

## Chapter 2

# CHAIN STRUCTURE & CONFIGURATION






# Conformation vs configuration

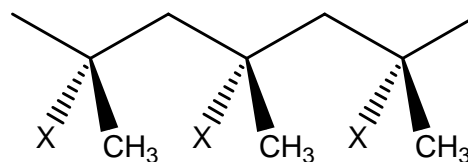
- conformation
  - rotation of bond
  - conformer
  - trans-gauche → *Chapter 5*
  - extended/folded, zigzag/helical → *Chapter 6*
- configuration
  - breaking bond
  - isomer

# Structure of polymers

- Chemical structure
  - Repeat unit (atomic) structure
  - Isomeric structure ← configuration
  - Sequence structure
  
- Physical Structure
  - Single chain structure ← conformation
  - Aggregation structure
    - Amorphous
    - (Semi)crystalline

# Isomers

- structural isomer 구조이성질체
  - $[\text{CH}_2\text{CH}_2\text{O}]_n$  &  $[\text{CH}_2\text{CH}(\text{OH})]_n$
  - 1,2-PBD & 1,4-PBD  p43
- geometric isomer 기하이성질체  p43
  - cis-1,4-PBD & trans-1,4-PBD
- head-to-tail vs head-to-head  p30
  - $[\text{CH}_2\text{CH}(\text{Y})\text{CH}_2\text{CH}(\text{Y})]$  &  $[\text{CH}_2\text{CH}(\text{Y})\text{CH}(\text{Y})\text{CH}_2]$
- optical isomer 광학이성질체
  - $[\text{OC}^*\text{H}(\text{CH}_3)\text{CH}_2]$   p42
  - vinyl polymers?  p37



pseudochiral

# Isomers 2

- Tacticity
  - stereoisomer
  - 입체이성질체
  - isotactic, syndiotactic, and atactic
  - determines crystallizability
  - affects thermal/mechanical properties

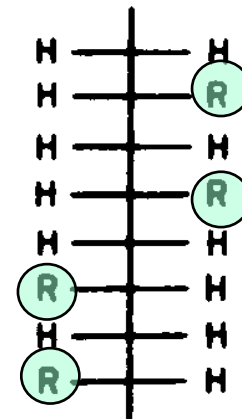
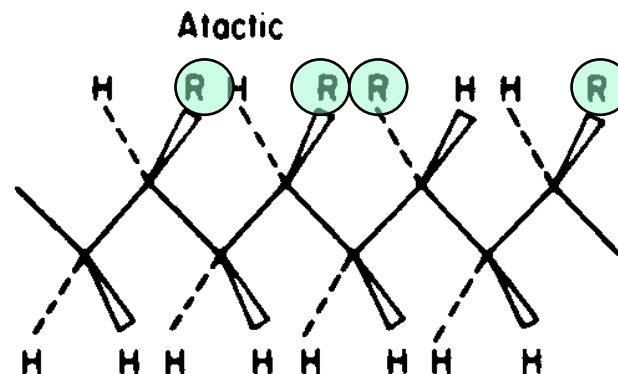
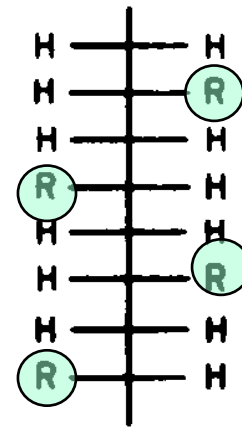
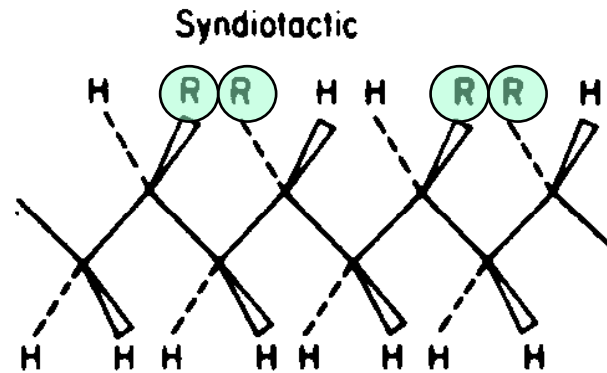
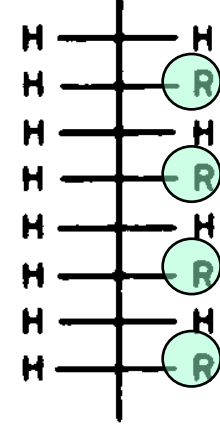
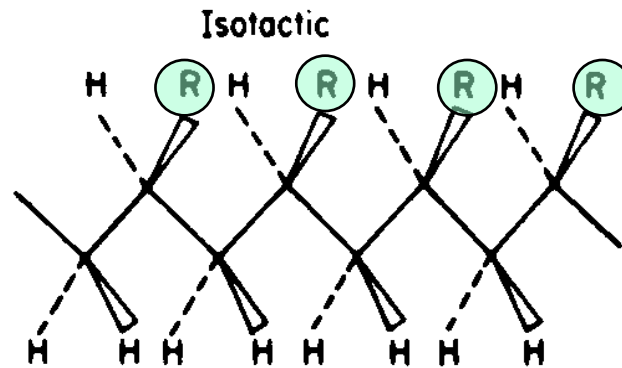


Fig 2.3

# ✓ Characterizing tacticity by NMR

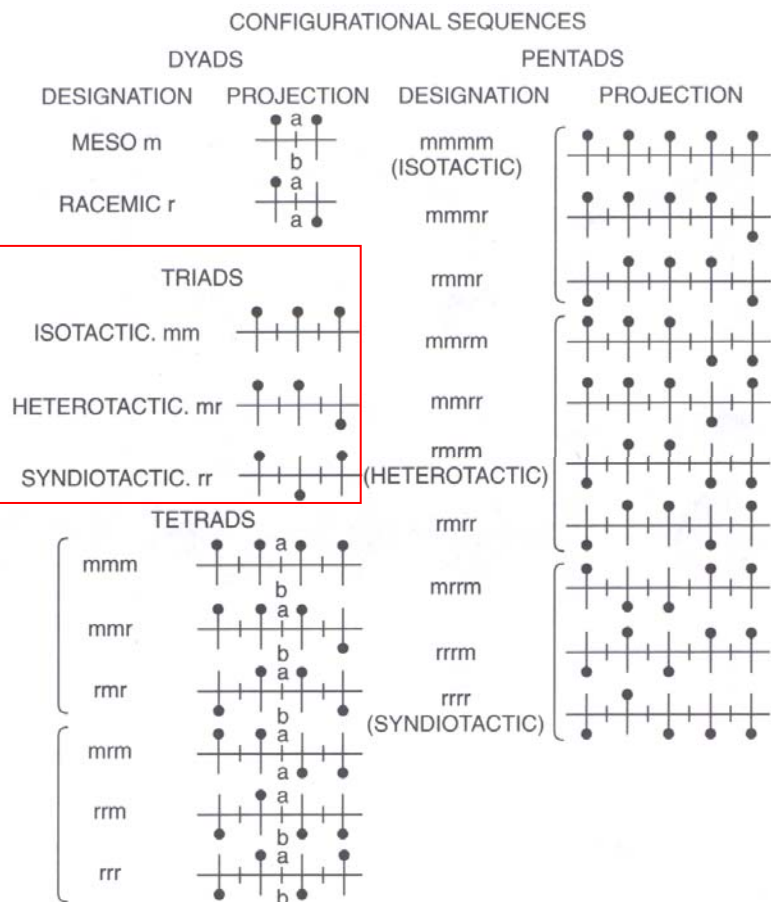
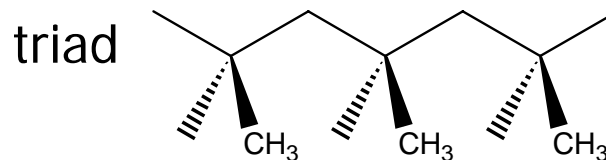
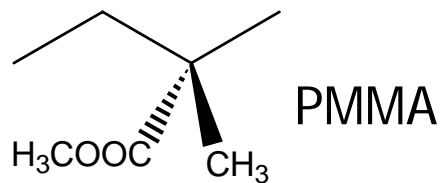


Fig 2.5

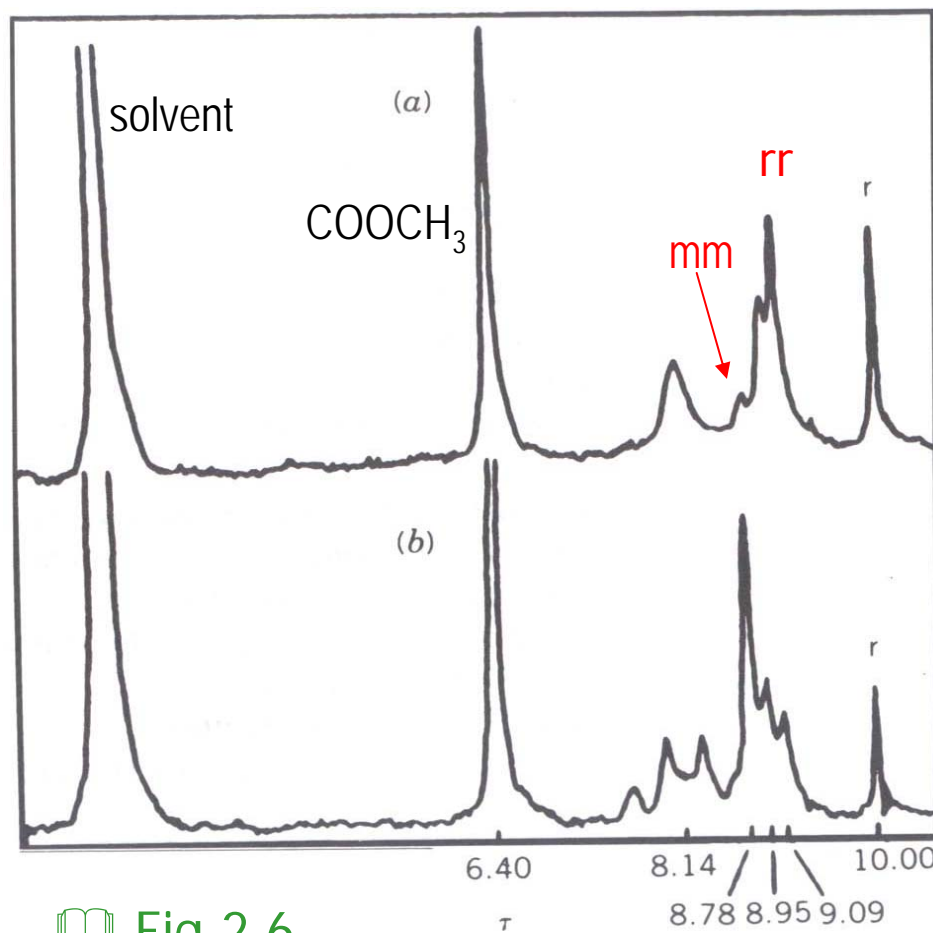
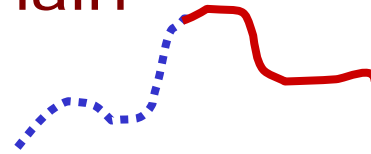


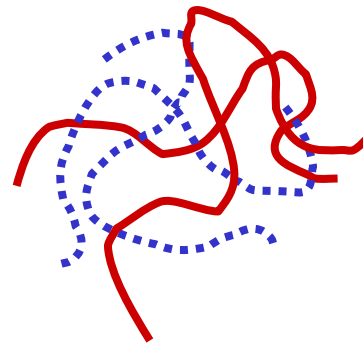
Fig 2.6

# Copolymer vs blend

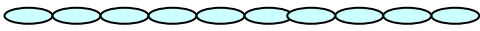


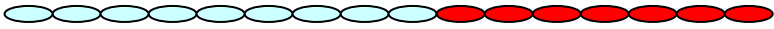
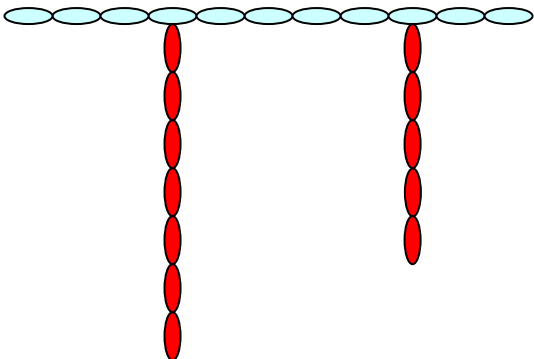
- copolymer
  - 2 or more different repeat units linked by covalent bond **in a chain**



- blend
  - **Mixture** of 2 or more different polymers



# Types of copolymers

- homopolymer 
- copolymer
  - random copolymer 
  - alternating copolymer 
  - block copolymer
    - diblock, triblock, multiblock
    - symmetric, asymmetric
  - graft copolymer 
  - terpolymer



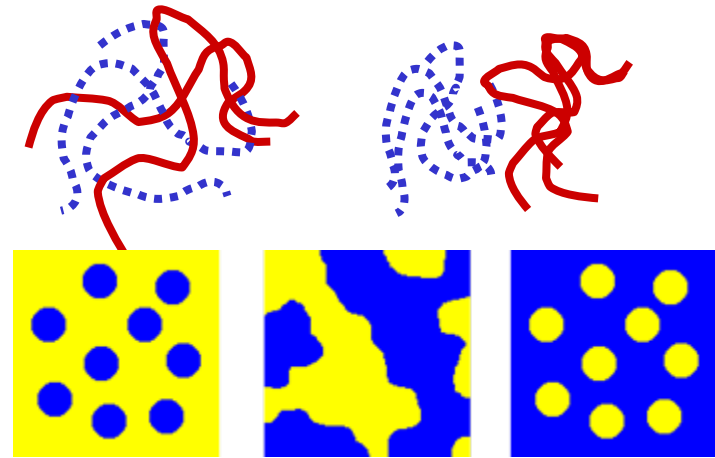
# Types of copolymers 2

Table 2.5 Some copolymer terminology (19,20)

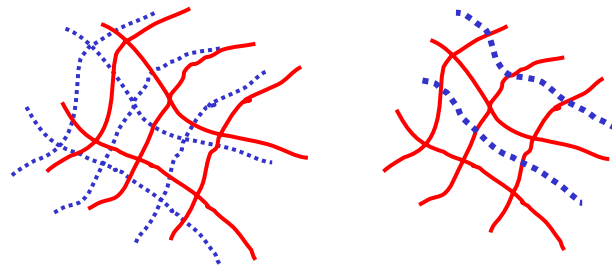
Type	Connective	Example
<i>Short Sequences</i>		
Unspecified	-co-	poly(A-co-B)
Statistical	-stat-	poly(A-stat-B)
Random	-ran-	poly(A-ran-B)
Alternating	-alt-	poly(A-alt-B)
Periodic	-per-	poly(A-per-B-per-C)
<i>Long Sequences</i>		
Block	-block-	<del>poly A block poly B</del> poly(A-b-B)
Graft	-graft-	<del>poly A graft poly B</del> poly(A-g-B)
Star	-star-	star-poly A
Blend	-blend-	<del>poly A blend poly B</del> polyA/polyB
Starblock	-star- . . . -block-	star-poly A-block-poly B
<i>Networks</i>		
Cross-linked	-net-	net-poly A
Interpenetrating	-inter-	cross-poly A-inter-net-poly B
AB-cross-linked	-net-	poly A-net-poly B

# Blends

- mixture of 2 or more different polymers
- miscible or immiscible
- Most pairs are immiscible.



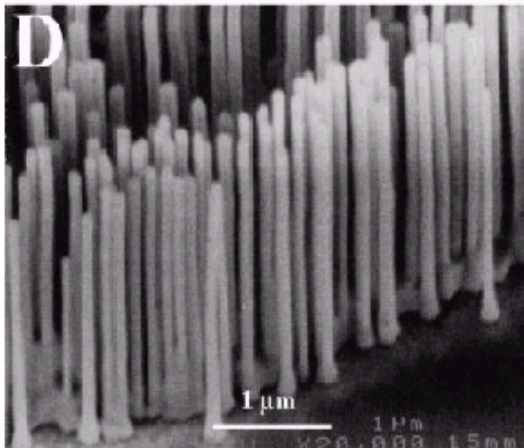
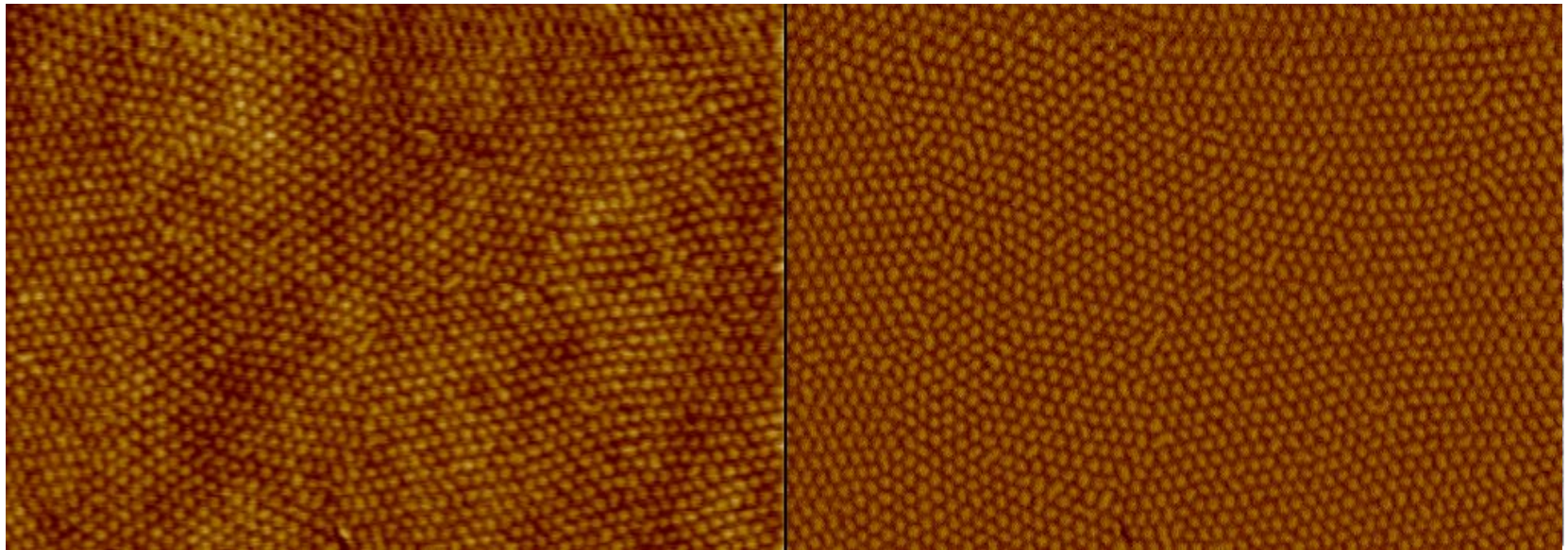
- special type: IPN and SIPN



- ✓ random, alternating copolymers ~ miscible
- ✓ block, graft copolymers ~ immiscible

# Block copolymer

poly(styrene-*b*-methyl methacrylate)

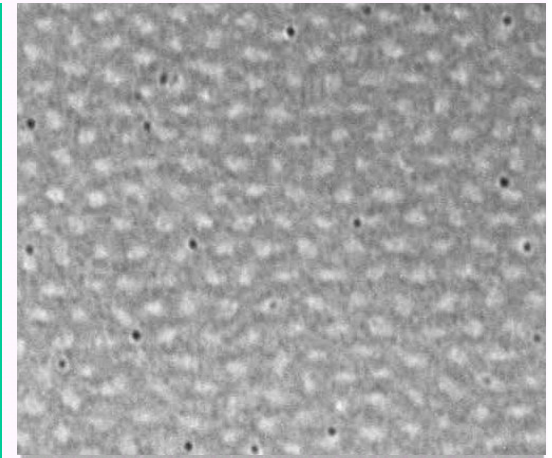


Array structure of

← nanotube

← nanowire

nanocrystal →



# Multicomponent systems

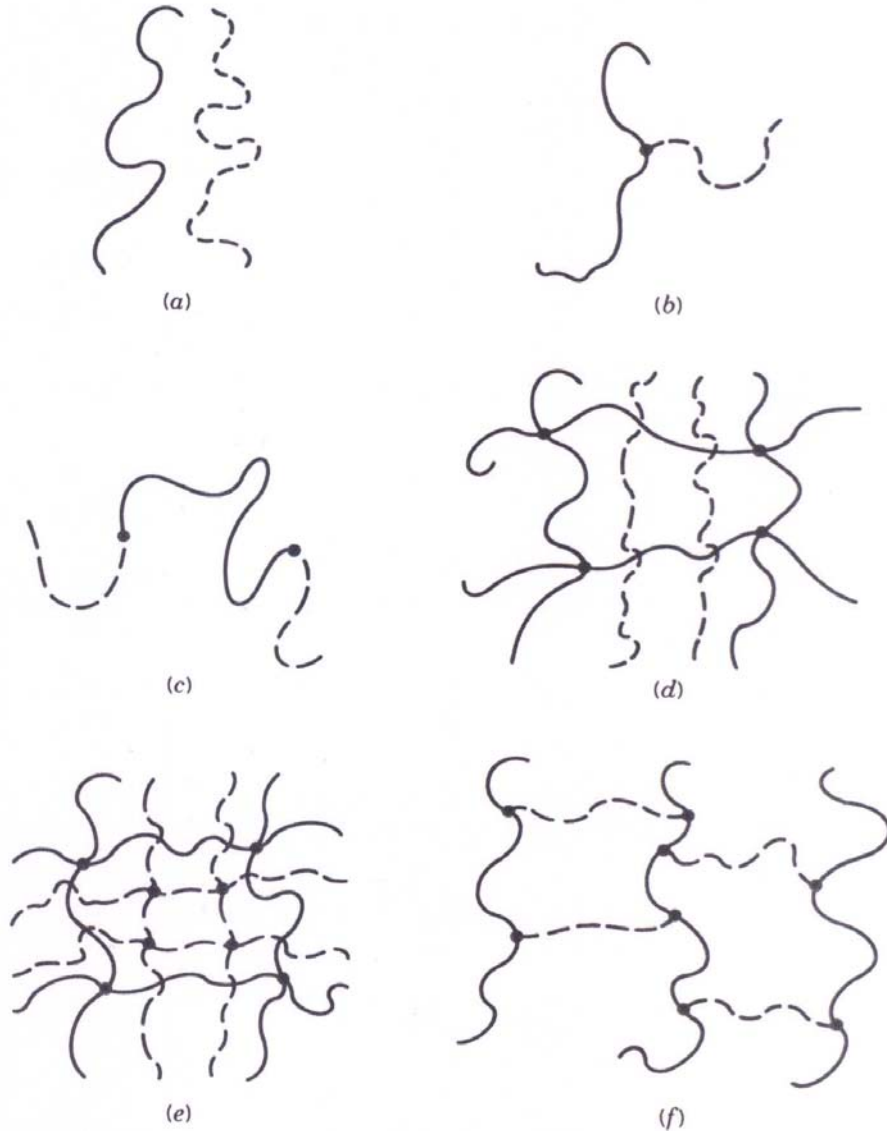


 Fig 2.10

# Conformational states & changes

- conformational states  
 $t, g^+, g^-$
- conformational changes
  - $ttt \rightleftharpoons g^+ tg^-$
  - by heat, load, light, etc
  - examined by NMR, IR, etc

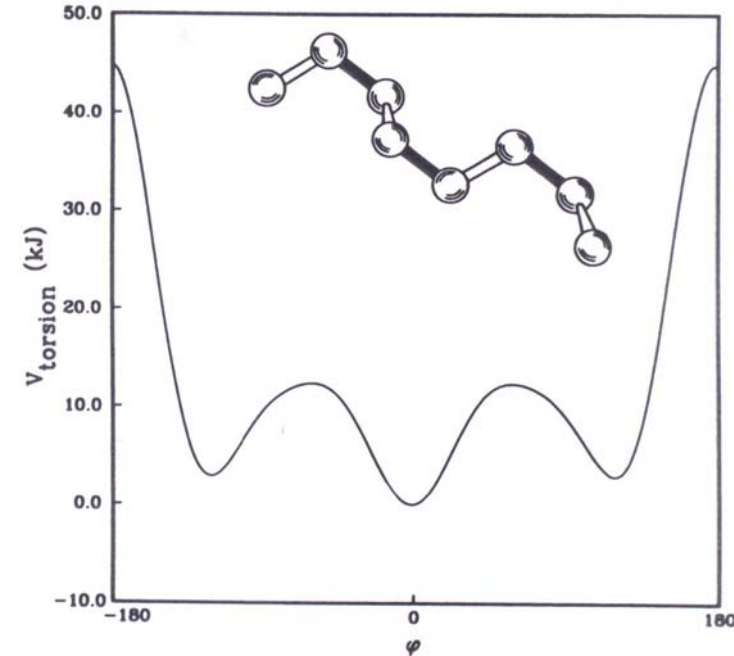


 Fig 2.11

# Resin, fiber, and rubber

- synthetic resin (합성수지)
  - linear (thermoplastic) or crosslinked (thermosetting)
  - amorphous or **semicrystalline**
  - at  $T < T_g$  (and/or  $T_m$ )
- synthetic fiber (합성섬유)
  - linear and semicrystalline, typically
  - highly drawn
- synthetic rubber (합성고무), elastomer (탄성체)
  - crosslinked, typically
  - at  $T > T_g$