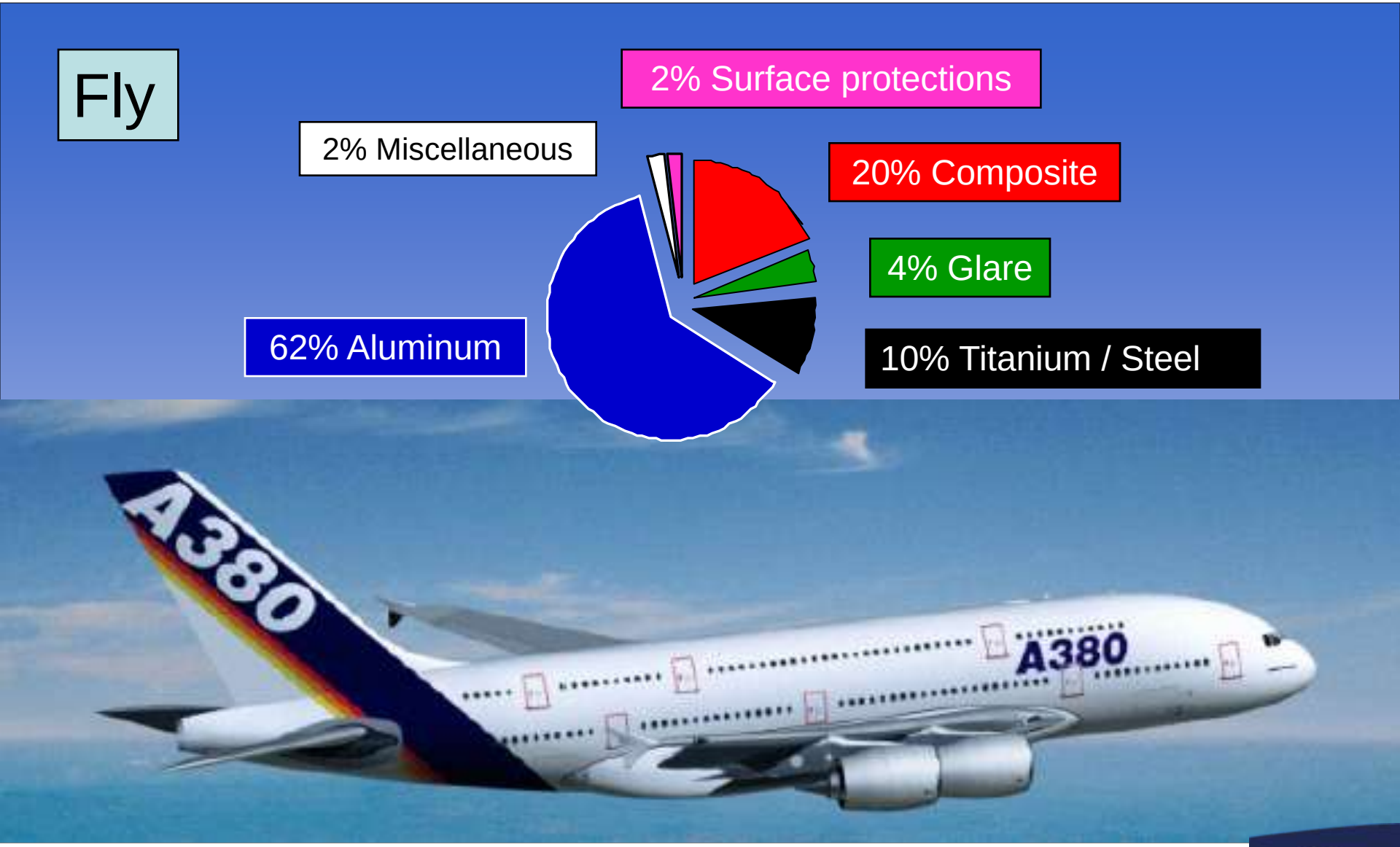
Class 2013

Technology Status A380 – Material Distribution (courtesy Airbus)



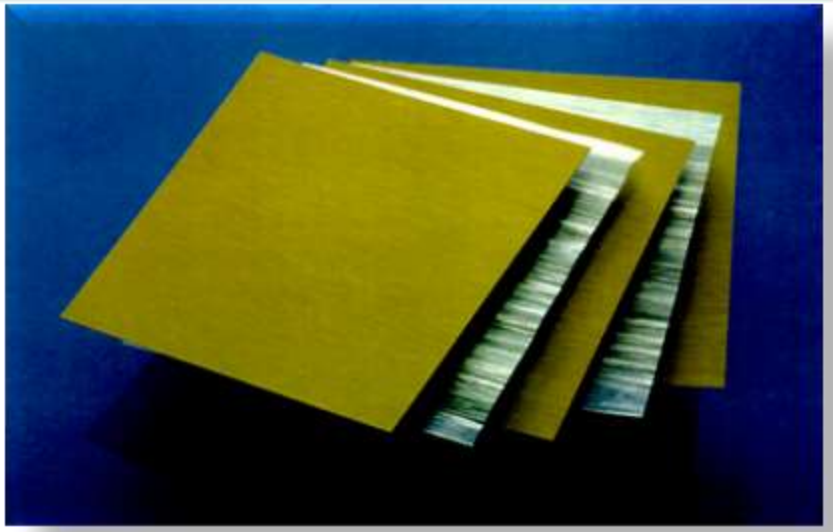
Technology Status A380 – Material Distribution (courtesy Airbus)

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.

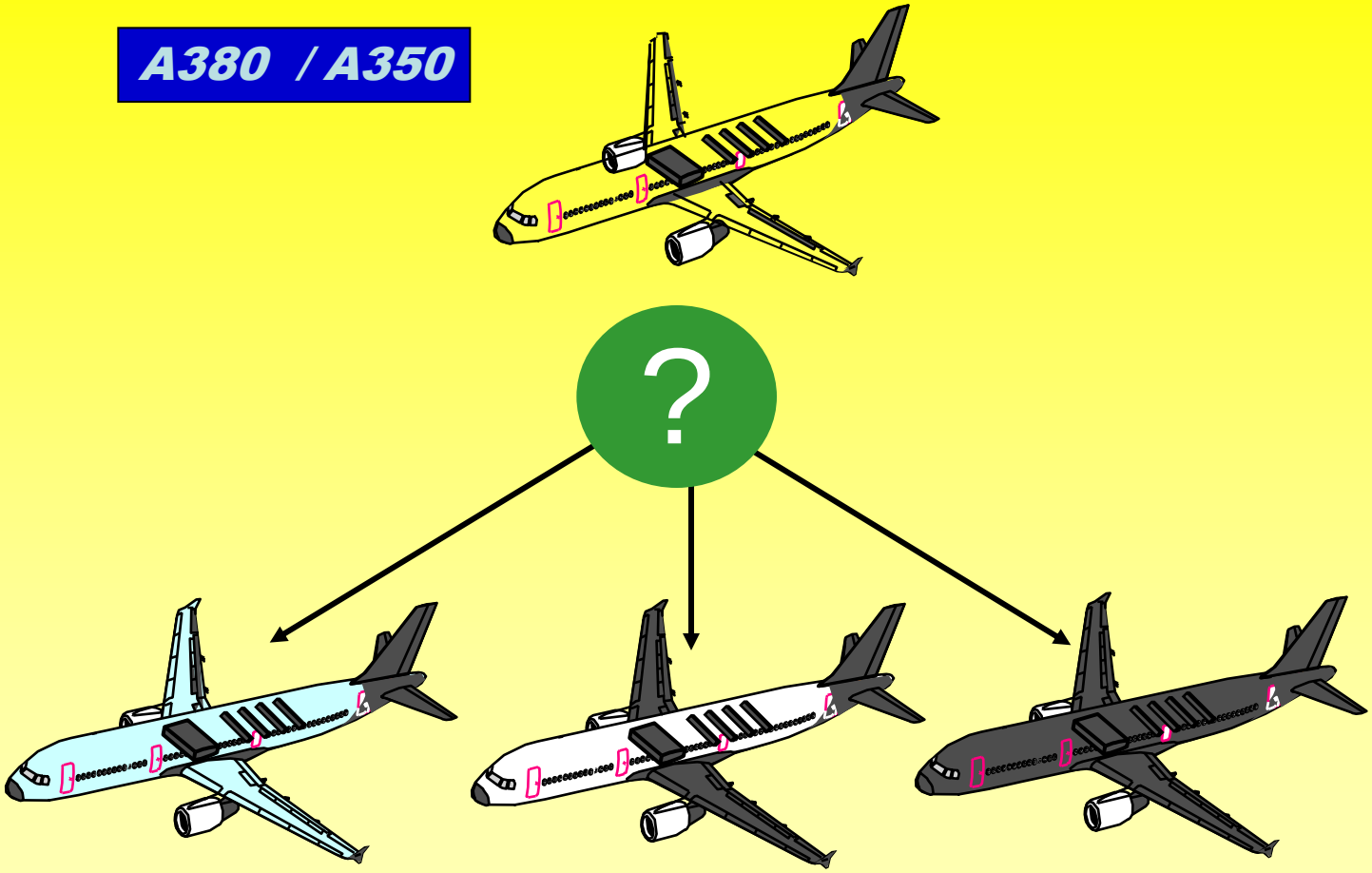
Uni-directional pre-preg layers may be aligned in different directions to suit the predicted stress conditions.

Next generation: CFK



- Improved Stiffness
- Improved hot-wet shear
- Material Optimised Hybrid
- Cost reduction
- Design rules
  - *Fiber dominated*
  - *Bonded Metal laminate*

Technology Status A380 – Material Distribution (courtesy Airbus)



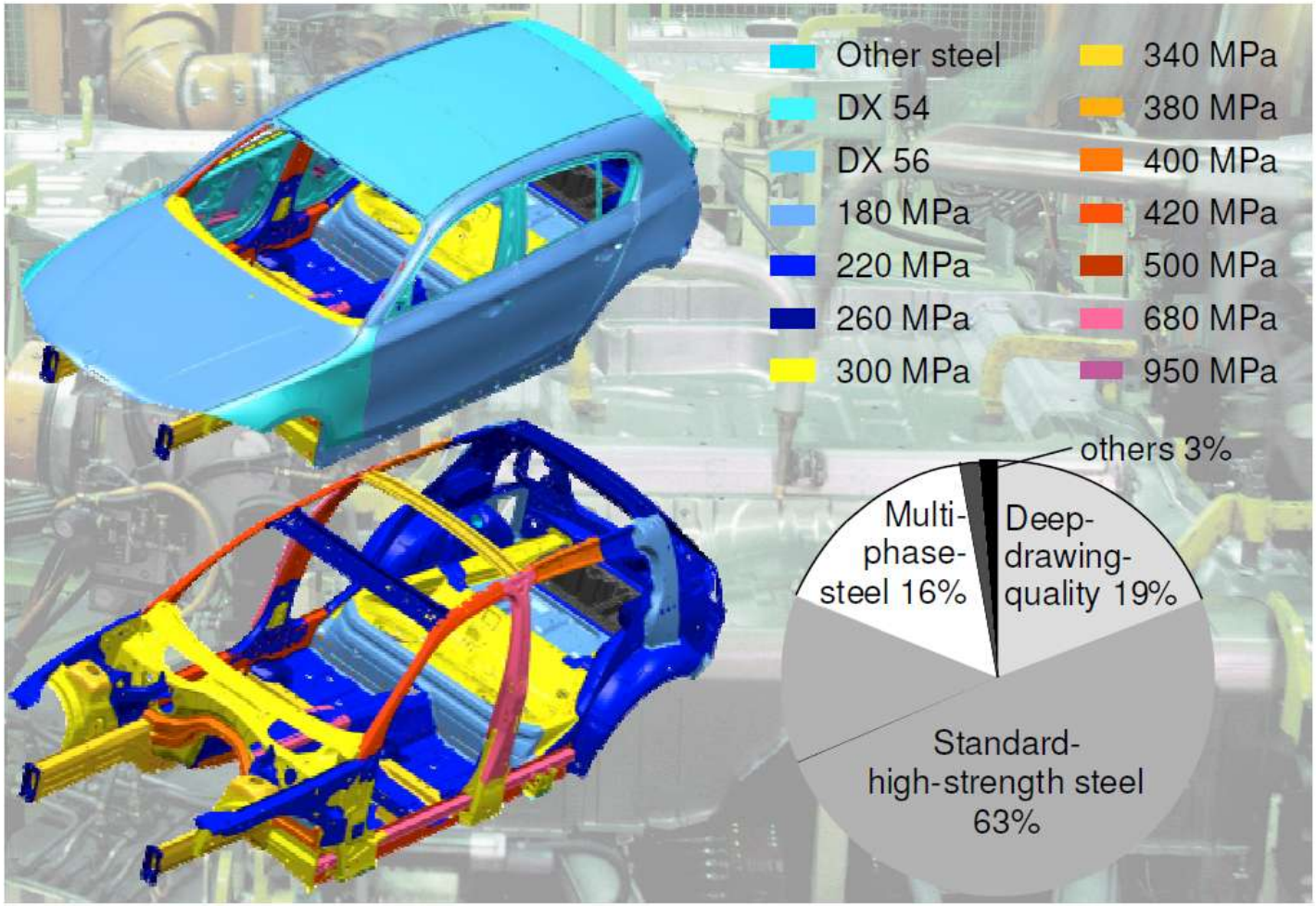
Status: A380 – Advanced . Advanced Metal-Technologies in Fuselage and Wing

Status: Composite Wing . Advanced Metal-Technologies in Fuselage

Status: Full Composite

New materials automotive (courtesy BMW)

Car Body Structure.
High Strength Steel.
BMW 1 Series.

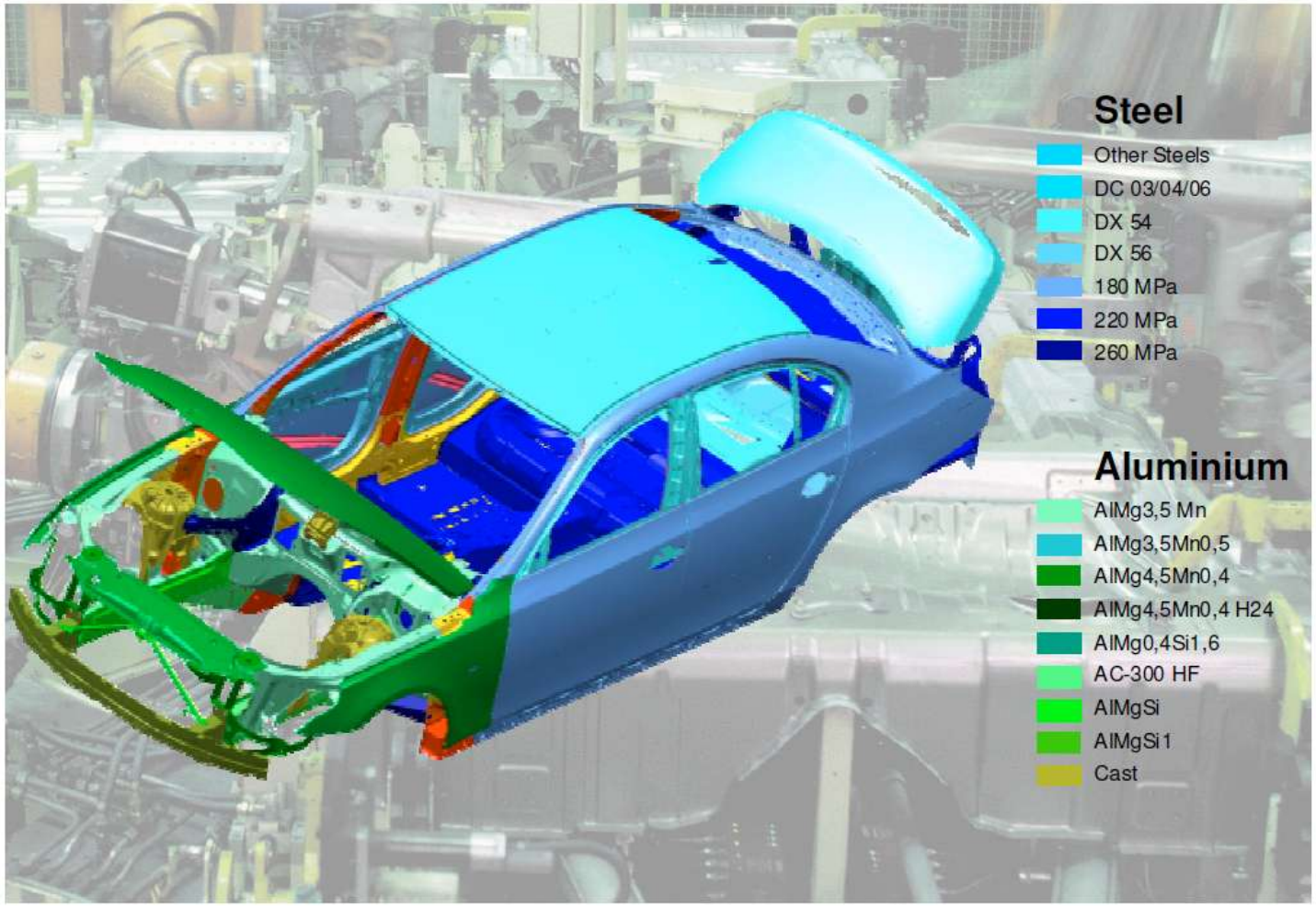


New materials automotive (courtesy BMW)

Car Body Structure.

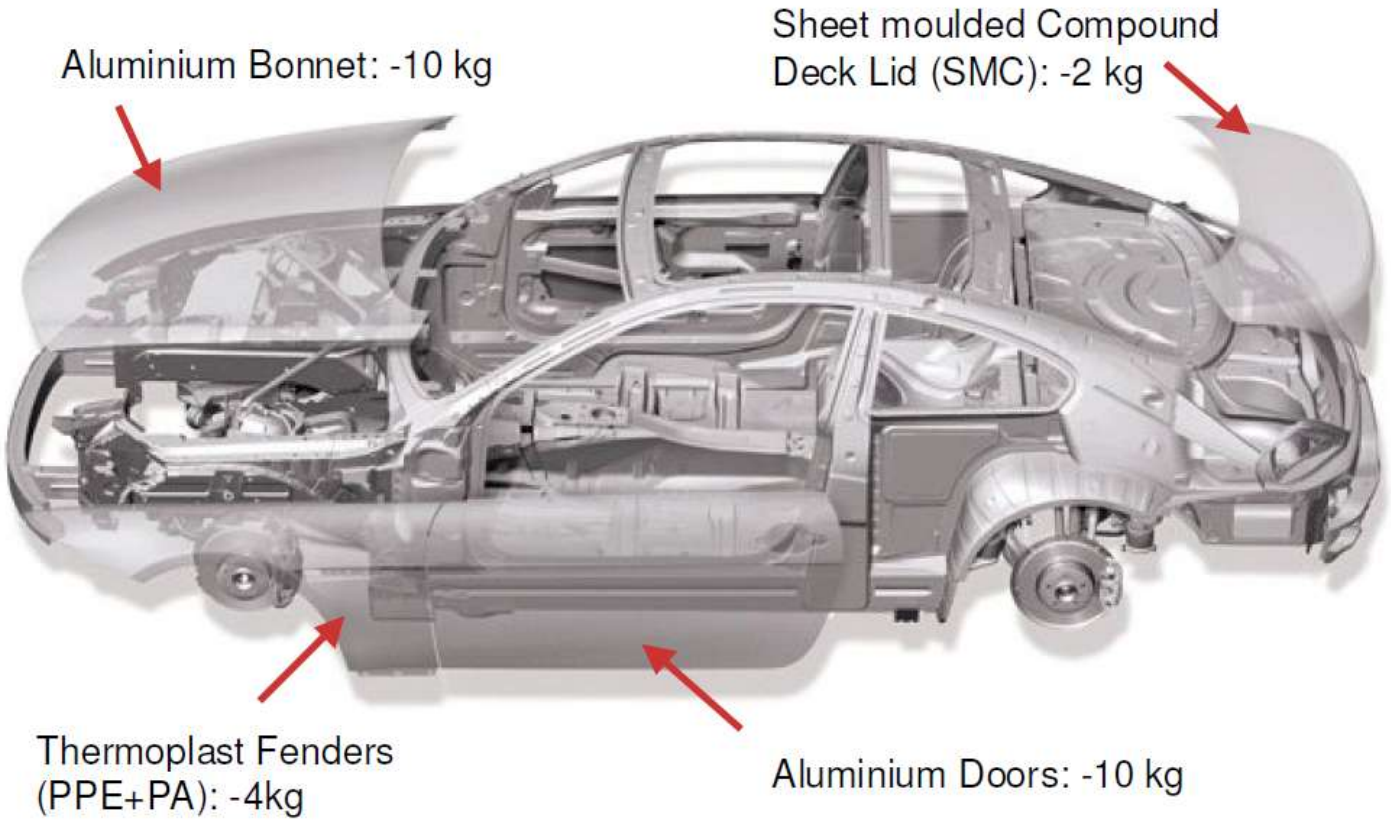
Aluminium Front End / Steel passenger Cab.

BMW 5 Series.



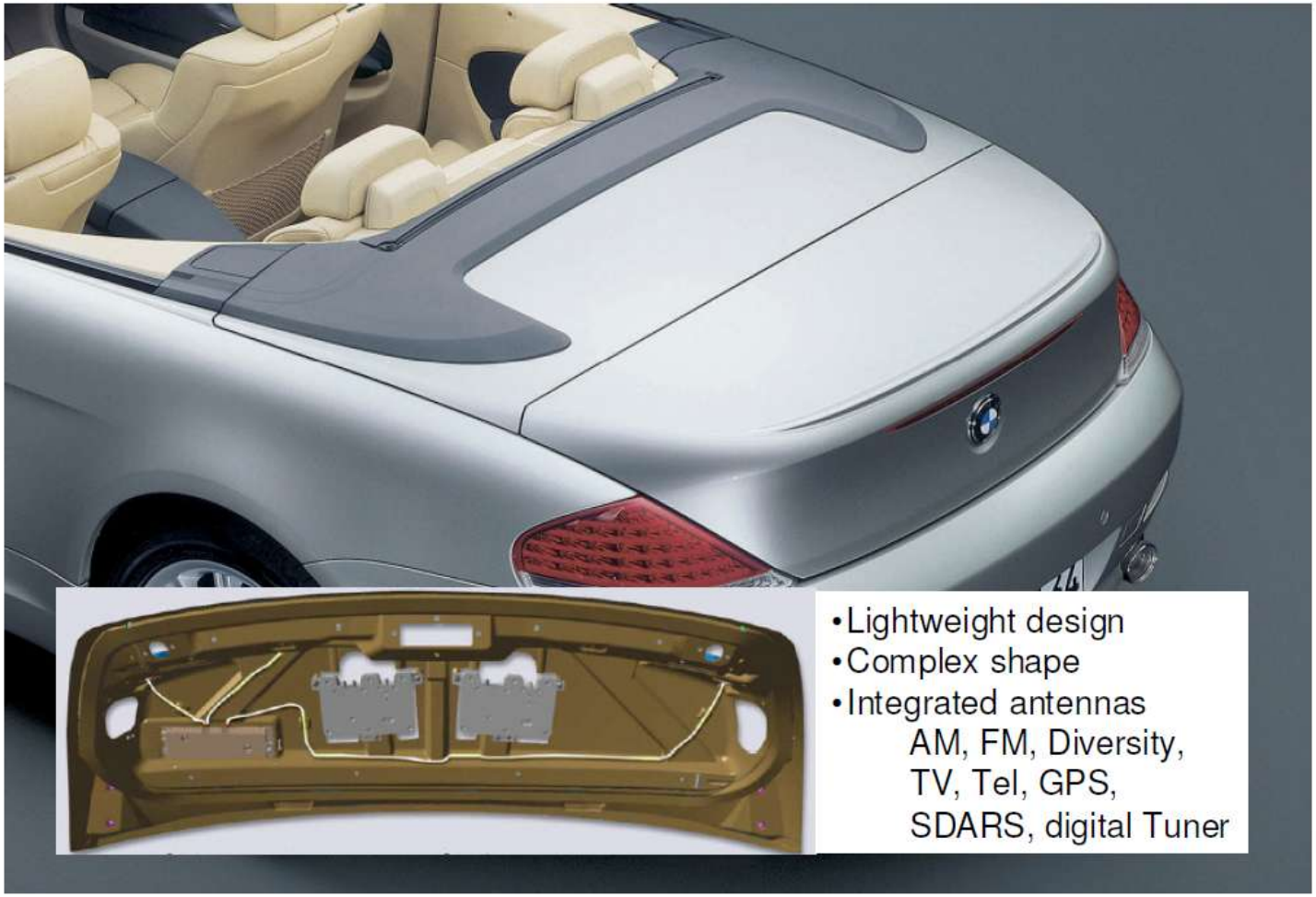
Car Body Shell.

Materials for the BMW 6 Series.
Weight savings compared to Steel



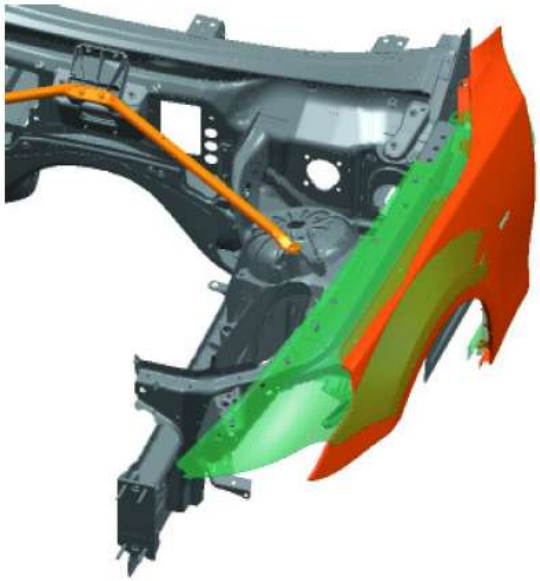
New materials automotive (courtesy BMW)

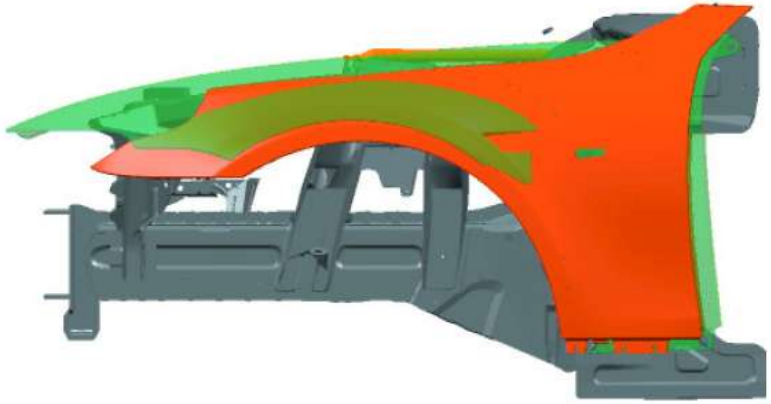
Car Body Shell.
Sheet Moulded Compound (SMC).
Deck Lid BMW 6 Series.



New materials automotive (courtesy BMW)

Car Body Shell.
Aluminium and Thermoplastic.



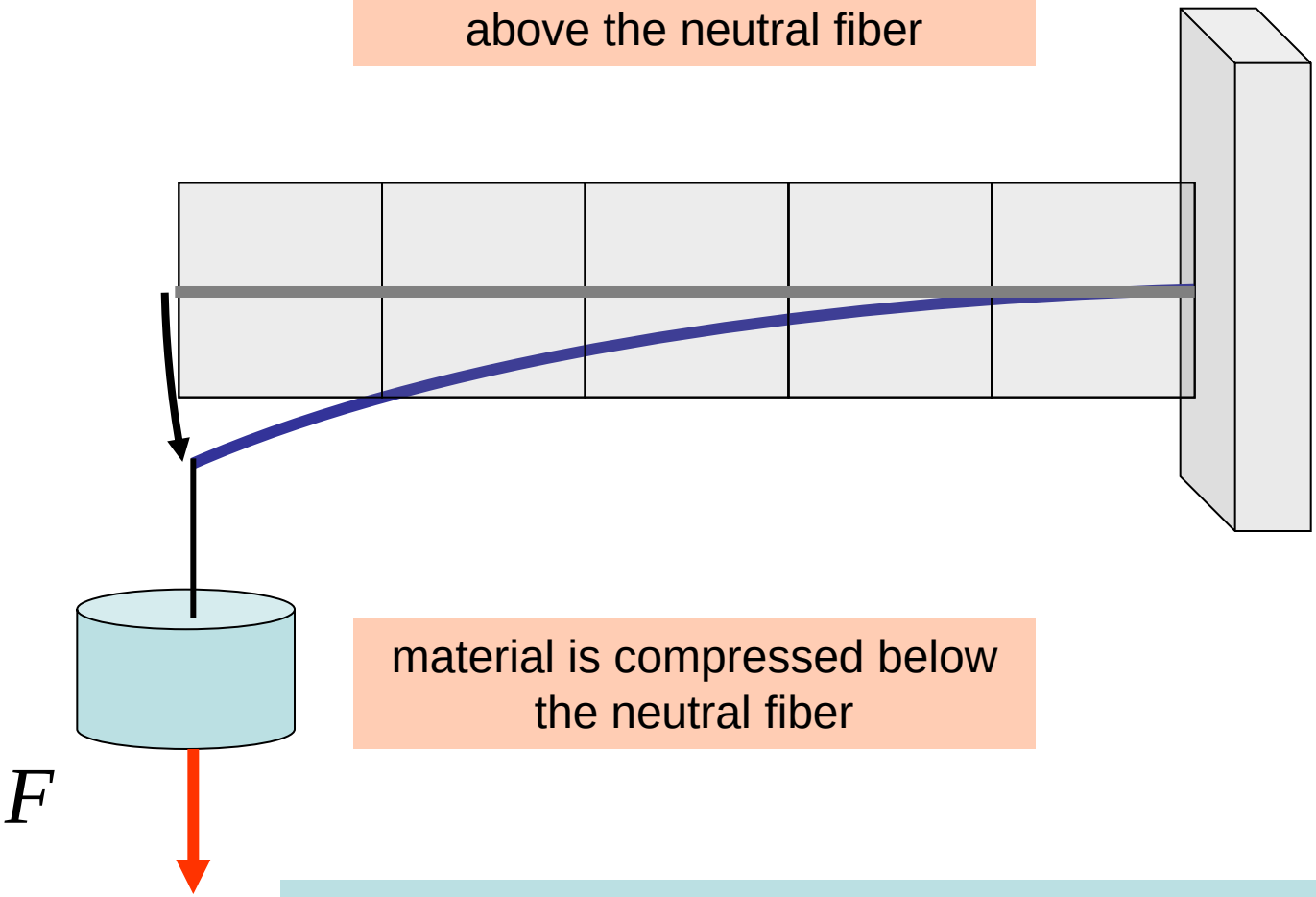


BMW 5 Series (Aluminium)

BMW 6 Series (Thermoplastics)

Construction stiffness: how design parts with light-weight materials

Material is under tensile stress above the neutral fiber



material is compressed below the neutral fiber

„***Neutral Fiber*** “: Center line remains unchanged during bending

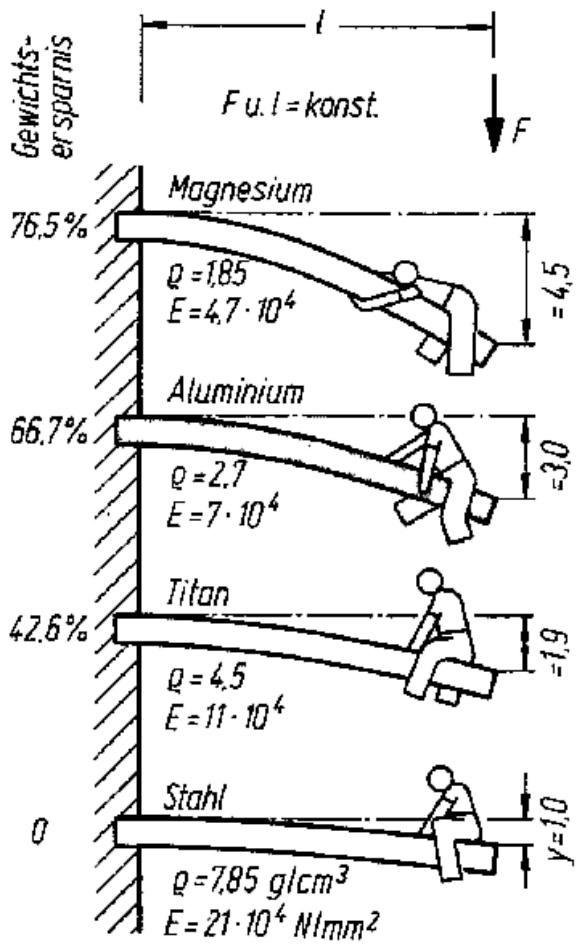
Construction stiffness: beam bending

$\Delta h = \frac{4 \cdot F \cdot l^3}{E \cdot b \cdot a^3}$	1 m	supported on one end
$\Delta h = \frac{F \cdot l^3}{4 \cdot E \cdot b \cdot a^3}$	1 m	supported on both ends
Δh	1 m	displacement
F	1 N	load
a	1 m	beam thickness
l	1 m	beam length
b	1 m	beam width
E	1 N/m^2	Elastic modulus

Beam thickness a: 3rd power against displacement, modulus acts only linear

1) instrinsic 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)



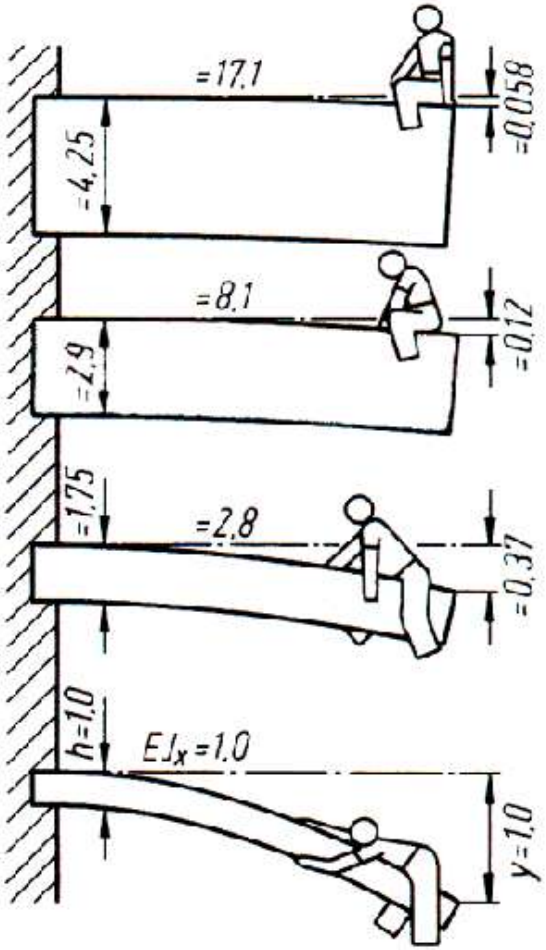
same force
same <u>cross section</u>
different materials

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

Construction stiffness: how design parts with light-weight materials

1) instrinsic 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)



same force
same <u>mass of beam</u>
same material

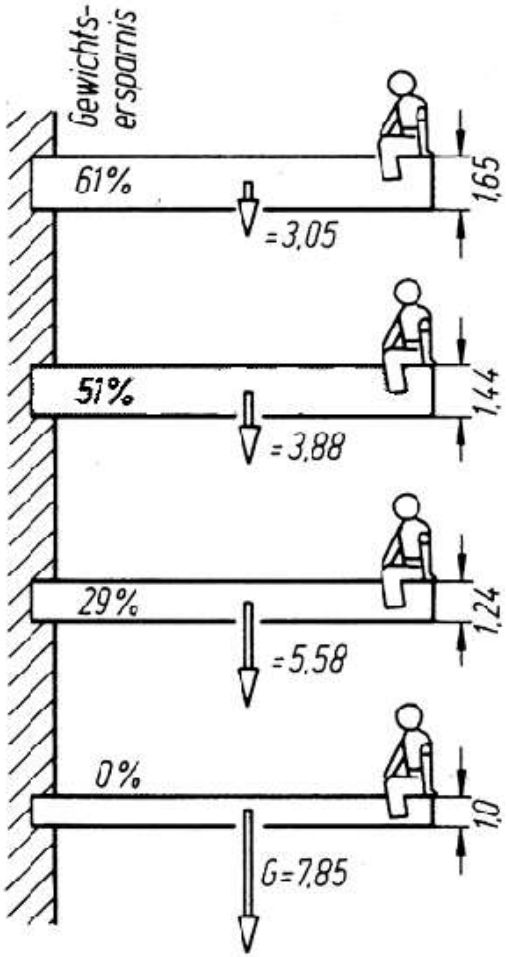
$$\Delta h = \frac{4 \cdot F \cdot l^3}{E \cdot b \cdot a^3}$$

Construction stiffness: how design parts with light-weight materials

1) instrinsic 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)

weight saving

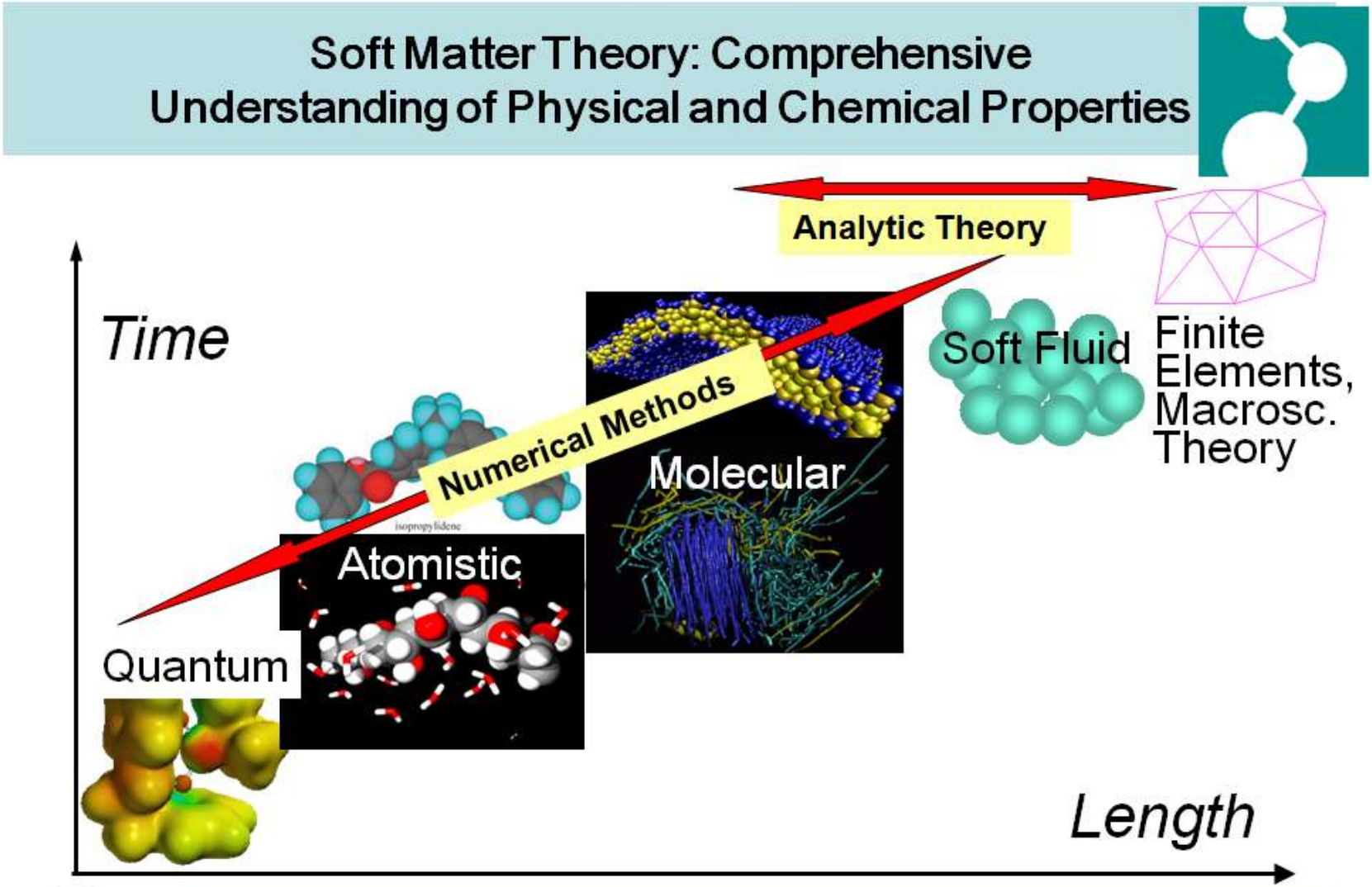


same force
same total stiffness
(intrinsic and cross section)

Overview

- Structures

Theory of polymers (slide with courtesy from Prof. Kurt Kremer)



Local Chemical Properties ⇔ Scaling Behavior of Nanostructures
Energy Dominance ⇔ Entropy Dominance of Properties

Polymers: Introduction

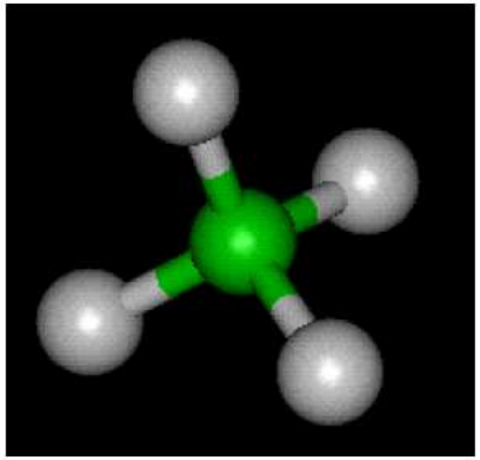
- **Polymers** – materials consisting of *polymer molecules* that consist of repeated chemical units (`mers') joined together, like beads on a string. Some polymer molecules contain hundreds or thousands of monomers and are often called *macromolecules*.

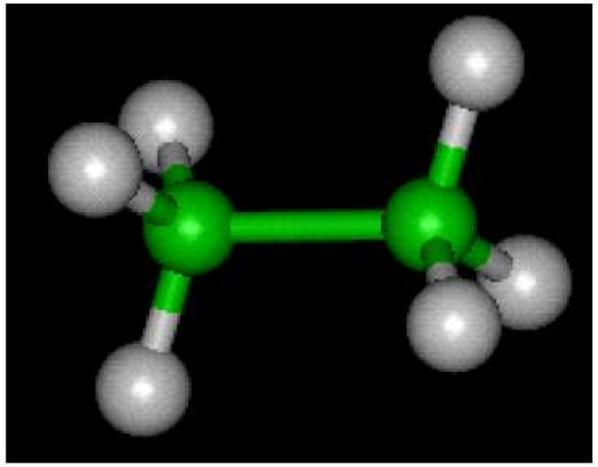
- Polymers may be **natural**, such as leather, rubber, cellulose or DNA, or **synthetic**, such as nylon or polyethylene.

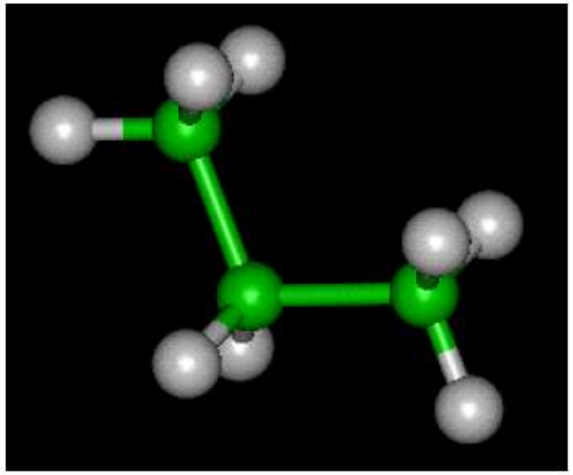
Structure of polymers

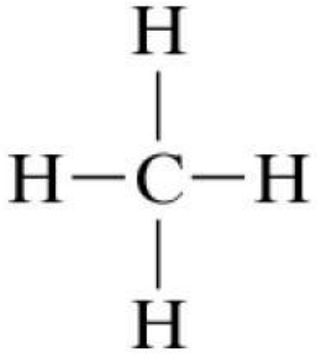
- Macromolecule that is formed by linking of repeating units through covalent bonds in the main backbone
- Properties are determined by
  - molecular weight
  - length
  - backbone structure
  - side chains
  - crystallinity
- Resulting macromolecules have huge molecular weights

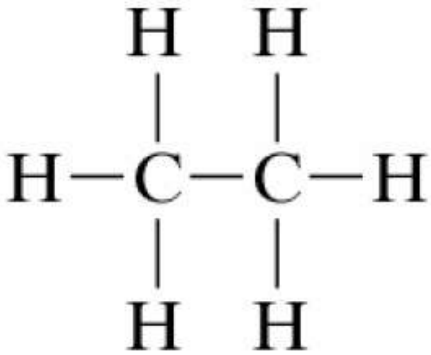
Types of polymers

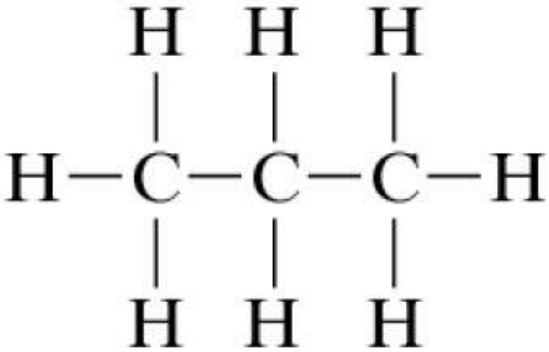








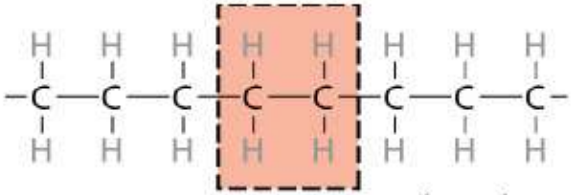




Methane, CH_4 **Ethane, C_2H_6** **Propane, C_3H_8**

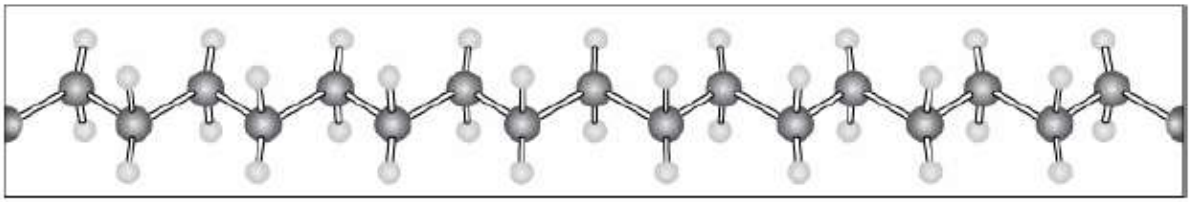
Types of polymers

- 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.



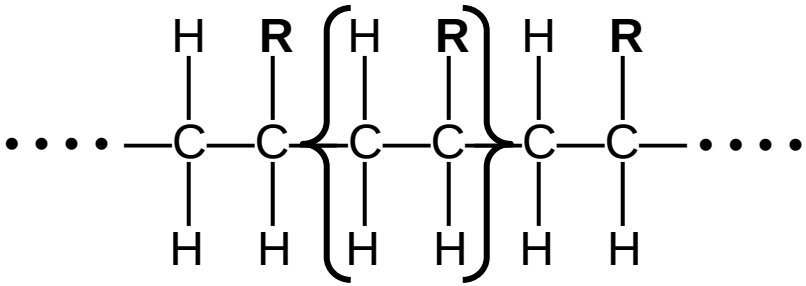
Repeat unit (mer)

polyethylene (e.g. paraffin wax for candles)



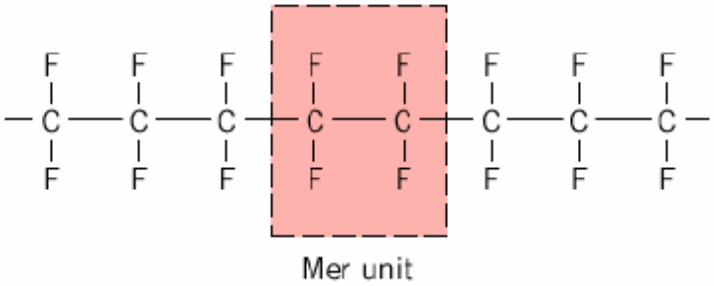
C H

Types of polymers



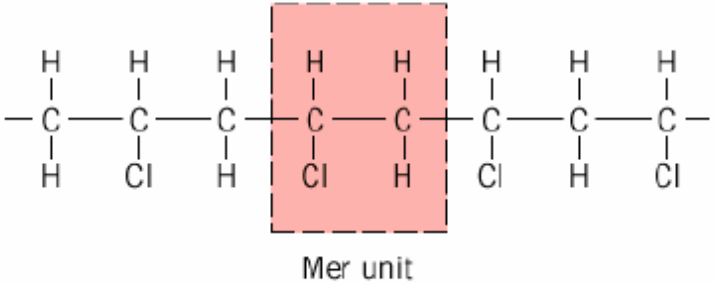
Structure	Source-Based Name	Application
R = -H	Polyethylene	Plastic
R = $-CH_3$	Polypropylene	Rope
R = -Cl	Poly(vinyl chloride)	"Vinyl"
X = -H, R = $-C_2H_5$	Poly(ethyl acrylate)	Latex paints
X = $-CH_3$, R = $-CH_3$	Poly(methyl methacrylate)	Plastic
R = -H	Polybutadiene	Tires
R = $-CH_3$	Polyisoprene	Tires
X = -F, R = -F	Polytetrafluoroethylene	Teflon®

Types of polymers



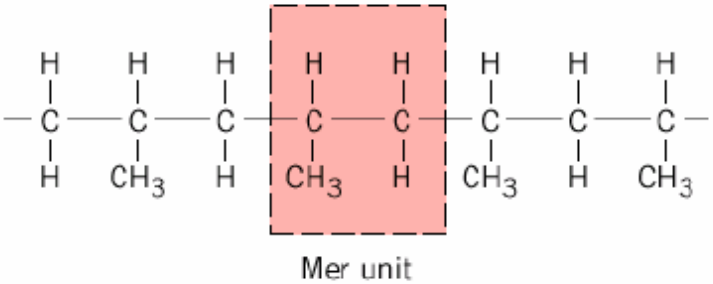
(a)

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



(b)

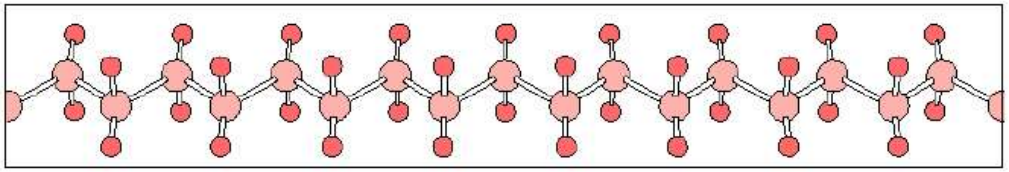
every fourth hydrogen atom in polyethylene is replaced with chlorine: poly(vinyl chloride) PVC



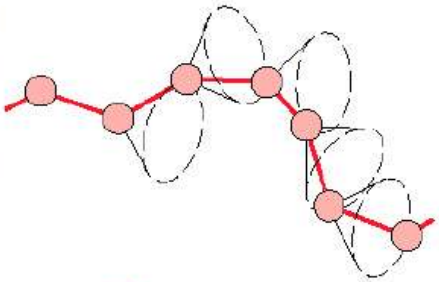
(c)

every fourth hydrogen atom in polyethylene is replaced with methyl group (CH_3): polyproplylene PP

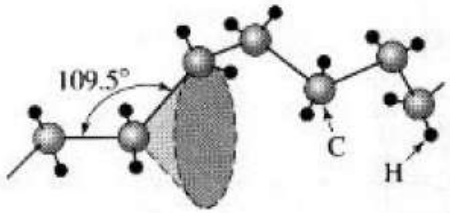
Molecular shape (conformation)

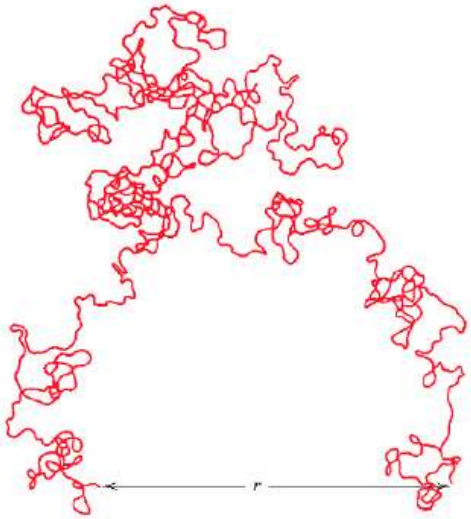


- The angle between the singly bonded carbon atoms is ~109° – carbon atoms form a zigzag pattern in a polymer molecule.
- Moreover, while maintaining the 109° angle between bonds polymer chains can rotate around single C-C bonds (double and triple bonds are very rigid).

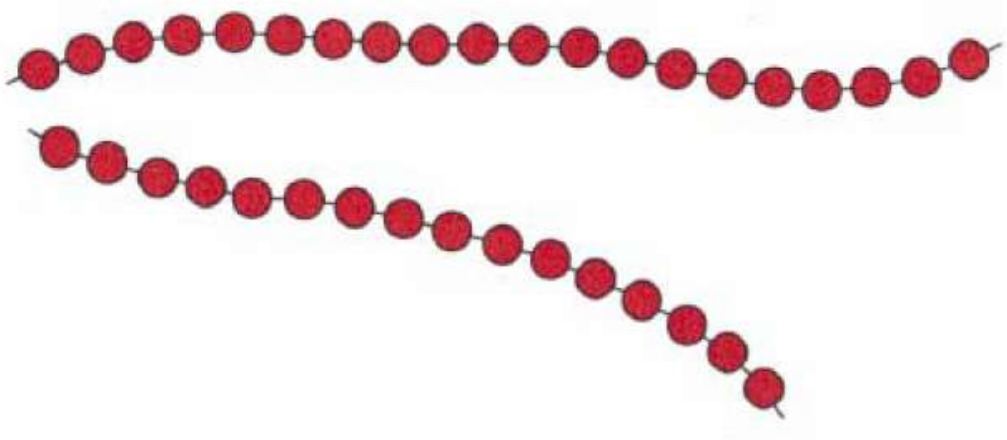


- Random kinks and coils lead to entanglement, like in the spaghetti structure:

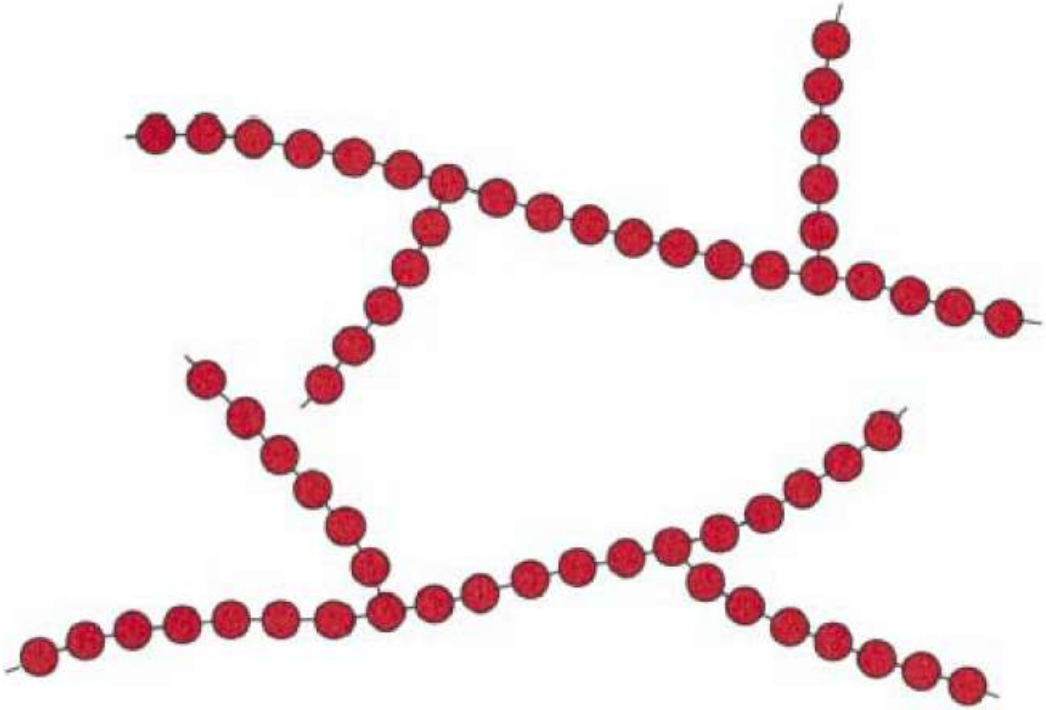




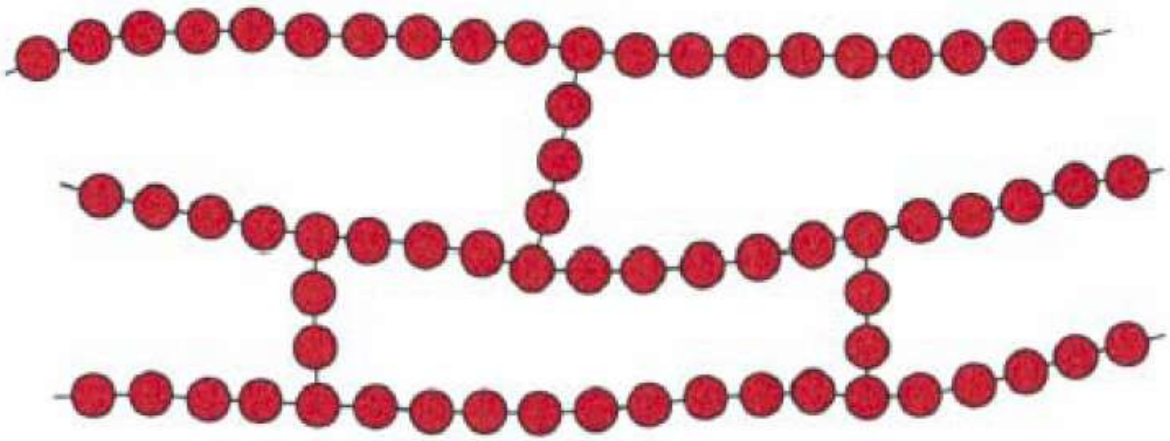
1 **Linear polymers**: Van der Waals bonding between chains. Examples: polyethylene, nylon.



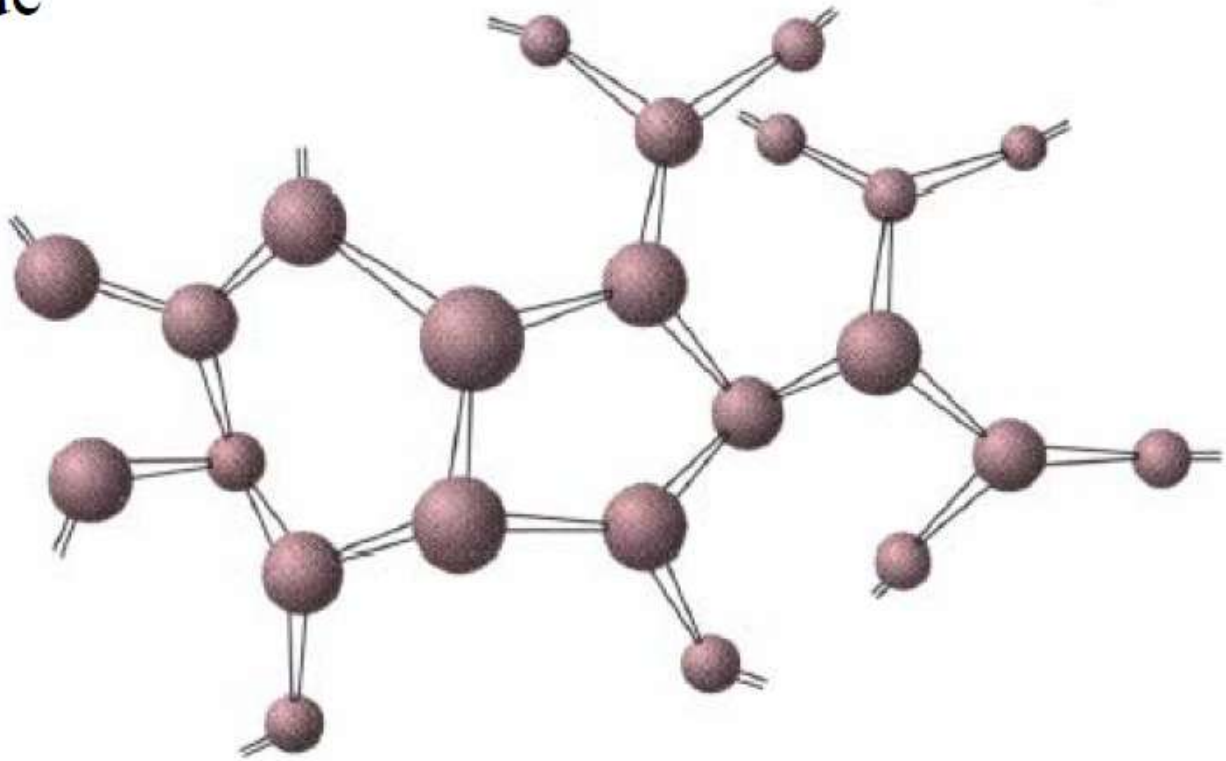
2 **Branched polymers**: Chain packing efficiency is reduced compared to linear polymers - lower density



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.

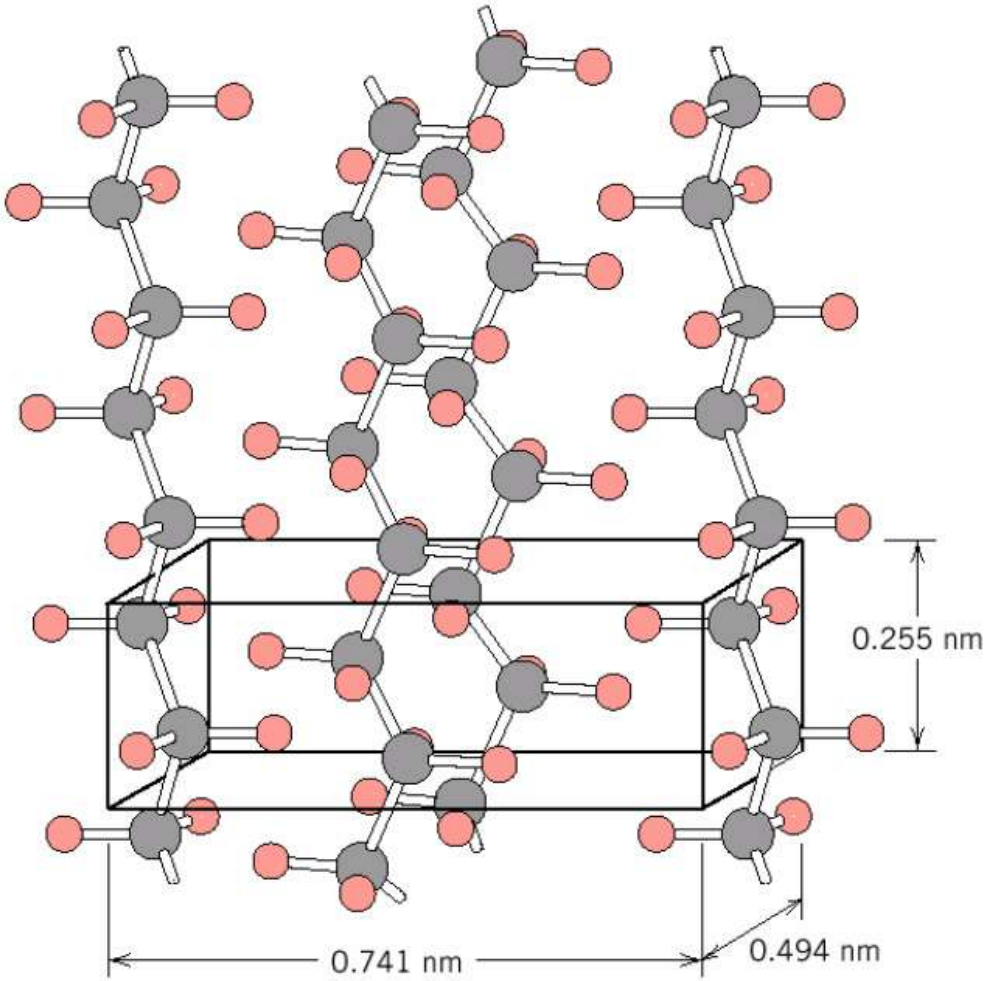


4 **Network polymers**: 3D networks made from trifunctional mers. Examples: epoxies, phenol-formaldehyde



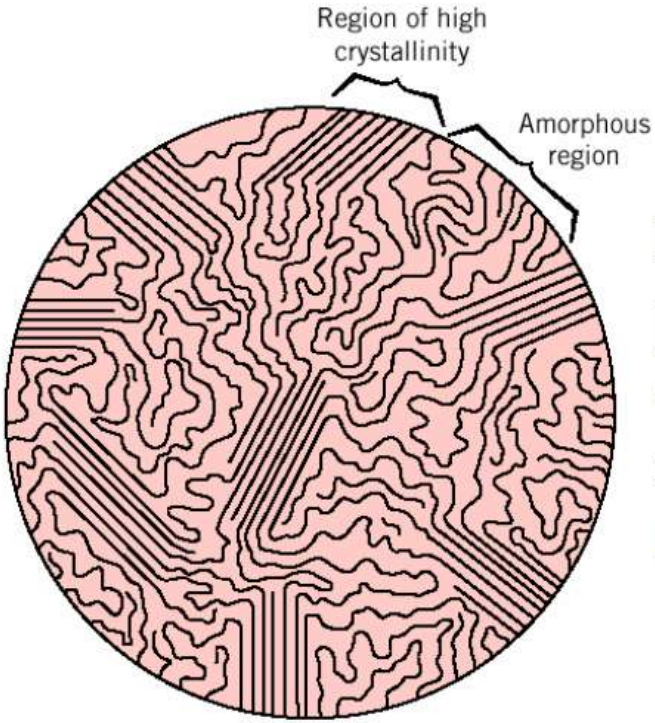
Polymer structure, crystals

Atomic arrangement in polymer crystals is more complex than in metals or ceramics (unit cells are typically large and complex).



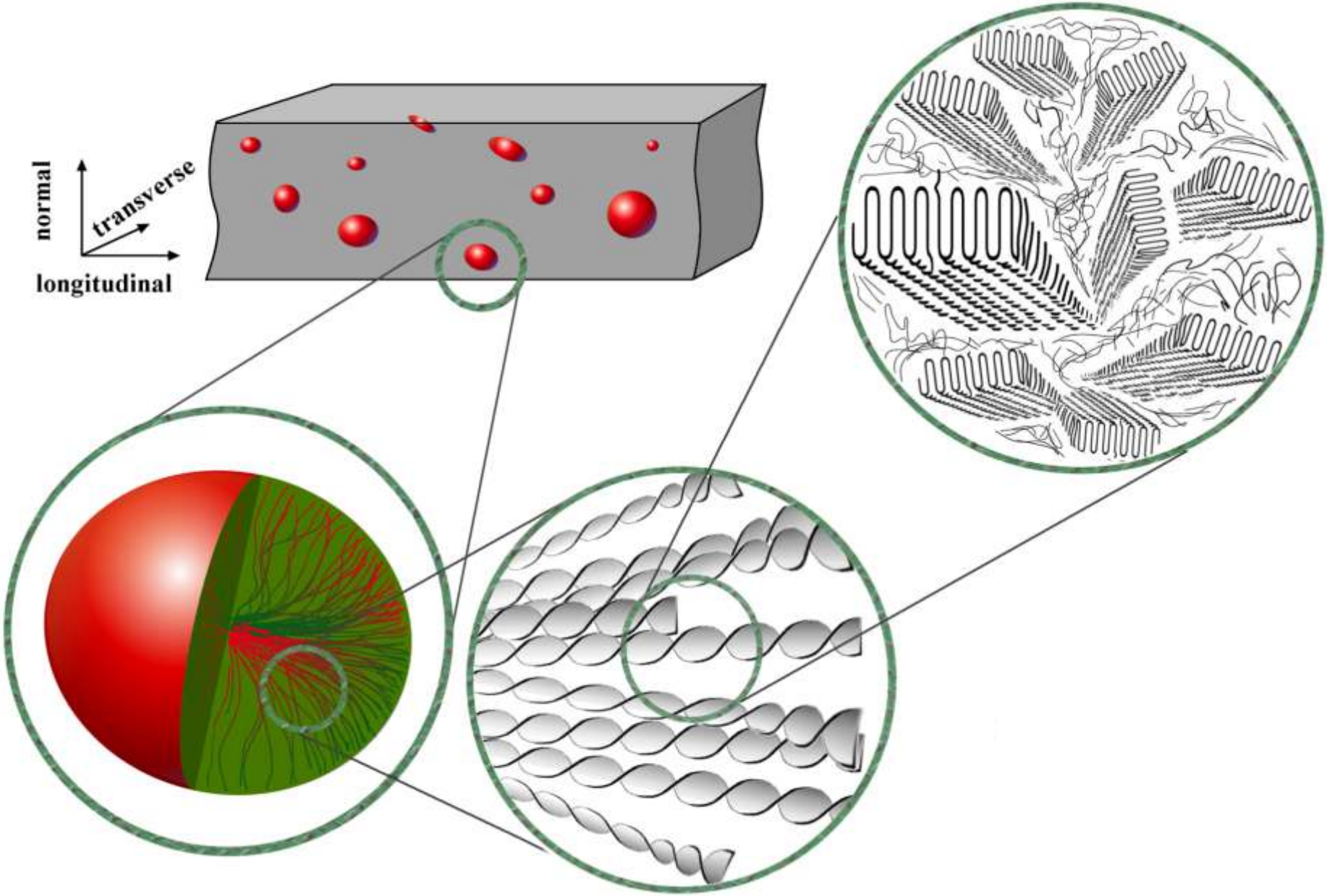
Polyethylene

Polymer structure, crystals and amorphous structure

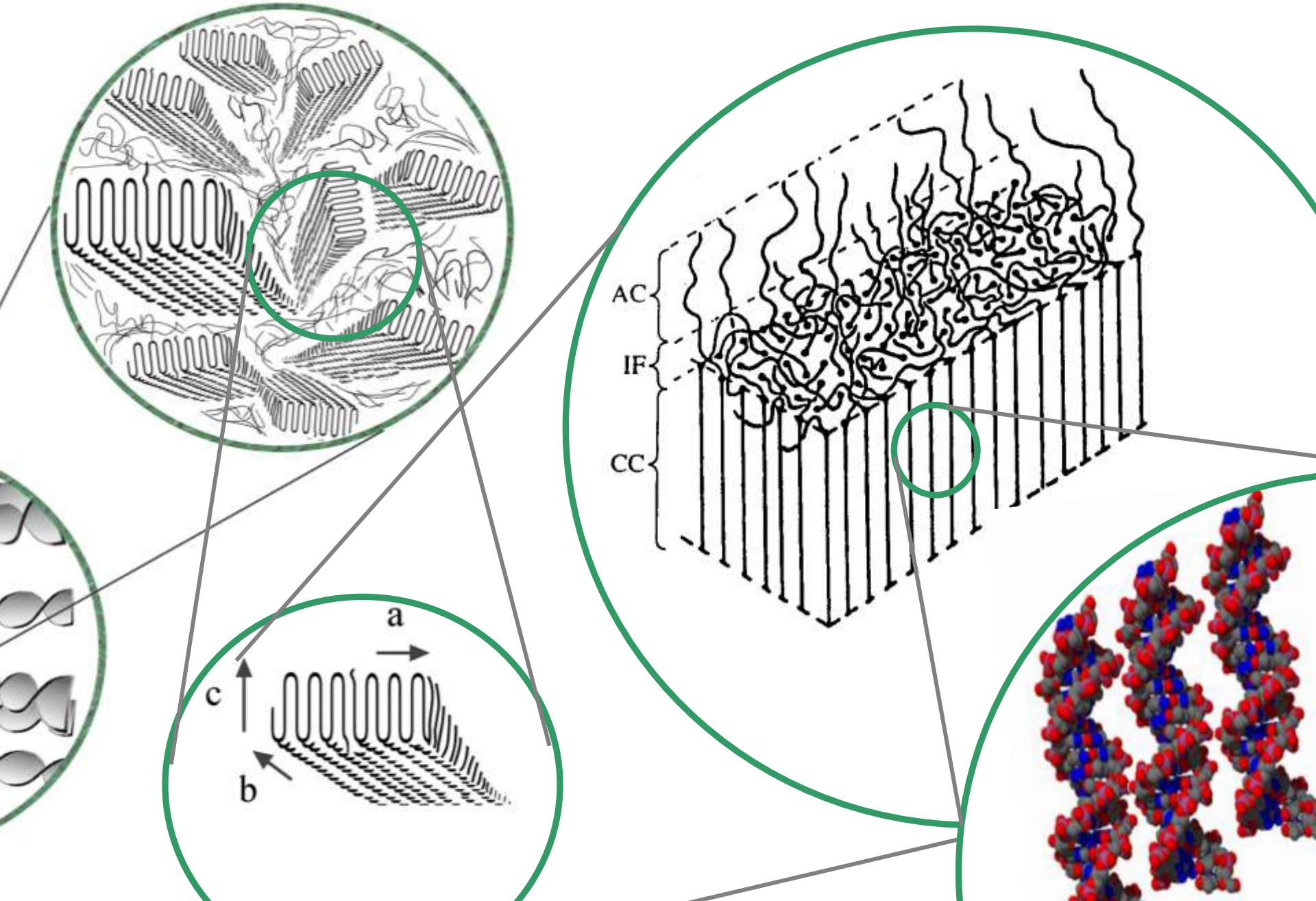


Polymer molecules are often partially crystalline (semi-crystalline), with crystalline regions dispersed within amorphous material.

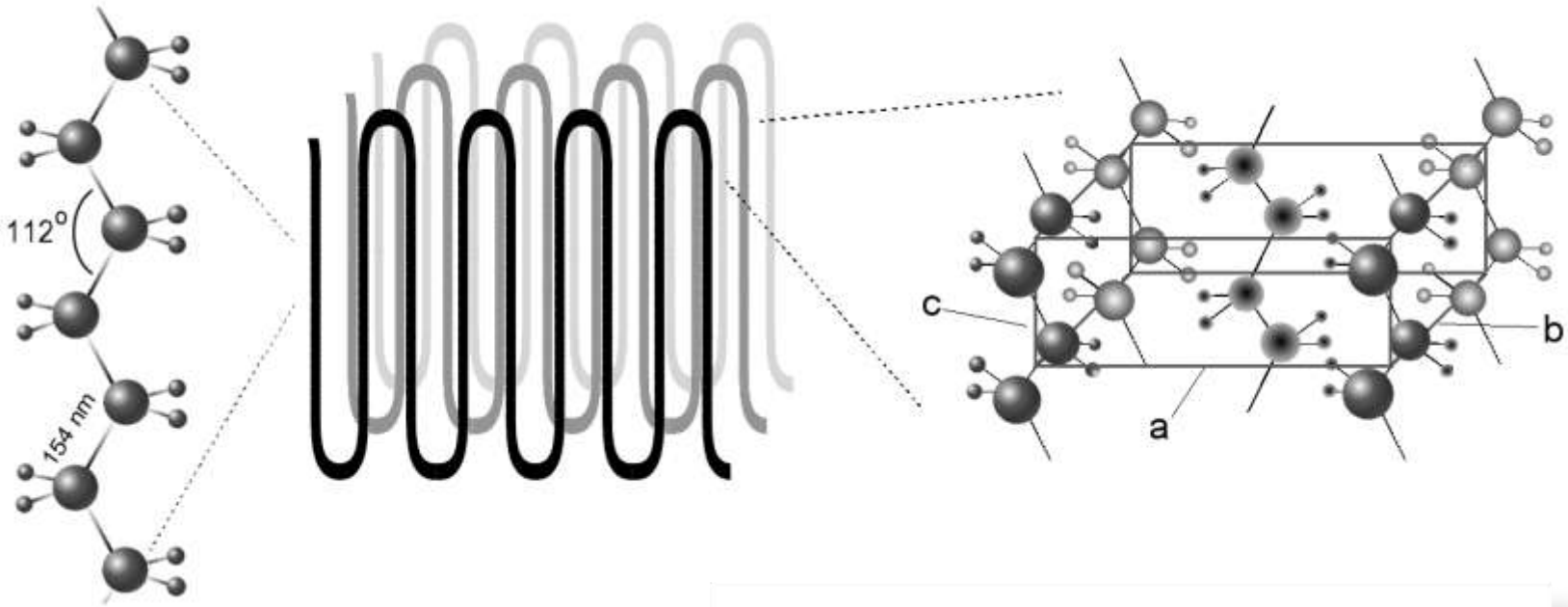
Structure, scales, partially crystalline polymers



Structure, scales, partially crystalline polymers

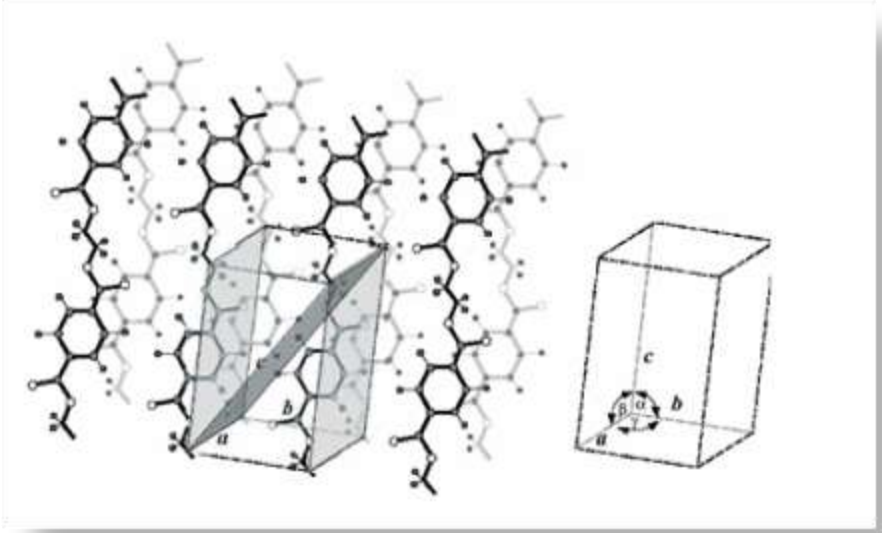


Structure, scales, partially crystalline polymers

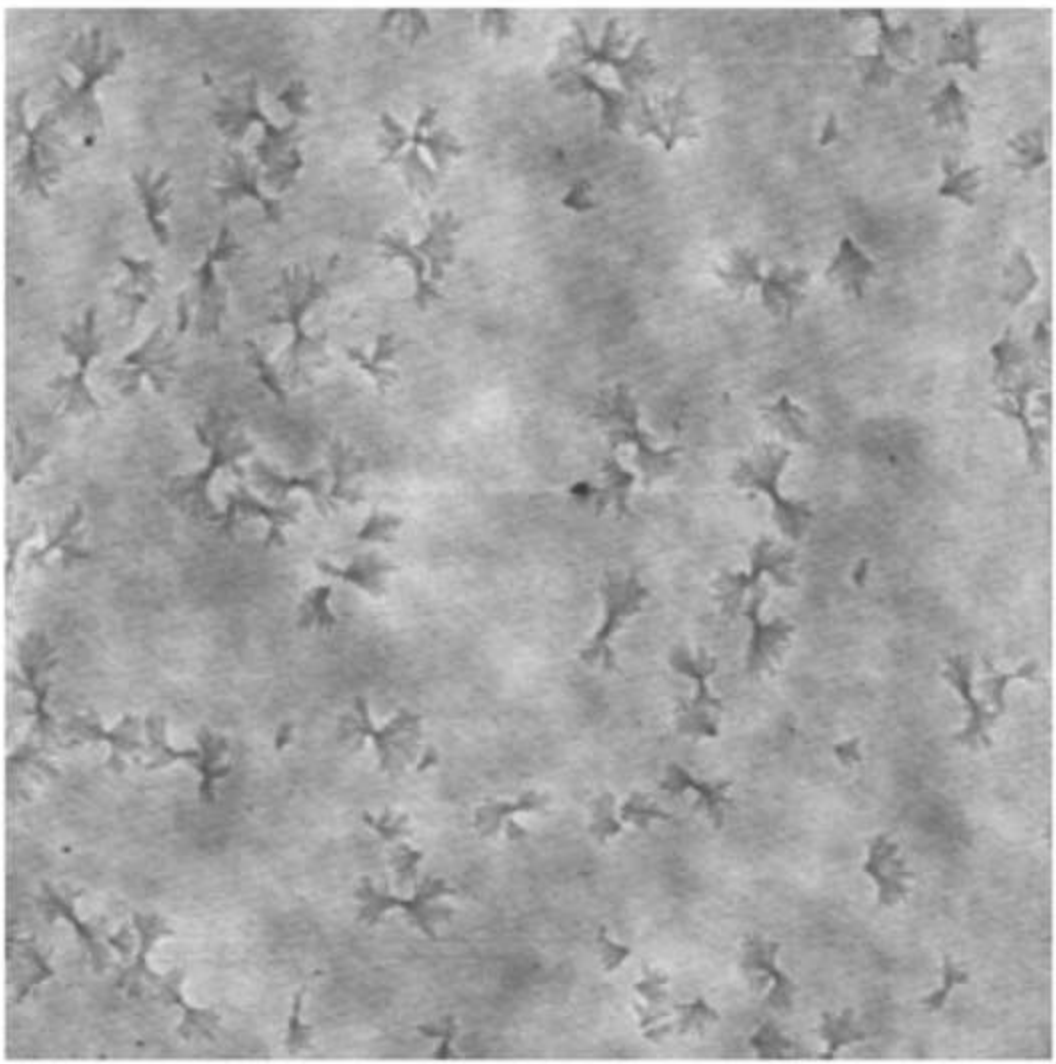


The crystalline unit cell for PET (a = 4.56 Å, b = 5.94 Å, c = 10.75 Å; α = 98.5°, β = 118°, γ = 112°),

M Durell (2002)



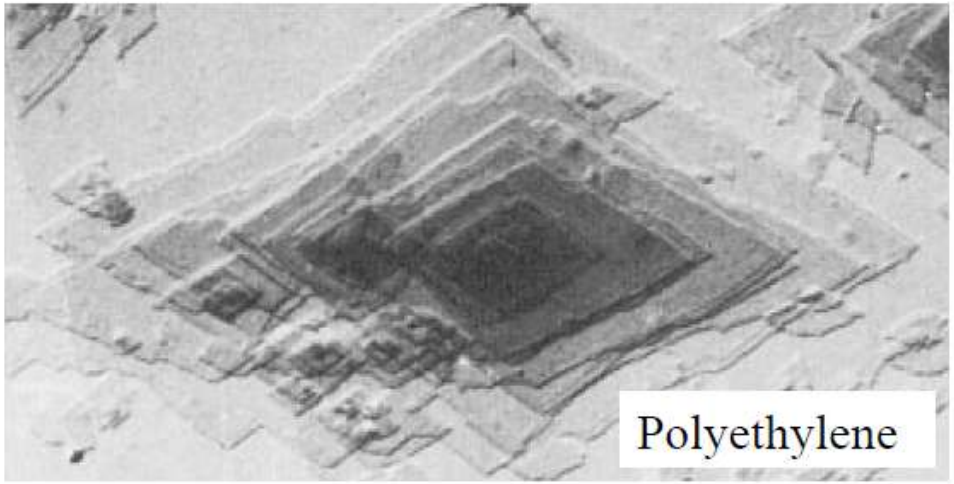
Polymer structure: spherulite growth



PET / AFM: M Durell, J E Macdonald, D Trolley, Europhysics Letters (2002)

Polymer structure: spherulite growth

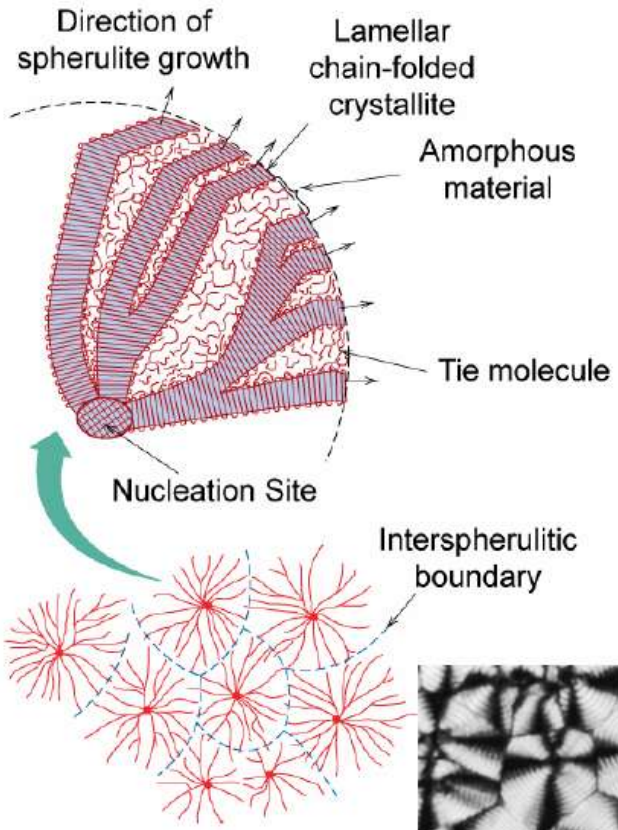
Thin crystalline platelets grown from solution - chains fold back and forth: chain-folded model



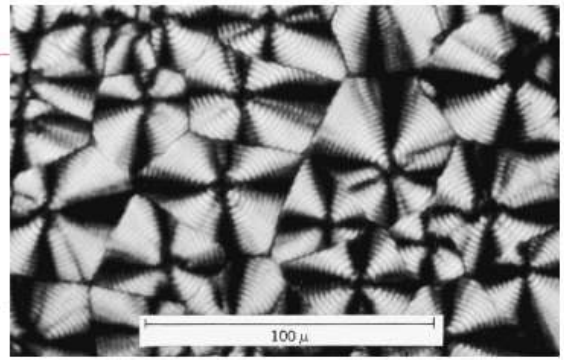
The average chain length can be much greater than the thickness of the crystallite

Polymer structure: spherulite growth

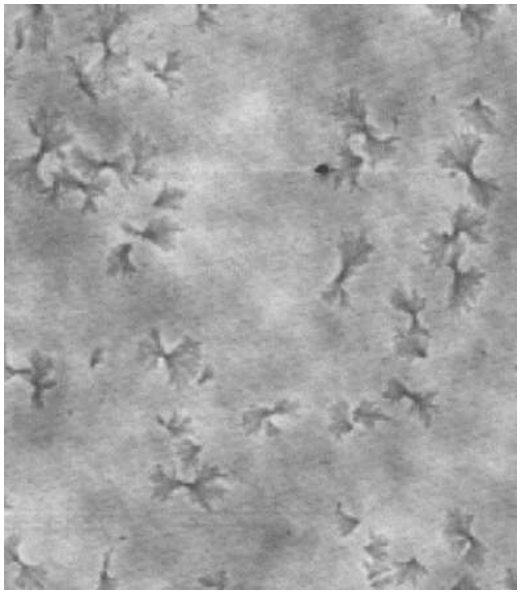
Spherulites: Aggregates of lamellar crystallites ~ 10 nm thick, separated by amorphous material. Aggregates are formed upon solidification from a melted state and are approximately spherical in shape.

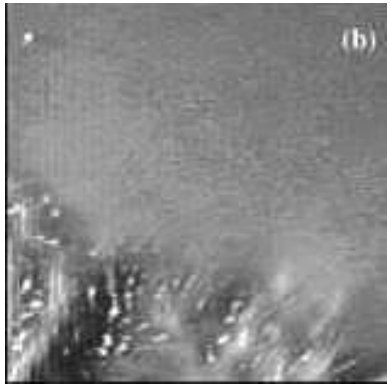


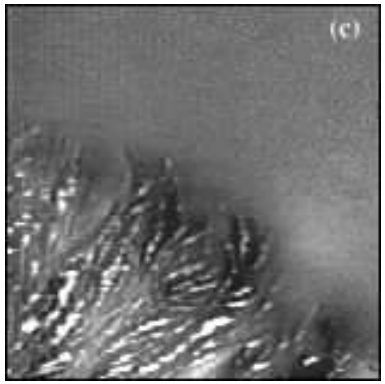
Photomicrograph of spherulite structure of polyethylene



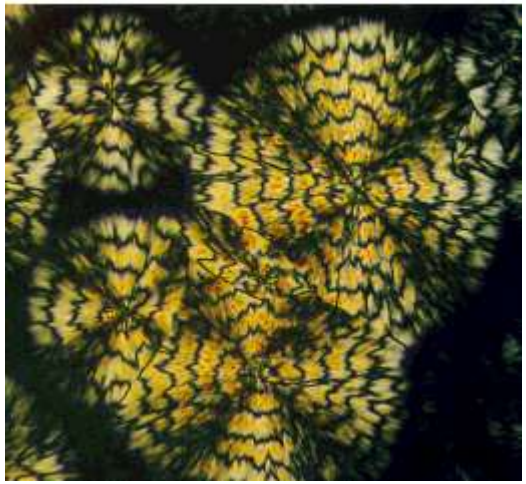
Polymer structure: spherulite growth







1 micron square, AFM



1 millimeter square, OM

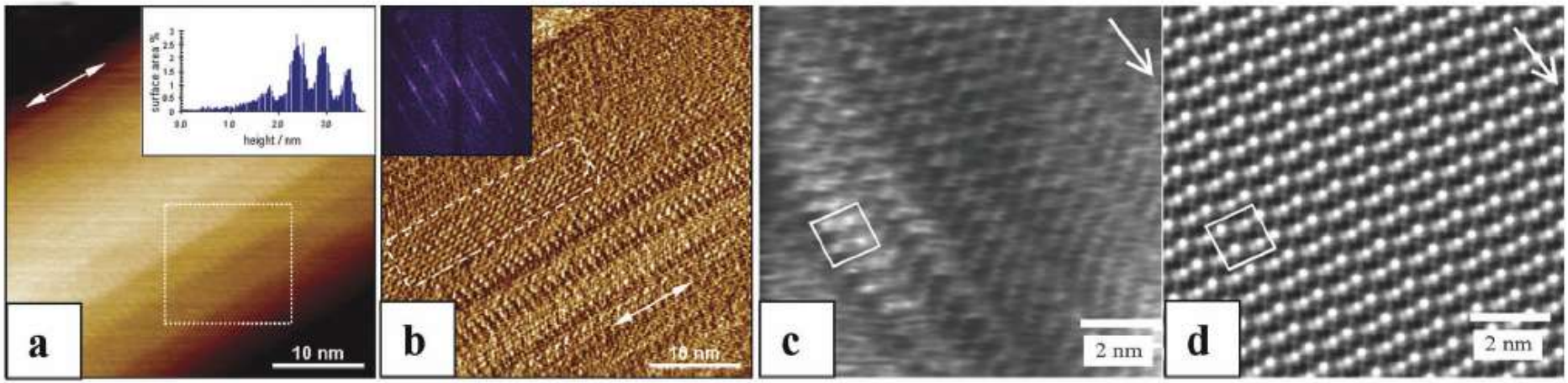
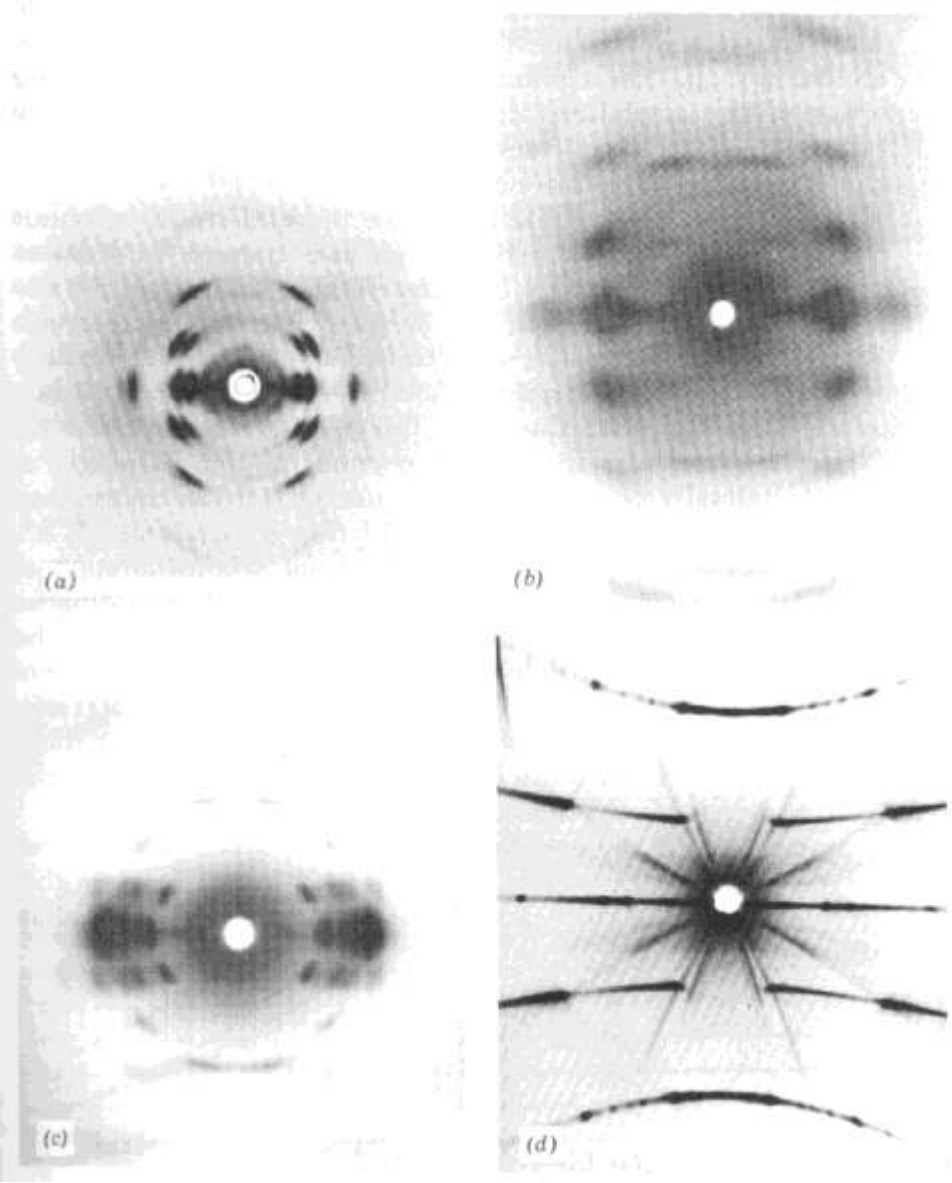
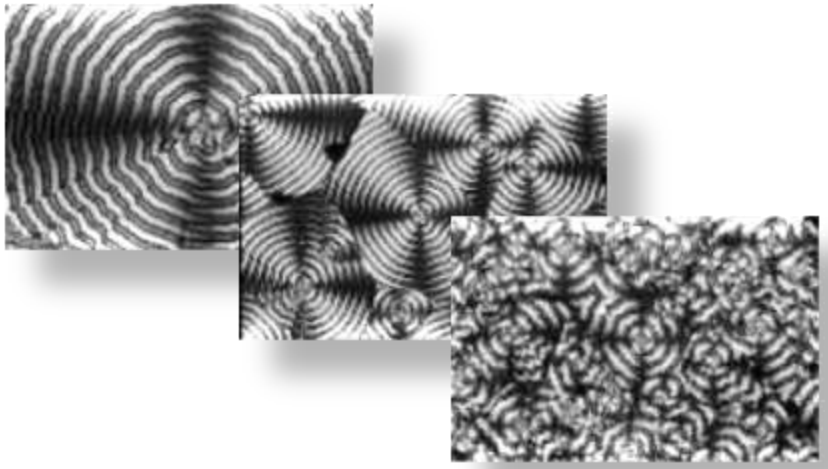


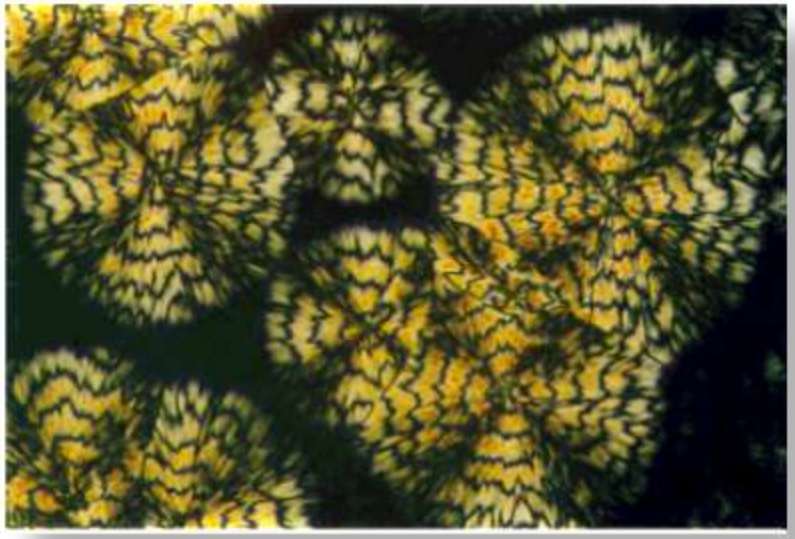
Fig. 2 AFM contact mode images. Cellulose molecules in micro-fibril crystal: (a) topographic image; and (b) error-signal image. Polybutene-1 molecules: (c) topographic image; and (d) simulated AFM image based on crystallographic data.

M. Miles, M. Antognozzi, H. Haschke, J. Hobbs, A. Humphris, T. McMaster
H.H. Wills Physics Laboratory, University of Bristol, Materials Today, Feb. 2003

Polymer structure: spherulite growth



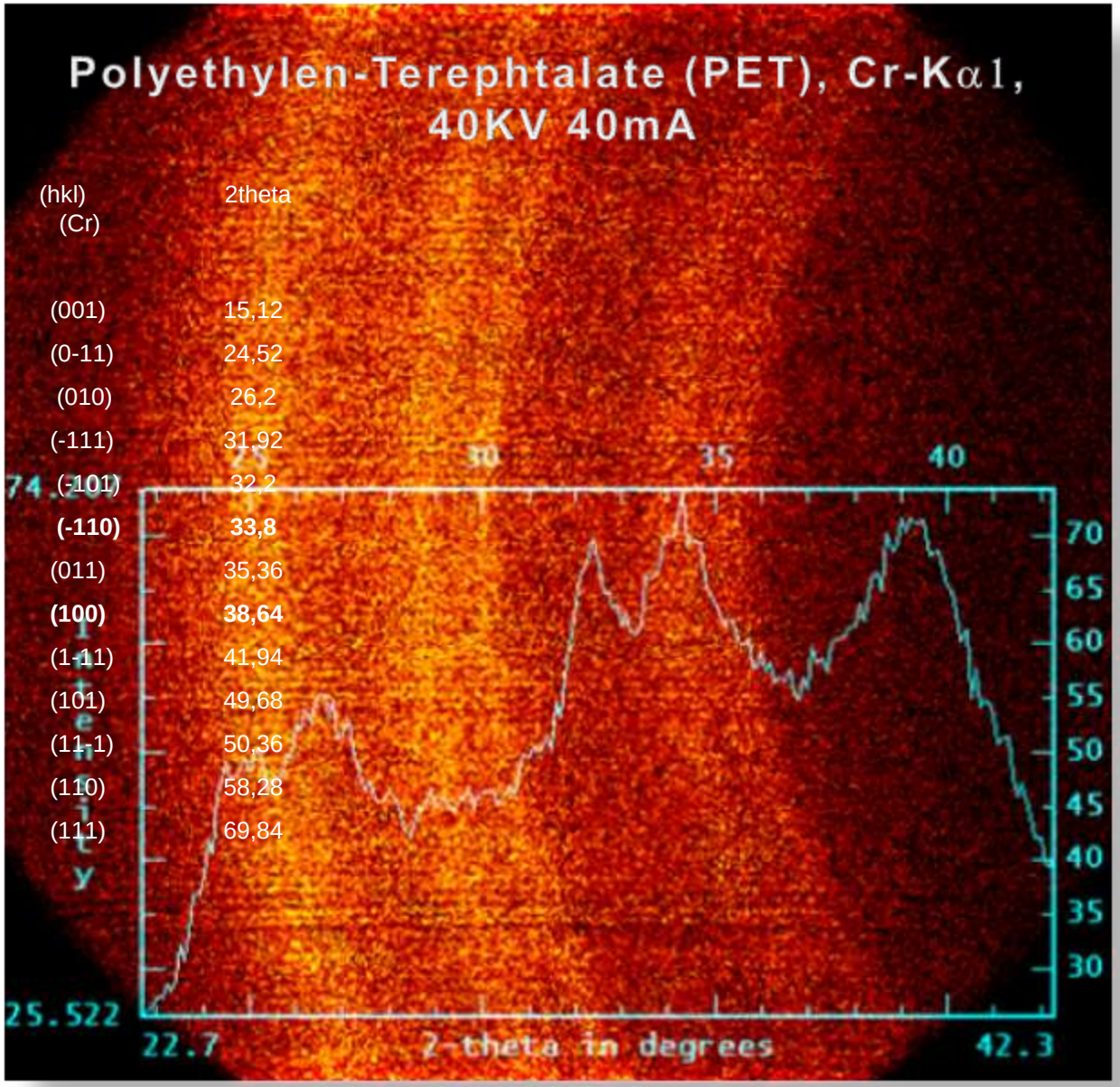


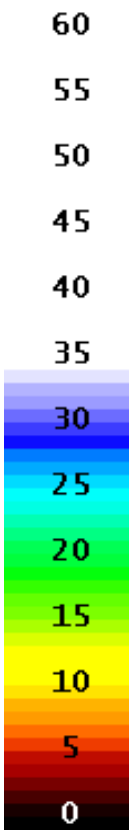


1 millimeter square, OM

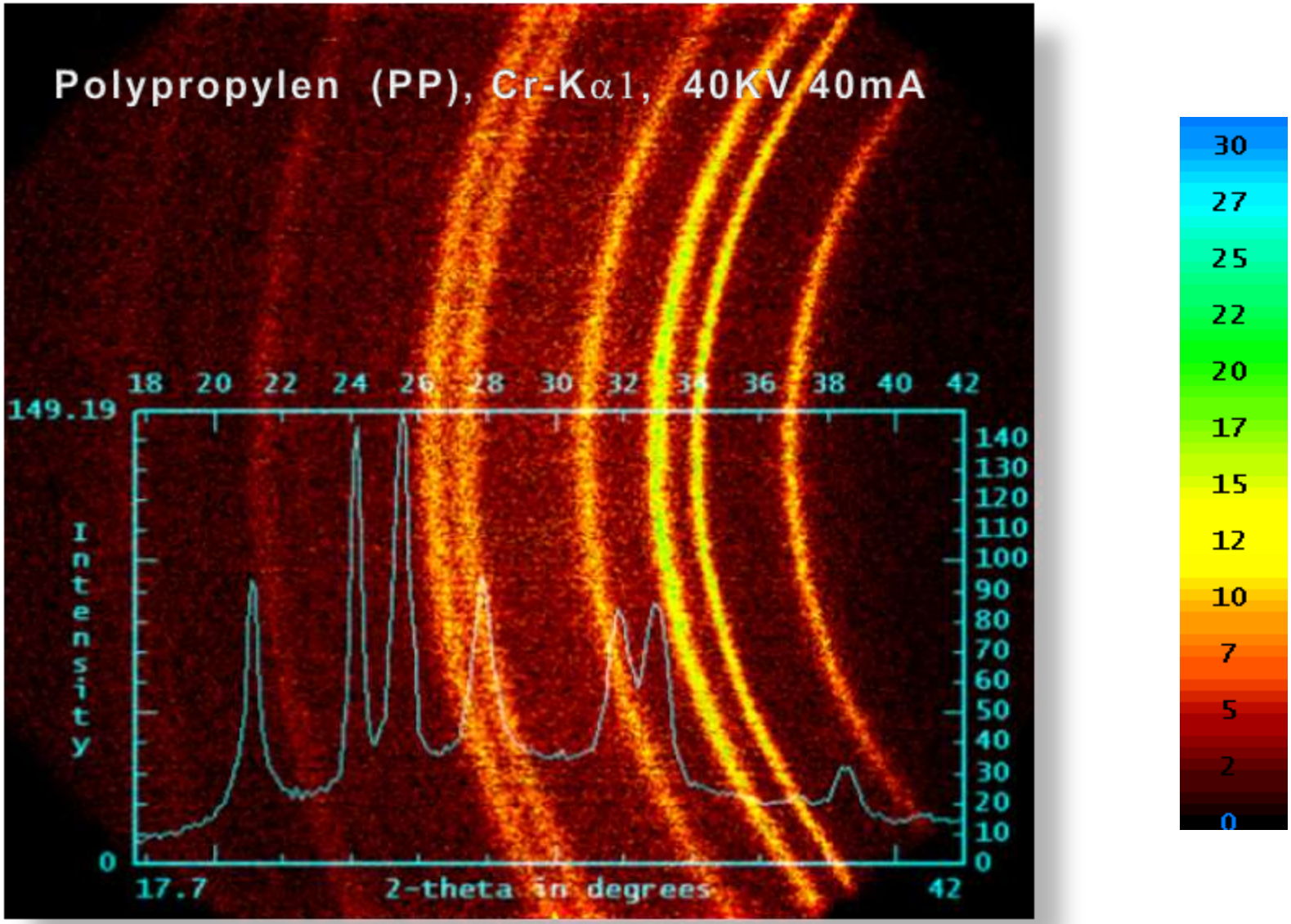
Bamford, Nature 173 (1954) p. 27; Astbury, Endeavor 1(1942) p. 70

Polymer structure: PET: XRD

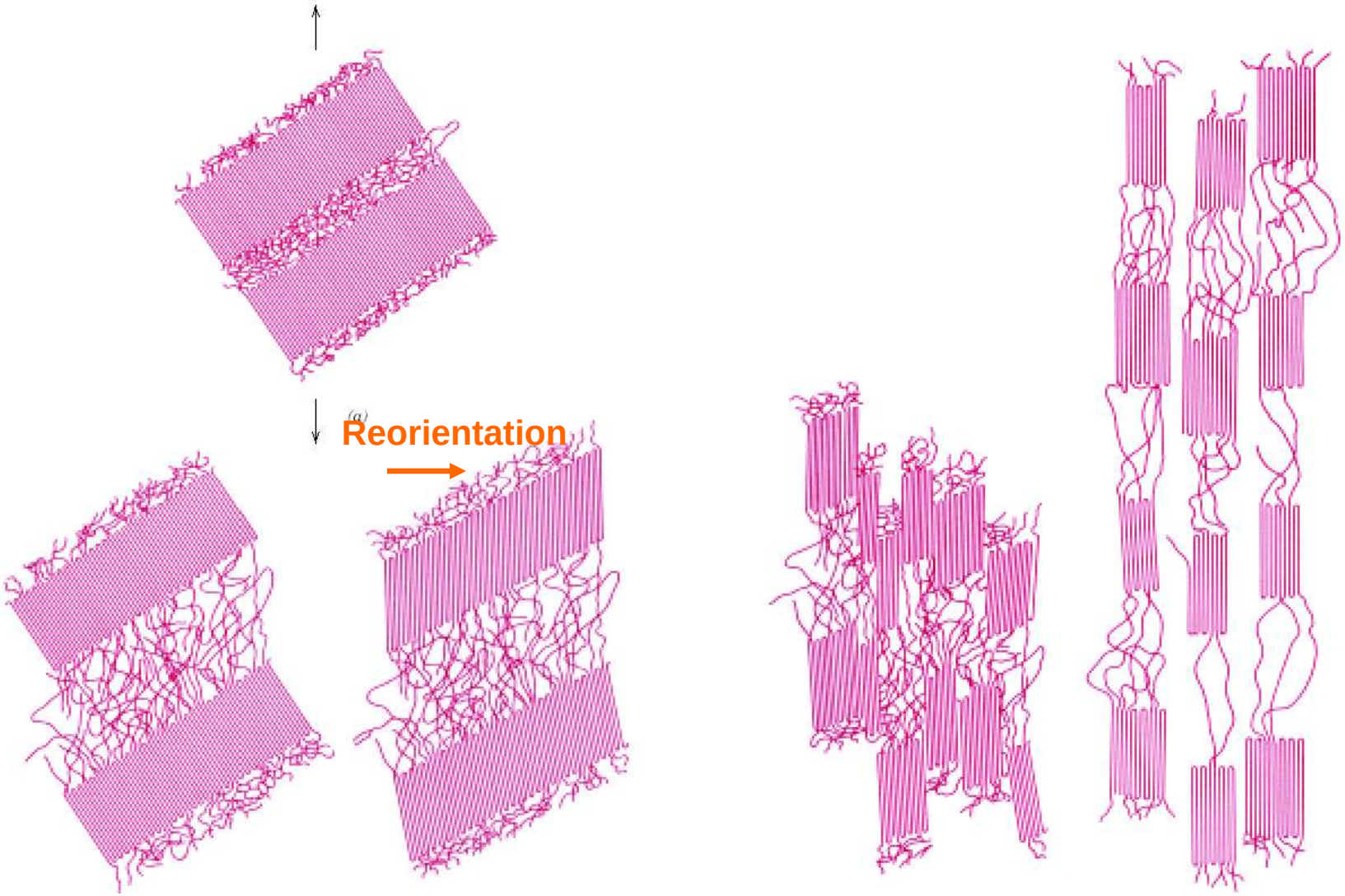




Polymer structure: PP: XRD



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

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

Performance is controlled by

- **vol. fraction of fibers**
- **properties of fibers and matrix**
- **bond between the two**