

Chapter 1. A Brief Introduction to Polymer Science

1.1 Fundamental definitions

Polymer (IUPAC 정의) : A substance composed of molecules characterized by the multiple repetition of CRU(constitutional repeating units).
(poly: many, mer: part)

CRUs are linked by covalent bonds.

Atoms of CRU are linked by covalent bonds.

Oligomer : A molecule with only a few CRUs.

Monomer : The substance that the polymer is made from.

Polymerization : The process that converts a monomer to a polymer.

Dissociation energy

- . Covalent bonds (or primary bonds) : 300 ~ 500 kJ/mol
- . Weak secondary bonds
 - Van der Waals 10 kJ/mol
 - Hydrogen bond 10 ~ 50 kJ/mol

- cf. Thermal energy 2.5 kJ/mol (at 300K)
 4 kJ/mol (at 500K)

Polymer crystals : direction-dependent (anisotropic)

- . Young's modulus of PE :
 - 300GPa in chain axis direction (strong, stiff bonds)
 - 3GPa in transverse direction (weak, soft, secondary bonds)

- Refractive index (굴절률)

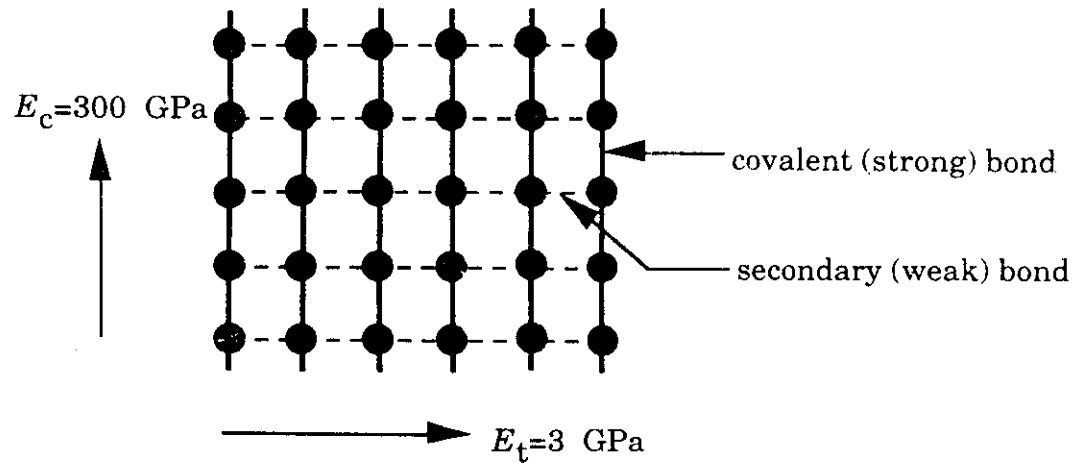


Figure 1.2 Schematic representation of a polymer crystal illustrating its anisotropic nature. The moduli for polyethylene parallel (E_c) and transverse (E_t) to the chain axis are shown.

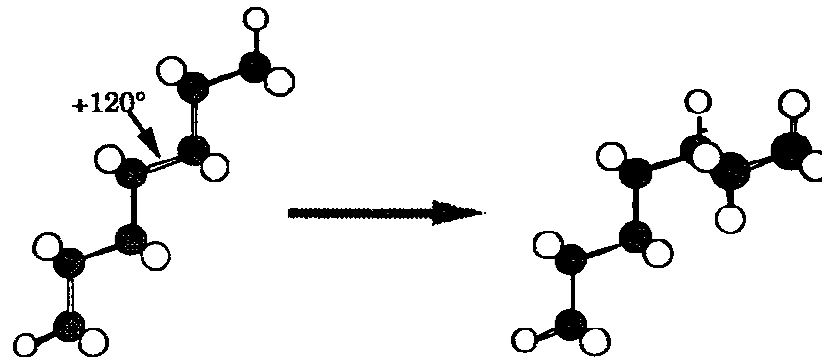
1.2 Configurational states

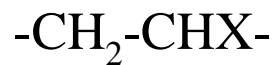
Configuration (配位) : the permanent stereostructure of a polymer

A permanent stereostructure that cannot be changed without a chemical reaction.

Conformation (配座) : the stereostructure of a molecule defined by its sequence of bonds and torsion angles

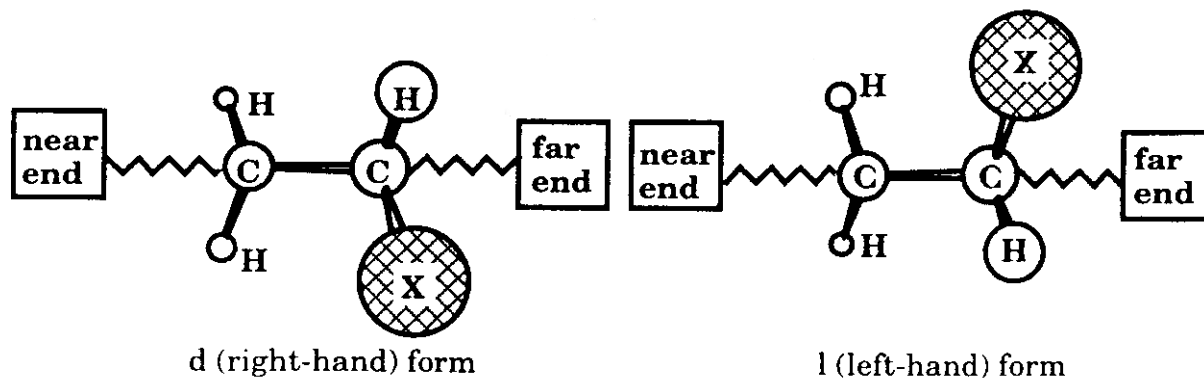
A stereostructure that can be changed by torsion about the sigma bond.





: Two stereo forms

- D (dextro) form : right-hand
- L (levo) form : left-hand



Tacticity : The orderliness of the succession of configurational base units in the main chain of a polymer molecule

Isotactic : all-d chain or all-l chain

Syndiotactic :dlldl....

Atactic : equal numbers of randomly distributed configurational base units

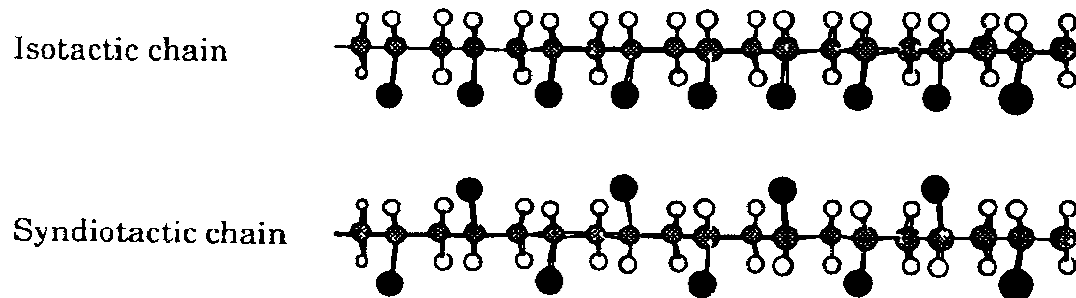


Figure 1.4 Regular tactic chains of $[-\text{CH}_2-\text{CHX}-]_n$, where X is indicated by a filled circle.

Dyads (2가지) : m (meso)
r (racemic)

Triads (3가지) : mm, mr, rr

Tetrads (6가지) : mmm, mmr, mrm, mrr, rmr, rrr

Pentads (10가지)

100% meso sequence : isotactic

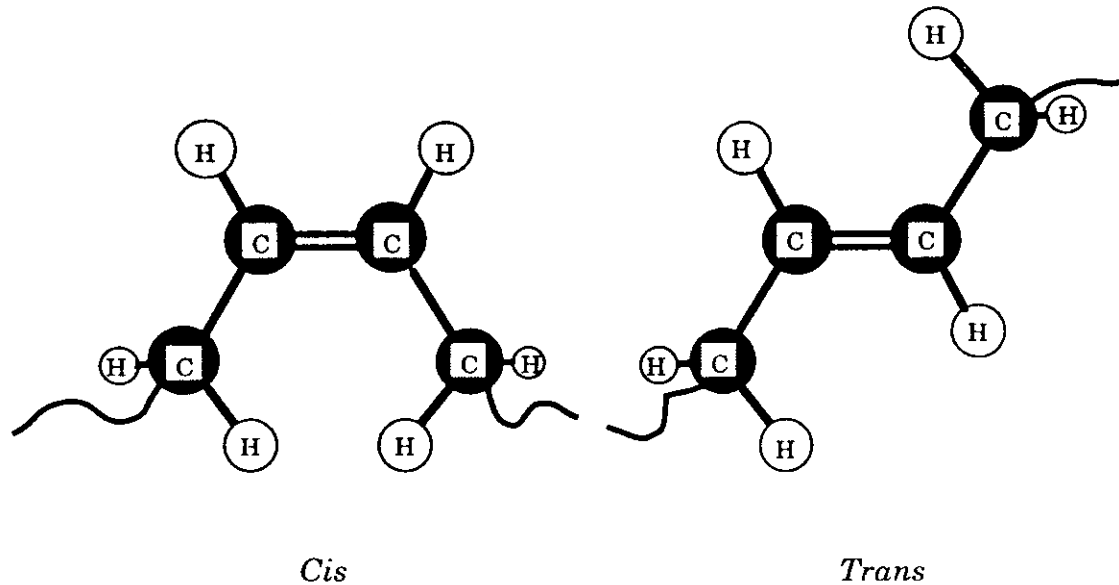
100% racemic sequence : syndiotactic

Polymers with double bonds in the main chain

1,4-polybutadiene : cis & trans

polyisoprene - natural rubber (cis form)

- gutta percha (trans form)

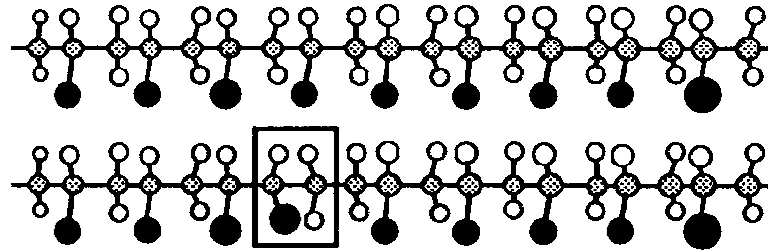


Atactic polymers : never crystallize, and freeze to a glassy structure

Isotactic polymers : crystallize at some temperature

Head-to-tail configuration (head: $-\text{CHX}-$, tail: $-\text{CH}_2-$)

Head-to-head-tail-to-tail configuration



Change of conformation : due to a torsion about single (sigma) bonds
(Trans, Gauche and Gauche' states)

--> Chapter 2에서 고찰.

Source-based nomenclature rules

- poly(A-co-B) : unspecified type
- poly(A-alt-B)
- poly(A-stat-B)
- poly(A-graft-B)
- poly(A-ran-B)

- poly A semicrystalline → poly(A-stat-B) : amorphous
poly B block & graft copolymers
similar properties of homopolymers

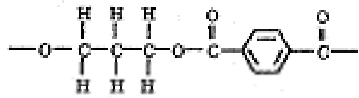
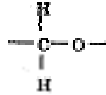

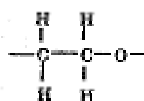

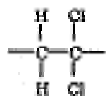



Terpolymers : three different CRUs (A,B,C), ex) ABS

Di-block copolymers (by living polymerization) – compatibilizers

Tri-block copolymers

1.4 Molecular Architecture

- Short-chain branches → reduce crystallinity
- Long-chain branches → affect rheological properties
- Network
- Dendrimer (or hyperbranched polymer) → spherical shapes
melt μ is lower than linear polymer

Polymer name, abbreviation	Constitutional repeating unit	Polymer name, abbreviation	Constitutional repeating unit
Poly(butylene terephthalate), PBTP		Polyoxymethylene, POM	
Polytetrafluoroethylene, PTFE		Polyethyleneoxide, PEO	
Polyamide 6, PA 6		Poly(vinylidene dichloride), PVDC	
Polyamide n, PA n		Poly(vinylidene difluoride), PVDF	
Polyamide 6.10, PA 6.10			

• Familiar polymers: PE, PP, PVC, PS, polybutadiene, polyisoprene, PAN, PMMA, PA6

• **Nomenclature**

structure-based : poly(CRU) - IUPAC name

source-based : poly(monomer) - popular

ex) poly(1-phenylethylene)

polystyrene