How do giant molecules wiggle?

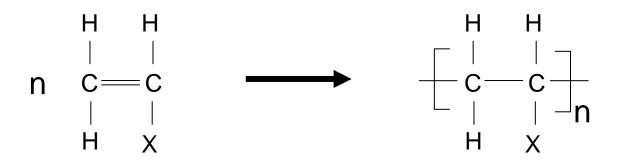
Ashish Lele National Chemical Laboratory

Acknowledgement: Chirag, Omkar, NCL Academy

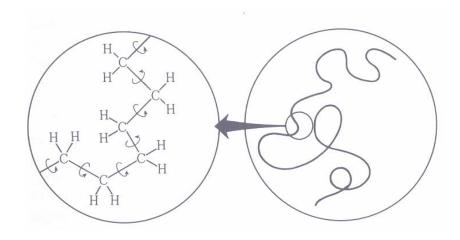
Contents

- Giant molecules and their applications
- Unusual flow behaviour
- Solids, liquids and....
- Wiggling motions

Giant molecules



Polymers OR Macromolecules

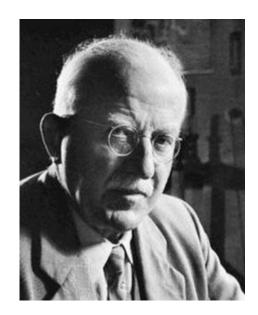


Giant molecules

Molecule	Molecular weight (g/mol)	Molecular size (Å)
H ₂	2	1.5
O_2	32	3.0
CO ₂	44	3.3
Ethylene	28	1.7
Benzene	78	2.8
Fullerene C ₆₀	720	10
Polyethylene	50,000 - 5,000,000	100
Silk	400,000	100
DNA	>106	7300

Long chains?

- Proposed the concept of polymers in 1920.
- Colloidal chemists rejected the idea.



Hermann Staudinger 1881-1965

- Awarded Nobel Prize in Chemistry in 1953.
- Rightfully called the father of polymer chemistry.

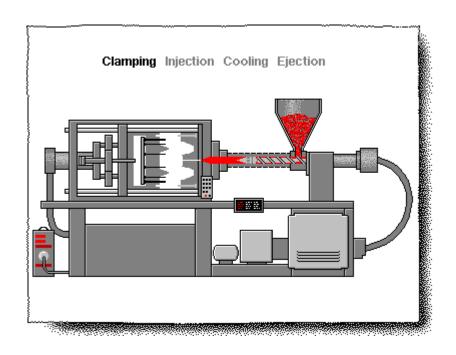
Can we live without them?



Why are they so popular?

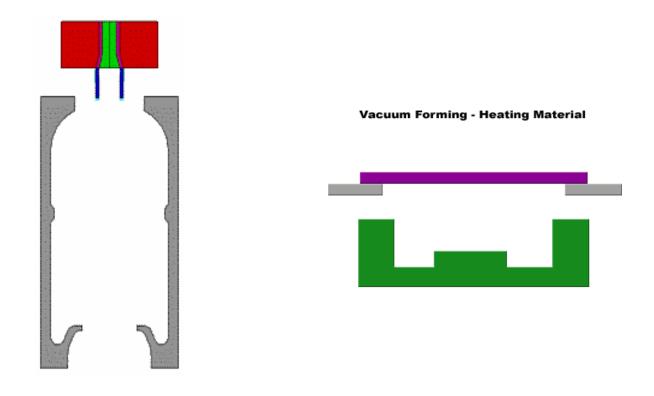
- Excellent properties
- Easy to shape into products
- Cheap
- Reusable
- Good service life
- _

We consumed 7 million tons in 2008!! (Mutha et al, 2006)









Flow behaviour demos...

- Rod climbing
- Extrudate swell
- Melt fracture
- Filament stretching
- Dilatency and yield stress

Is this solid or liquid?



Solids (Elastic)

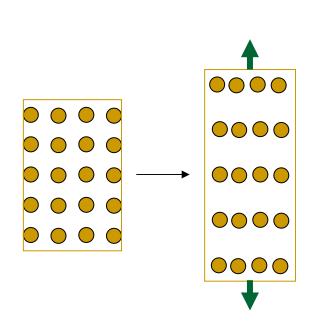
- Recovery (memory)
- Energy storage
- Hooke's law F = -k x



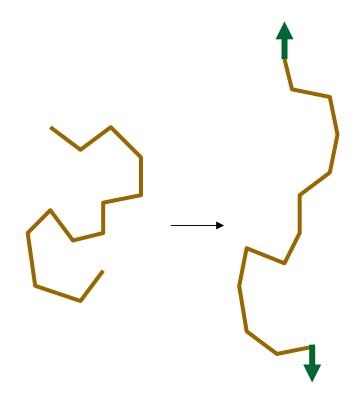
Robert Hooke 1635-1703

Homework: Can you render water elastic?

Molecular origin of elasticity

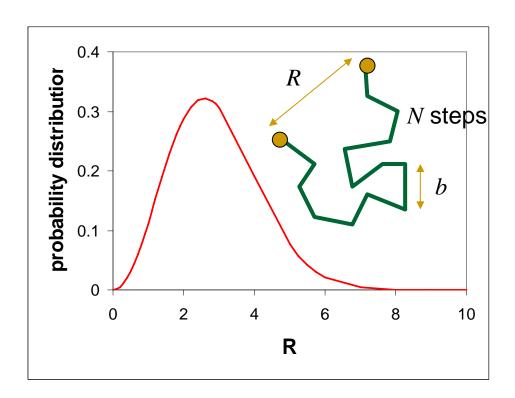


Bond stretching Enthalpic



Bond rotation Entropic

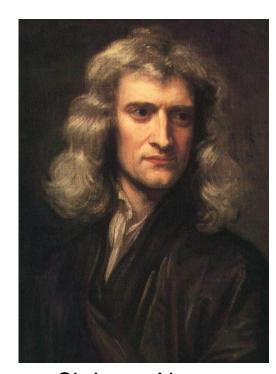
Molecular origin of elasticity



$$F = \frac{3k_B T}{Nb^2} R$$

Liquids (Viscous)

- Zero recovery (no memory)
- Energy dissipation
- Newton's law $F = -\eta A \frac{dv}{dy}$



Sir Isaac Newton 1642-1727

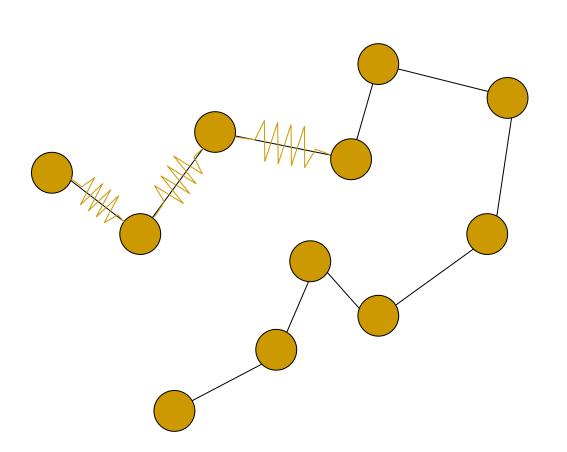
Viscoelasticity

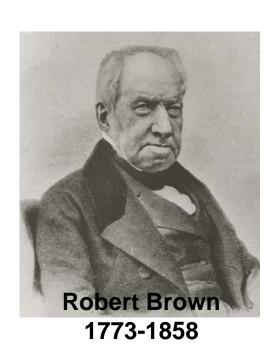
James Clerk Maxwell 1831-1879



- Fading memory
- Short time elastic, long time viscous
- "Mountains flow before the Lord" $De = \frac{\lambda}{t_p}$

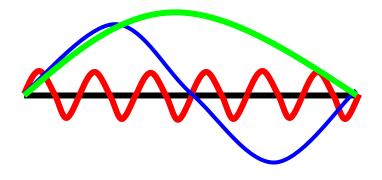
Wiggling in solutions







Wiggling in solutions

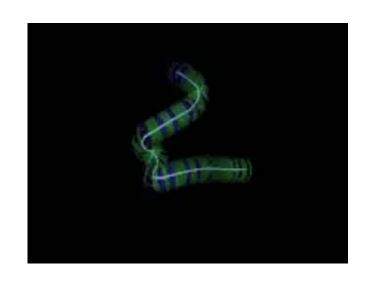


Plucked string of a guitar

Rouse, P.E. Jr., 1953

$$\lambda \approx \frac{b^2 \zeta}{k_B T} N^2$$

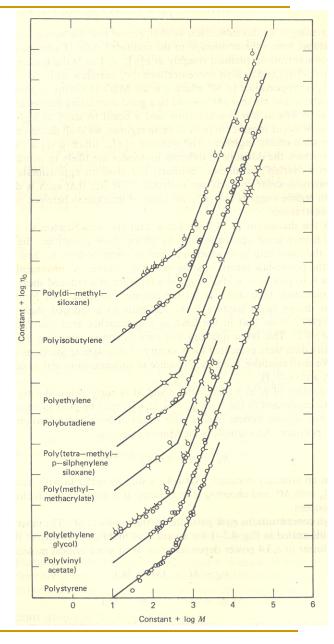
Wiggling in melts





Pierre de Gennes 1932-2007

$$D_c = \frac{k_B T}{N \zeta_{bead}} \qquad \lambda = \frac{L^2}{D_c} \sim N^3$$

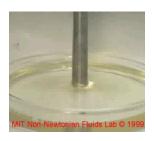


Why are wiggling motions important?

- Choosing the right polymer for an application.
- Choosing the right equipment for a polymer.
- Influence on solidification processes.
- Biological processes.

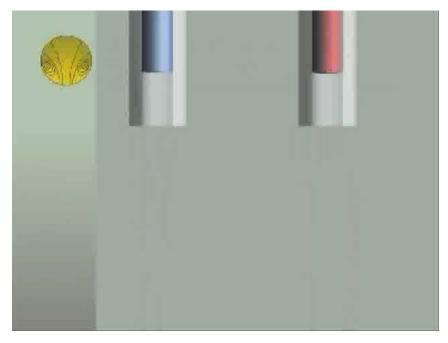
THANK YOU!

Rod climbing



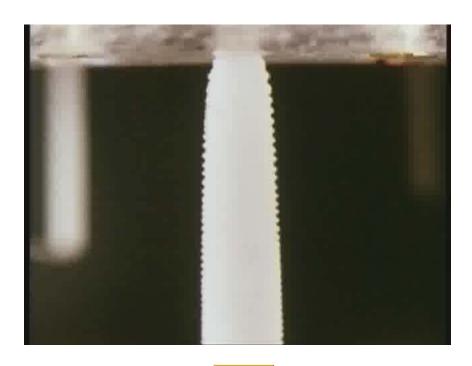


Extrudate swell





Melt fracture





Filament stretching



