



**From nano to macro: Introduction to atomistic
modeling techniques**

IAP 2007

Nanomechanics of hierarchical biological materials

Lecture 6



Department of
Civil & Environmental Engineering
Massachusetts Institute of Technology

Markus J. Buehler



Outline



1. **Introduction to Mechanics of Materials**
Basic concepts of mechanics, stress and strain, deformation, strength and fracture
Monday Jan 8, 09-10:30am
2. **Introduction to Classical Molecular Dynamics**
Introduction into the molecular dynamics simulation; numerical techniques
Tuesday Jan 9, 09-10:30am
3. **Mechanics of Ductile Materials**
Dislocations; crystal structures; deformation of metals
Tuesday Jan 16, 09-10:30am
4. **The Cauchy-Born rule**
Calculation of elastic properties of atomic lattices
Friday Jan 19, 09-10:30am
5. **Dynamic Fracture of Brittle Materials**
Nonlinear elasticity in dynamic fracture, geometric confinement, interfaces
Wednesday Jan 17, 09-10:30am
6. **Mechanics of biological materials**
Monday Jan. 22, 09-10:30am
7. **Introduction to The Problem Set**
Atomistic modeling of fracture of a nanocrystal of copper.
Wednesday Jan 22, 09-10:30am
8. **Size Effects in Deformation of Materials**
Size effects in deformation of materials: Is smaller stronger?
Friday Jan 26, 09-10:30am



Outline and content (Lecture 5)



- **Topic:** Elasticity in biological materials: Entropic versus energetic contributions
- **Examples:** Deformation of collagen, vimentin, ...: Protein mechanics
- **Material covered:** Covalent bonding and models, chemical complexity, reactivity, molecular potentials: CHARMM
- **Important lesson:** Models for bonding in proteins, entropic vs. energetic elasticity
- **Historical perspective:** AFM, single molecule mechanics



- **Very brief review:**

Material covered in last 2-3 lectures



Dislocation nucleation from a crack tip

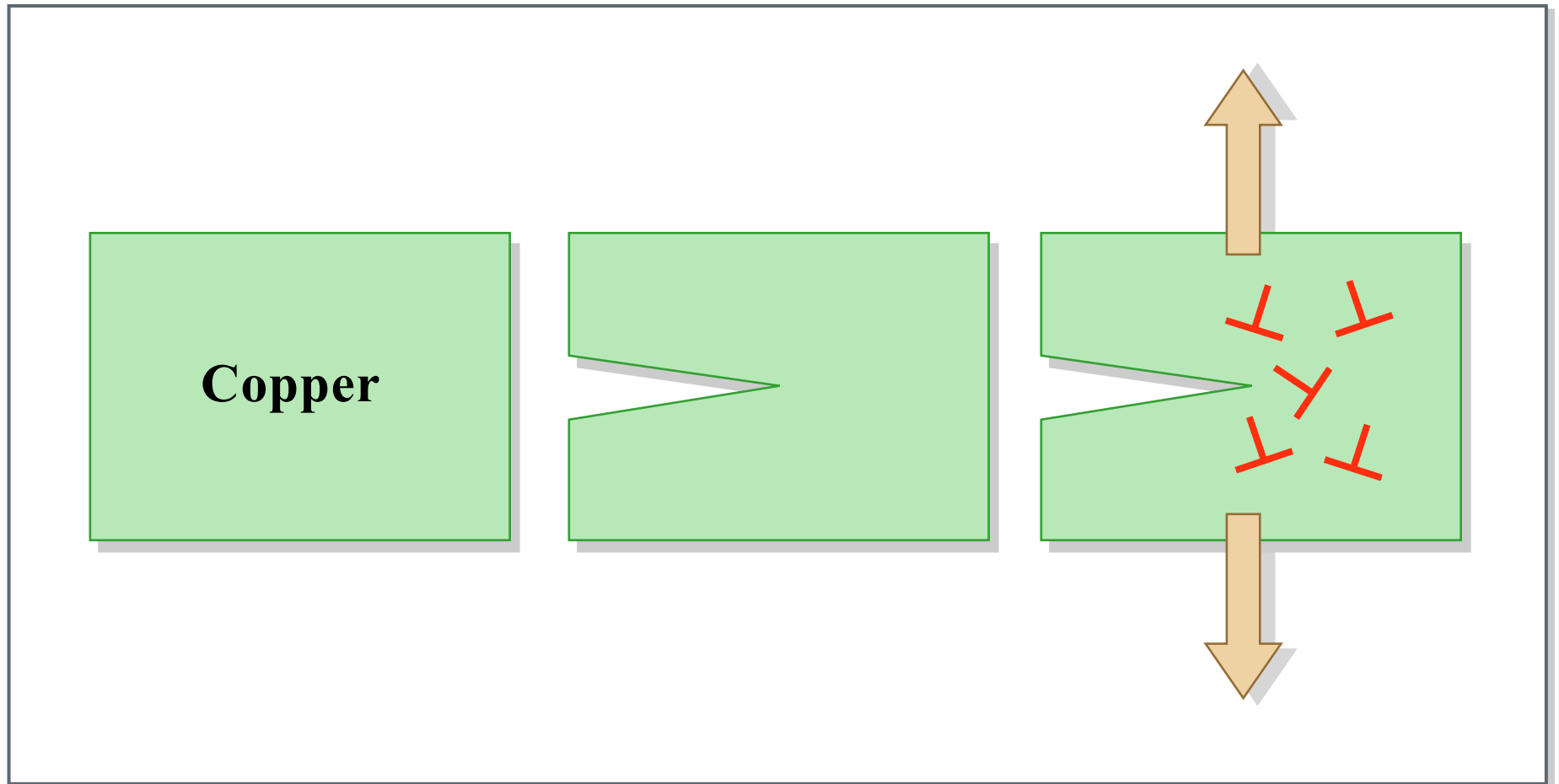


Figure by MIT OCW.

Ductile
vs. brittle
Depends on atomic
behavior at crack tip



Ductile materials are governed by the motion of dislocations: Introduction

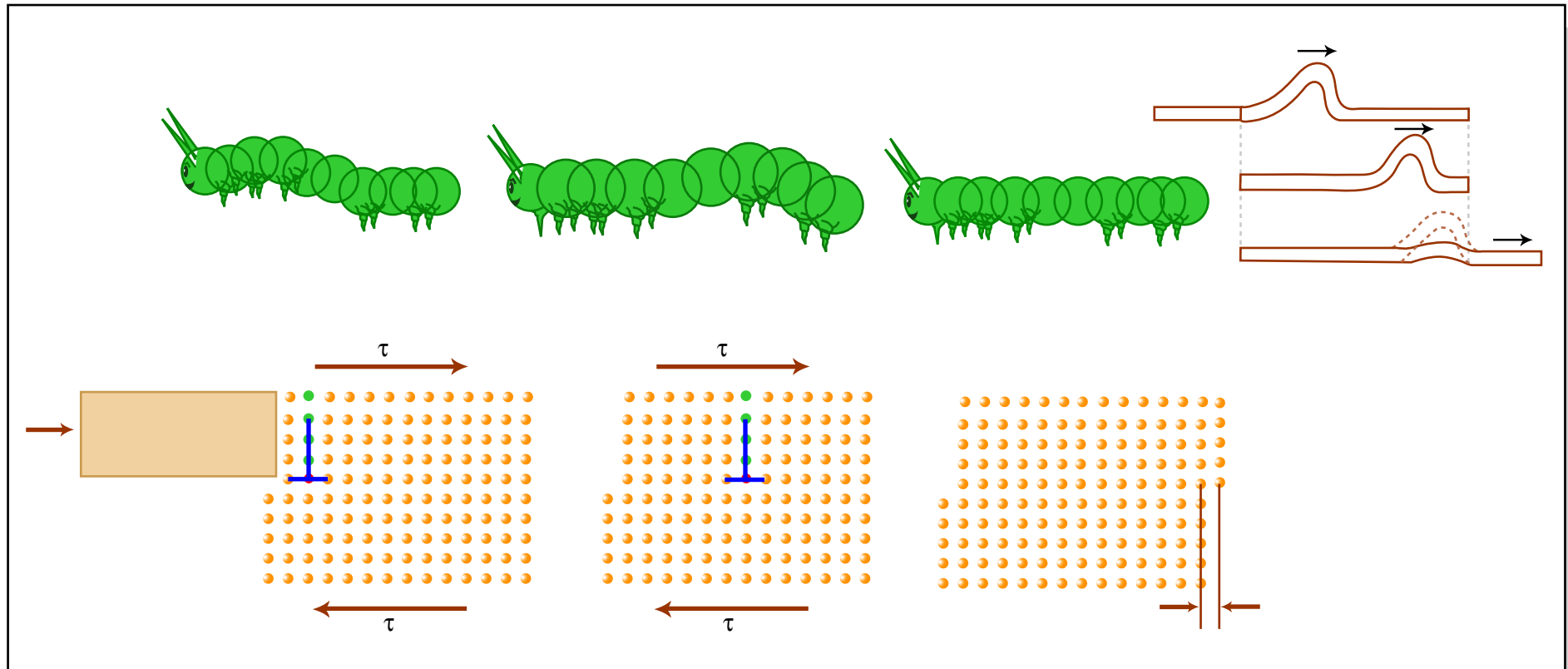


Figure by MIT OCW.

Dislocations are the discrete entities that carry plastic (permanent) deformation; measured by “Burgers vector”



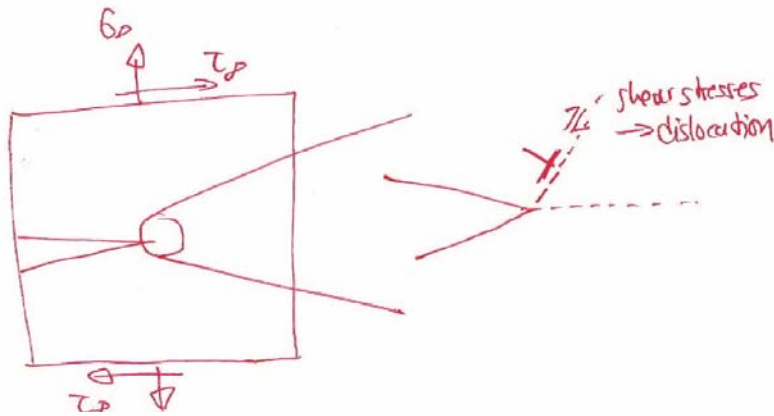
Brittle or ductile?



$$\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{r\theta} \end{Bmatrix} = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \begin{Bmatrix} 1 + \sin^2 \frac{\theta}{2} \\ \cos^2 \frac{\theta}{2} \\ \sin \frac{\theta}{2} \cos \frac{\theta}{2} \end{Bmatrix}$$

Critical conditions for dislocation nucleation / beginning of fracture

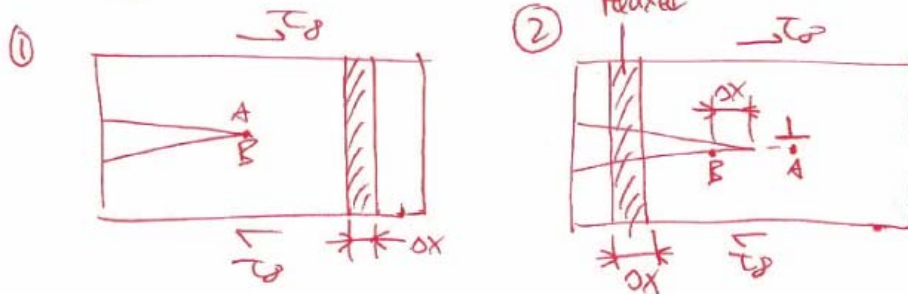
Rice-Thomson model



$$\sigma_\infty = \sqrt{\frac{2b}{a}} \frac{1}{f(\theta)} \frac{\mu}{4\pi(1-\nu)}$$

$$\sigma_\infty \sim \sqrt{\frac{b}{a}} \mu.$$

Rice-Pearls model



$$\tau_{\infty,disl} = \sqrt{\frac{2\gamma_{us}\mu}{H}}$$

$$\tau_{\infty,surf} = \sqrt{\frac{4\gamma_s\mu}{H}}$$

$$\alpha = \frac{\gamma_{us}}{2\gamma_s}$$



Strengthening mechanisms

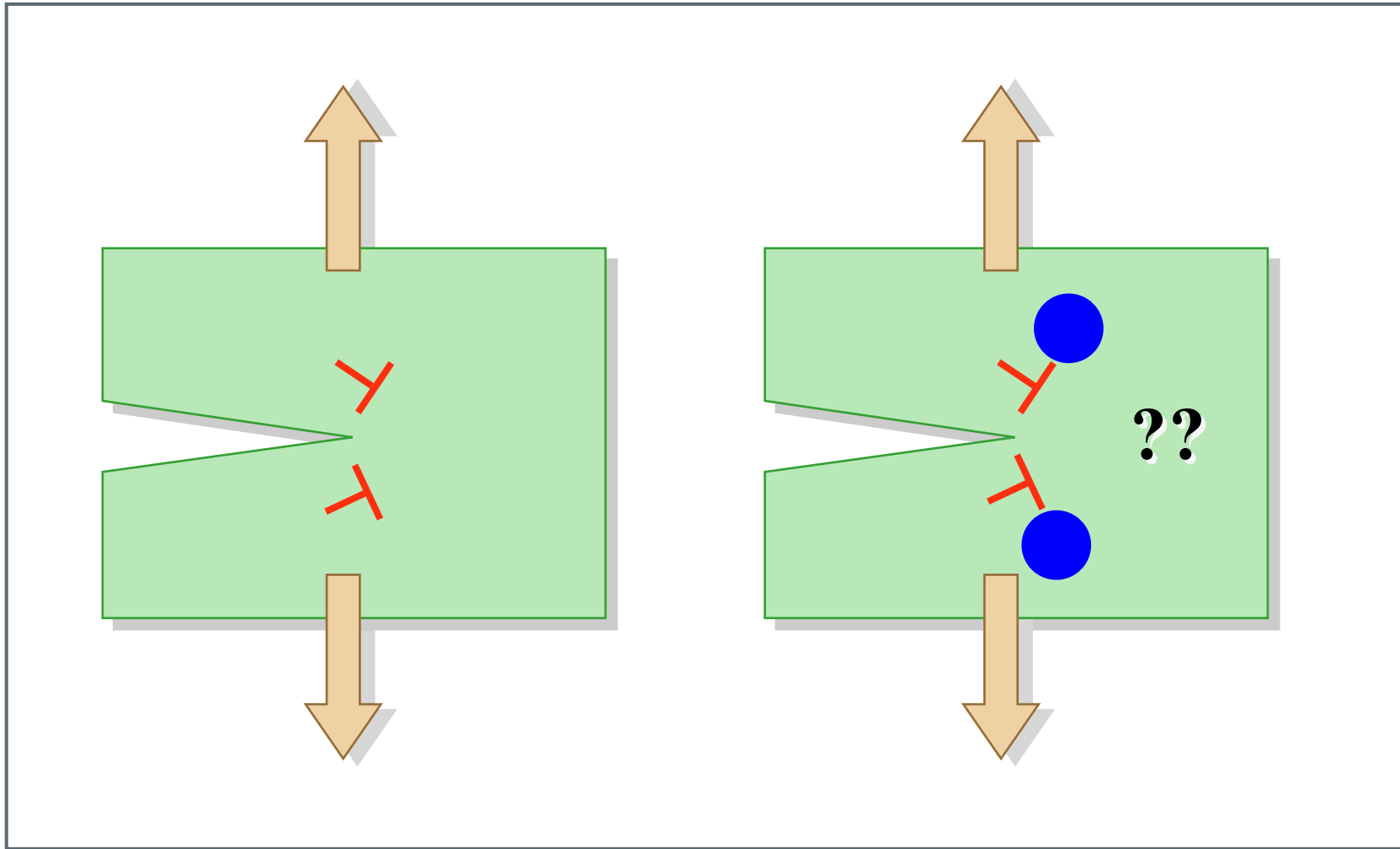
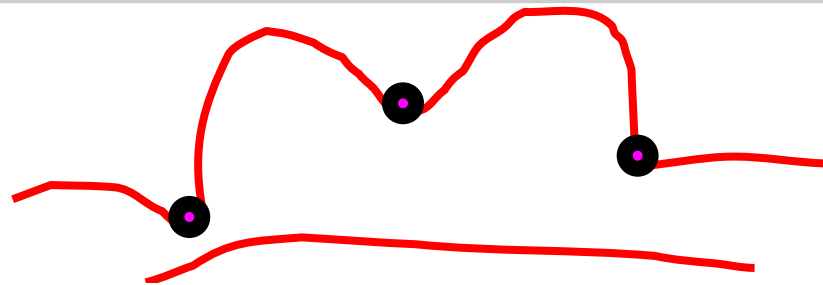


Figure by MIT OCW.





Final sessile structure



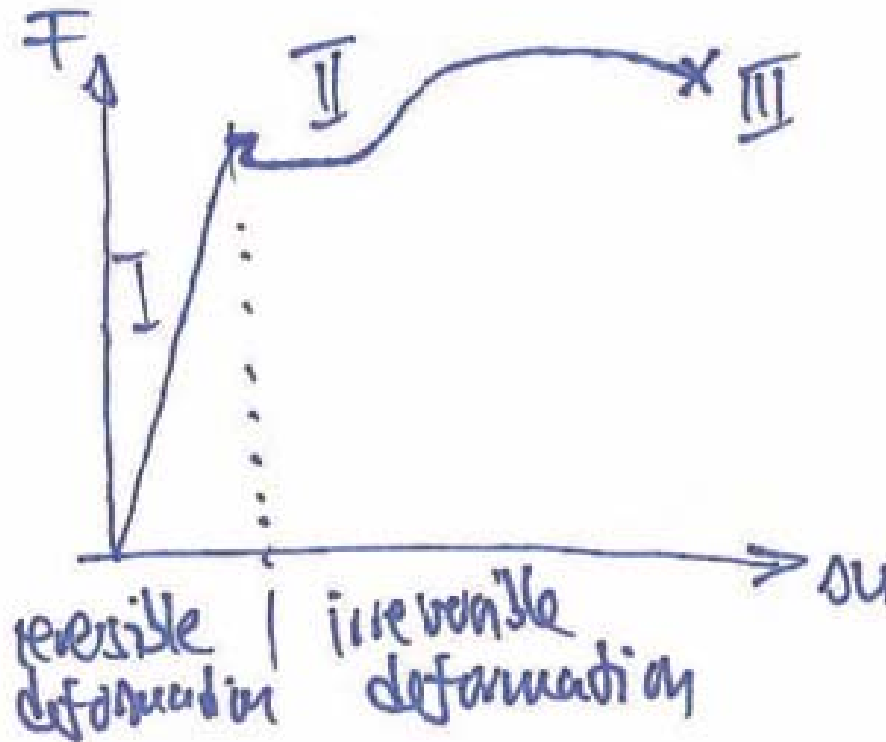
Image removed due to copyright restrictions.

See:

1. Buehler, M. J., et al. "The dynamical complexity of work-hardening: a large scale molecular dynamics situation." *Acta Mechanica Sinica* 21, no. 2 (2005): 103-111.
2. Buehler, M. J., et al. "Atomic plasticity: description and analysis of a one-billion atom simulation of ductile materials failure." *Computer Methods in Applied Mechanics and Engineering* 193, no. 48-51 (2004): 5257-5282.



Energy approach to elasticity



$$F = k_s \Delta u$$



Energy approach to elasticity



1st law of TD

$$\frac{dU}{dt} = \delta W + \delta Q$$

External work rate

$$\delta W = \dot{x}F_e$$

Applied force

2nd law

$$\frac{dS}{dt} \geq \frac{\delta Q}{T}$$

Change in entropy is always greater or equal than the entropy supplied in form of heat; difference is due to internal dissipation

$$\frac{dD}{dt} = T \frac{dS}{dt} - \delta Q \geq 0$$

Dissipation rate

$$\delta Q = dU/dt - \delta W$$

Dissipation rate after consider 1st law of TD:

$$\frac{dD}{dt} = \delta W - \frac{d}{dt} (U - TS)$$

Dissipation rate=External work rate
-change in usable energy U-TS`

$F = U - TS$ is defined as free energy or Helmholtz energy,



Energy approach to elasticity



Elastic deformation (no dissipation by definition):

$$\frac{dD}{dt} = 0$$

$$\delta W - \frac{dF}{dt} = 0 \quad \text{Assume only internal energy change}$$

$$\delta W = \dot{x}F_e$$

$$\dot{x} \left(F_e - \frac{dF}{dx} \right) = 0.$$

Expand equation
 $dU/dt = dU/dx \, dx/dt$

$$\dot{x}F_e - \frac{dF}{dx} \frac{dx}{dt} = 0$$

Therefore: If applied force equals change in free energy of the system, have elastic deformation`

$$F_e = \frac{dF}{dx} \quad F_e = \frac{dU}{dx}$$

With strain energy density: $\Psi = F/V \quad \Psi = U/V$

$$\sigma_{ij} = \frac{d\Psi}{d\varepsilon_{ij}} \quad c_{ijkl} = \frac{d^2\Psi}{d\varepsilon_{ij}d\varepsilon_{kl}}$$



Cauchy-Born rule



- Idea: Use thermodynamic approach to develop expression of elasticity of a atomic microstructure, provided a specific interatomic potential
- Assuming locally homogeneous deformation, take a unit cell representation (typically PBCs) and express free energy density as a function of strain tensor
- This provides direct link between interatomic potential and constitutive behavior
- For example: FCC crystal and EAM potential – can calculate elastic properties directly



Cauchy-Born rule



- Idea: Express elastic energy (strain energy density) for a atomistic representative volume element as a function of macroscopic applied strain

$$\Phi = \frac{1}{\Omega_0} \int_{\Omega_0^*} U(l) D_{\Omega} d\Omega \quad U(l) \text{ a function of deformation gradient}$$

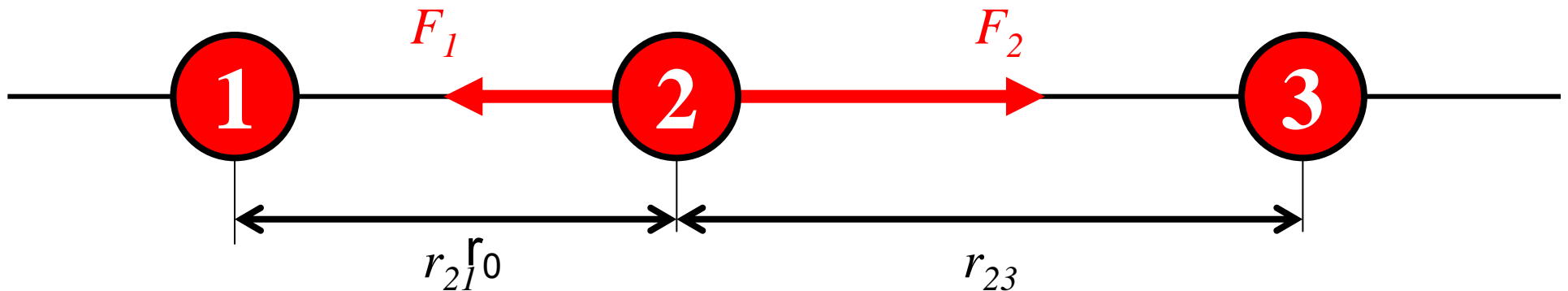
- D_{Ω} : Mapping function, e.g. $D(l_0, \theta, \phi) = \delta_D(l_0 - l_0^*) D_{\theta\phi}(\theta, \phi)$
- Impose macroscopic deformation gradient on atomistic volume element, then calculate atomic stress – this corresponds to the macroscopic stress
- Strictly valid only far away from defects in periodic lattice (homogeneous deformation, perfect lattice, amorphous solid-average)
- Allows direct link of potential to macroscopic continuum elasticity



1D example: Cauchy-Born rule



- Impose homogeneous strain field on 1D string of atoms
- Then get $\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$ from that



$$\Phi(\varepsilon) = \frac{1}{r_0 \cdot D} \phi(r) = \frac{1}{r_0 \cdot D} \phi((1 + \varepsilon) \cdot r_0) \quad \text{Strain energy density function}$$

$$r_0 \cdot D \quad \text{Atomic volume}$$



-
- Detailed write-up on 1D / 2D Cauchy-Born rule is included on line

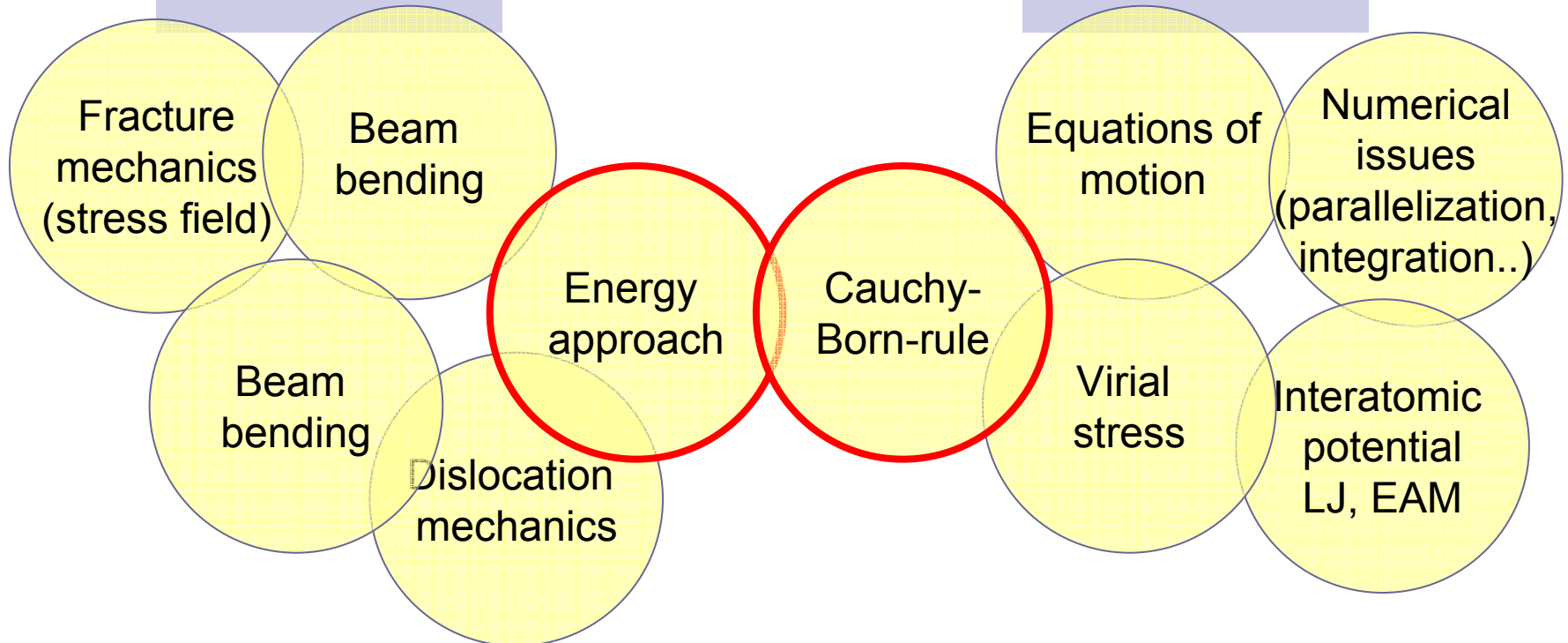


Review



**Continuum
mechanics**
 $\text{div } \sigma = -\rho g$

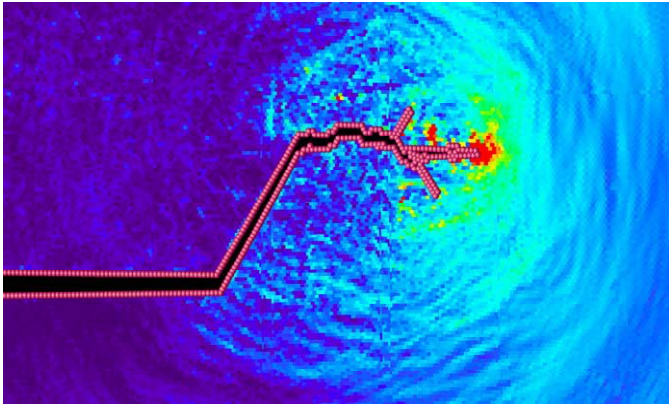
**Atomistic
modeling**
 $F=ma$



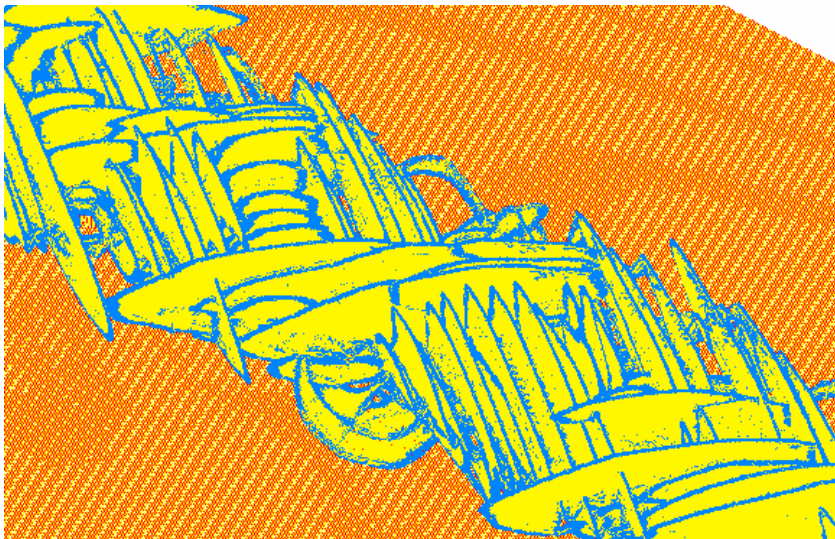


■ Mechanics of biological materials

(a) Brittle



(b) Ductile



Images removed due to copyright restrictions.



Example: Stretching of proteins



Images removed due to copyright restrictions.

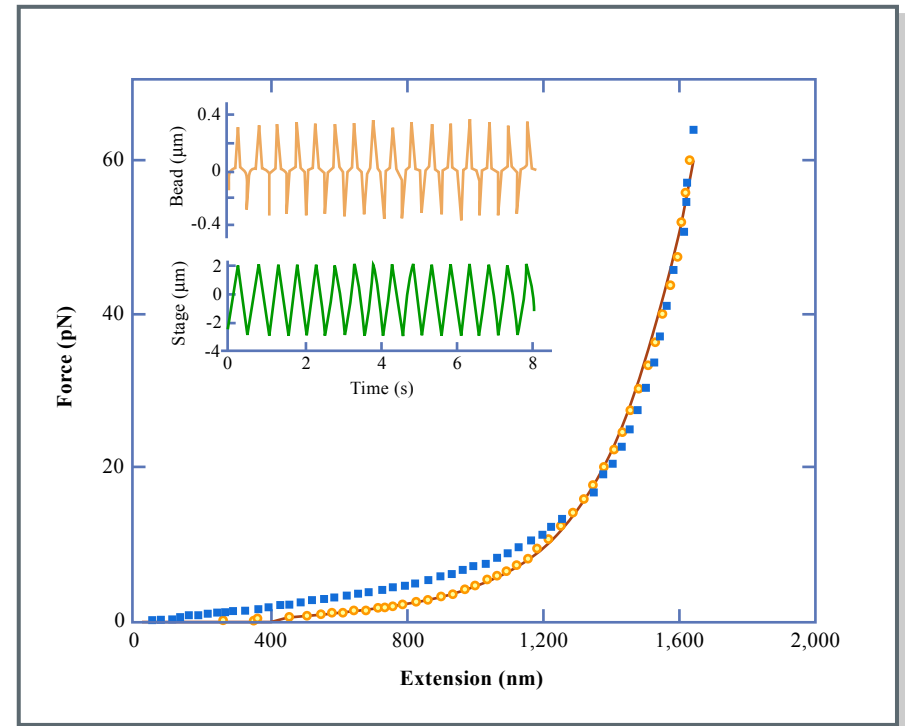


Figure by MIT OCW.

Physical origin?
Soft matter
Nonlinear
Viscoelastic (time dependent)

...



Additional Reading



Book Chapters

T. Courtney, Mechanical Behavior of Materials
Chapter 2

D.I. Bower
An Introduction to Polymer Physics (Chapter 6 [+7 and 3])

D. Boal
Mechanics of the Cell (Chapters 1+2)

D. Whitford
Proteins – Structures and Function (Chapters 1-4)



- Interactions between atoms, molecules and/or particles govern the elastic response of materials
- For a fundamental understanding of elasticity, need to consider atomic bonding (chemistry or quantum mechanics)
- Elastic response is governed by change of free energy as a function of deformation (yields stress versus strain); second derivative of free energy with respect to strain yields Young's modulus

$$F(T, V) = U - TS$$

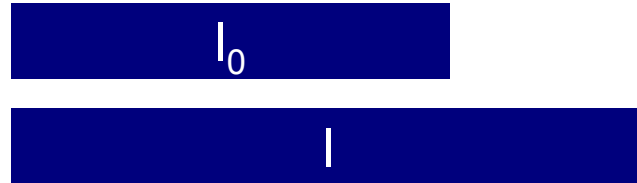
- Polymers
- Biological structures and materials (proteins, DNA, ...)



Extension ratios: Large-strain deformation



$$\epsilon_{ii} = \frac{\partial u_i}{\partial x_i}$$



Extension ratio
 $\lambda = l / l_0$

$$\lambda_i = 1 + \Delta_i$$

$$\epsilon_{ii} = \epsilon_i = \Delta_i$$

In small-strain elasticity

$$\lambda_i^2 = 1 + 2\Delta_i + \cancel{\Delta_i^2}^0 \quad \Delta_i \rightarrow 0 \quad \text{Leads to (small strains)}$$

$$\lambda_i^2 = 1 + 2\Delta_i$$

λ_i Extension ratios in three directions; pure tensile stress state (directions of principal stress)



Strain energy functions



- Phenomenological theory that uses the concept of strain-energy functions

$$U = f(\lambda_i)$$

- Shear strains are assumed to be zero (coordinate system of principal stresses)
- U is (physically) **not** equivalent to the thermodynamic internal energy function; instead it is a function that maps changes in entropy and internal energy into a mathematical function (phenomenological model) – **free energy density!**
- **Examples:** Rivlin, Neo-Hook, ...



Example: Neo-Hookean Solid



$$U = C(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3)$$

Express “strain energy density” as a function of extension ratios λ_i

C is a constant (parameter) that is related to the Young’s modulus (will be derived later)

The SED function is used to calculate the stress for a given deformation state

(note: 2nd derivatives=modulus=not constant!!)



Uniaxial deformation



Incompressible (retain volume during deformation)

$$U = C(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3)$$

Orthogonal to pulling direction:

$$\sigma_1 = \sigma_2 = 0 \quad \sigma_3 = \sigma$$

$$\underbrace{\lambda_1 \lambda_2 \lambda_3 = 1 \quad \lambda_1 = \lambda_2 \quad \lambda_3 = \lambda}_{\lambda_3 = \lambda_2 = 1/\sqrt{\lambda}}$$



→ λ_3

$$U = C(\lambda^2 + 2/\lambda - 3) \text{ for uniaxial tension}$$

$$dU / d\lambda = 2C(\lambda - 1/\lambda^2) = \sigma$$



Reduction to small-strain elasticity



Then, the relation between extension ratio and stress can be written as

$$\sigma = 2C(\lambda^2 - 1/\lambda)$$

Consider the nominal stress force/unit area of the undeformed medium:

$$\sigma = 2C(\lambda - 1/\lambda^2) \quad \text{For small strains: } \lambda_i = 1 + \varepsilon_i$$

$$\sigma = 2C((1 + \varepsilon)^2 - 1/(1 + \varepsilon)) \approx 2C[\overset{3}{1} + \cancel{2}\varepsilon - (\cancel{1} - \cancel{\varepsilon}) + O(0)]$$

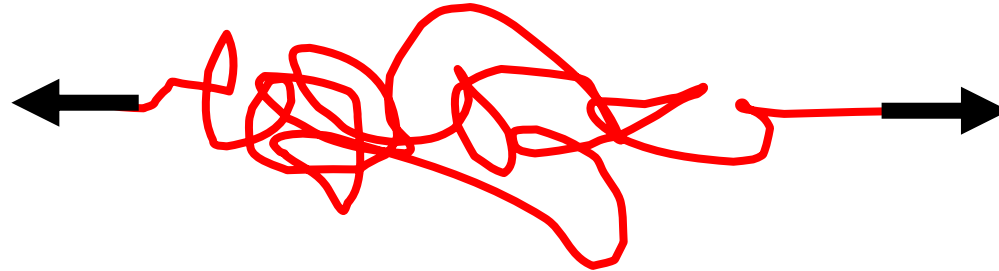
$$\sigma = 6C\varepsilon = E\varepsilon$$

Hooke's law (*linear* elasticity)

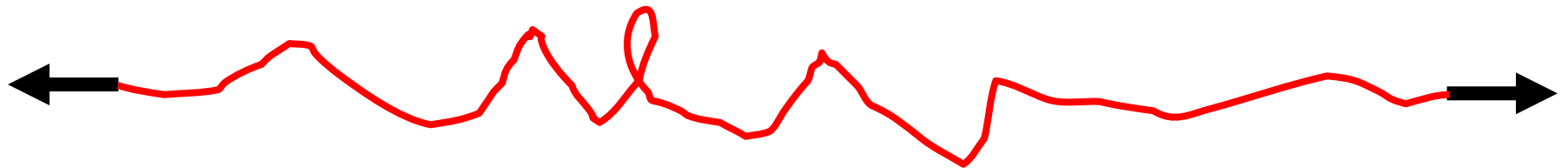
$$C = E / 6$$



Entropic change as a function of stretch



High entropy



Low entropy



Entropic change as a function of stretch

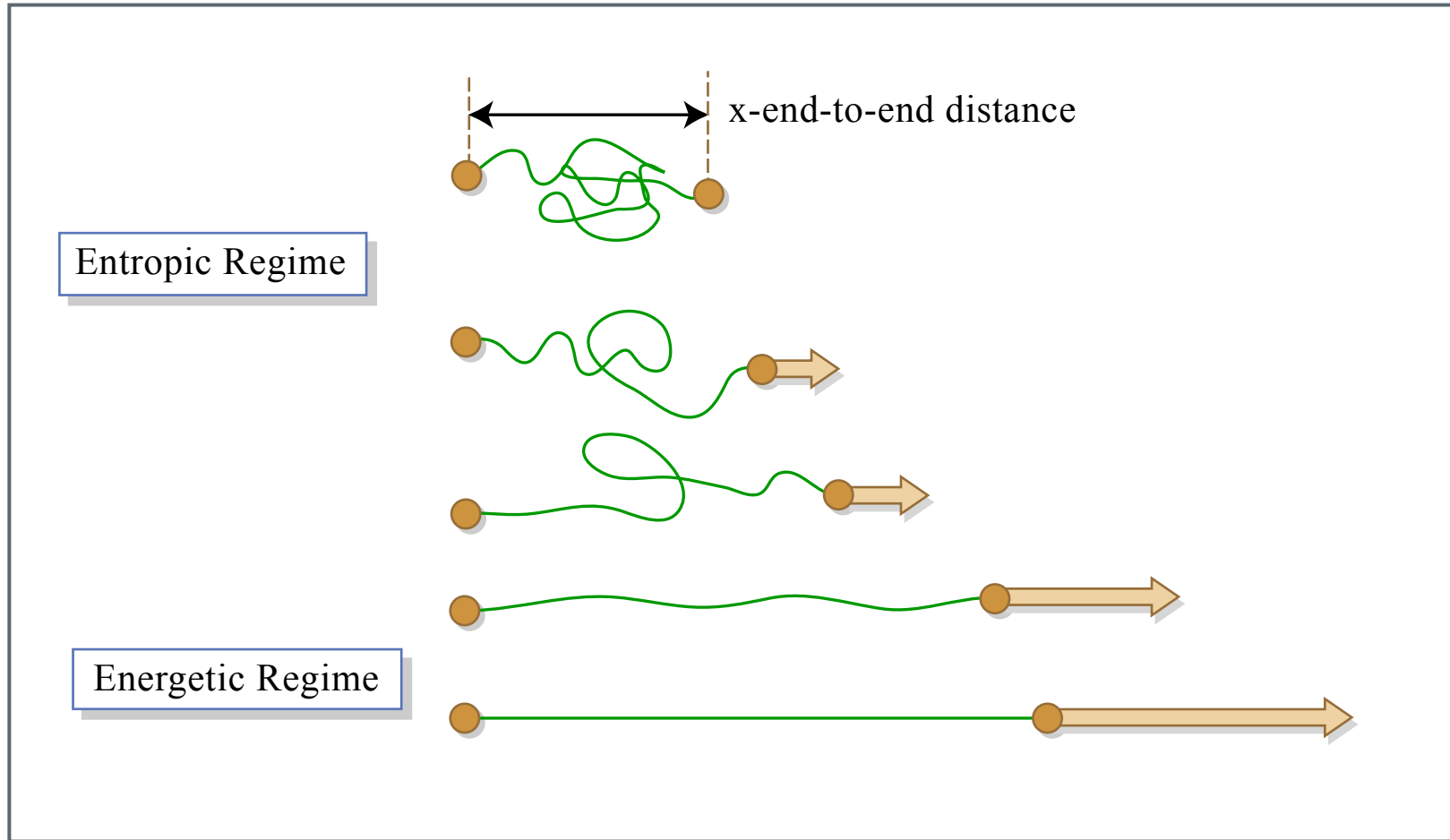


Figure by MIT OCW.



- Based on the assumption that the rubber entropy S can be calculated in terms of

$$\lambda = l / l_0$$

- For example, it can be shown that

$$U = C(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3) \quad C = E / 6$$

$$\sigma_n = C(\lambda - 1 / \lambda^2)$$

This is the result for a neo-Hookean solid



Note: No change in elastic energy of molecules

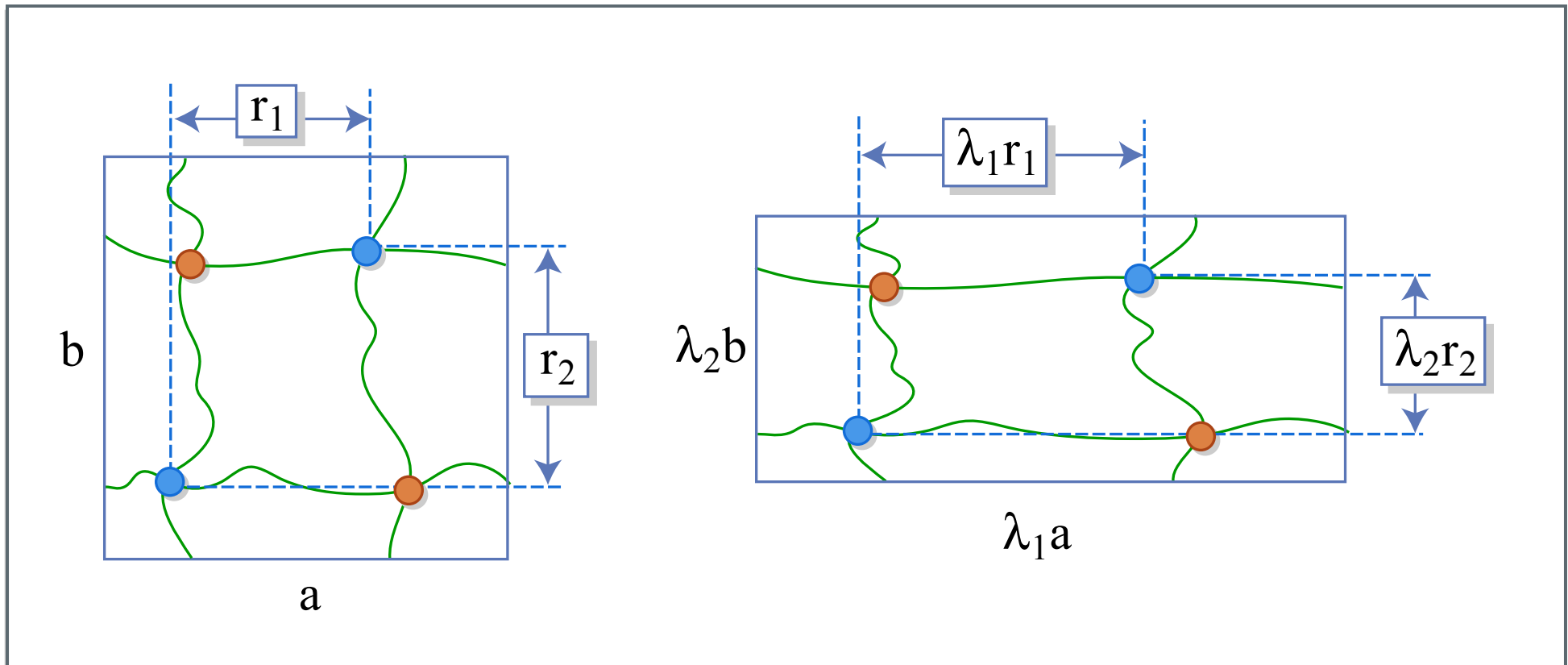


Figure by MIT OCW.

Needed to understand elasticity: Expression of free energy as a function of the applied strain!

Here: Entropic elasticity – therefore change in entropy



Single freely jointed chain

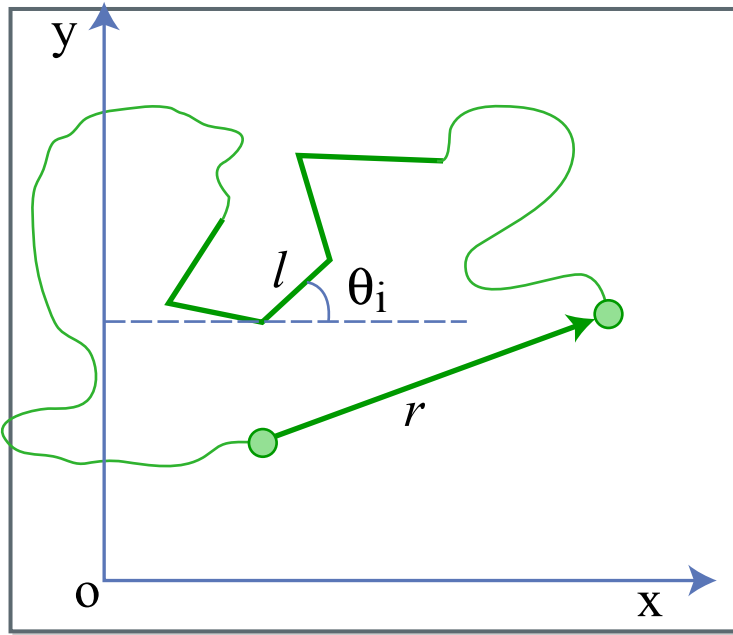


Figure by MIT OCW.

$$S = c - kb^2 r^2$$

$$b^2 = \frac{3}{2nl^2}$$

Total length: $nl=L$

$r^2 = \langle r_b^2 \rangle = n \cdot l^2$ RMS length of the chain (no force applied)

$\sqrt{n} \cdot l \rightarrow nl$ Maximum extension due to force

Physical meaning of l : Length at which molecular bending is uncorrelated



Entropic elasticity: Derivation



Freely jointed Gaussian chain with n links and length l each
(same for all chains in rubber)

$$S = c - kb^2 r^2 \quad \text{where} \quad b^2 = \frac{3}{2nl^2} \quad r \quad \begin{array}{l} \text{end-to-end} \\ \text{distance of} \\ \text{chain} \end{array}$$

$$\Delta S = -kb^2 \sum_{N_b} (\lambda_1^2 - 1)x^2 + (\lambda_2^2 - 1)y^2 + (\lambda_3^2 - 1)z^2$$

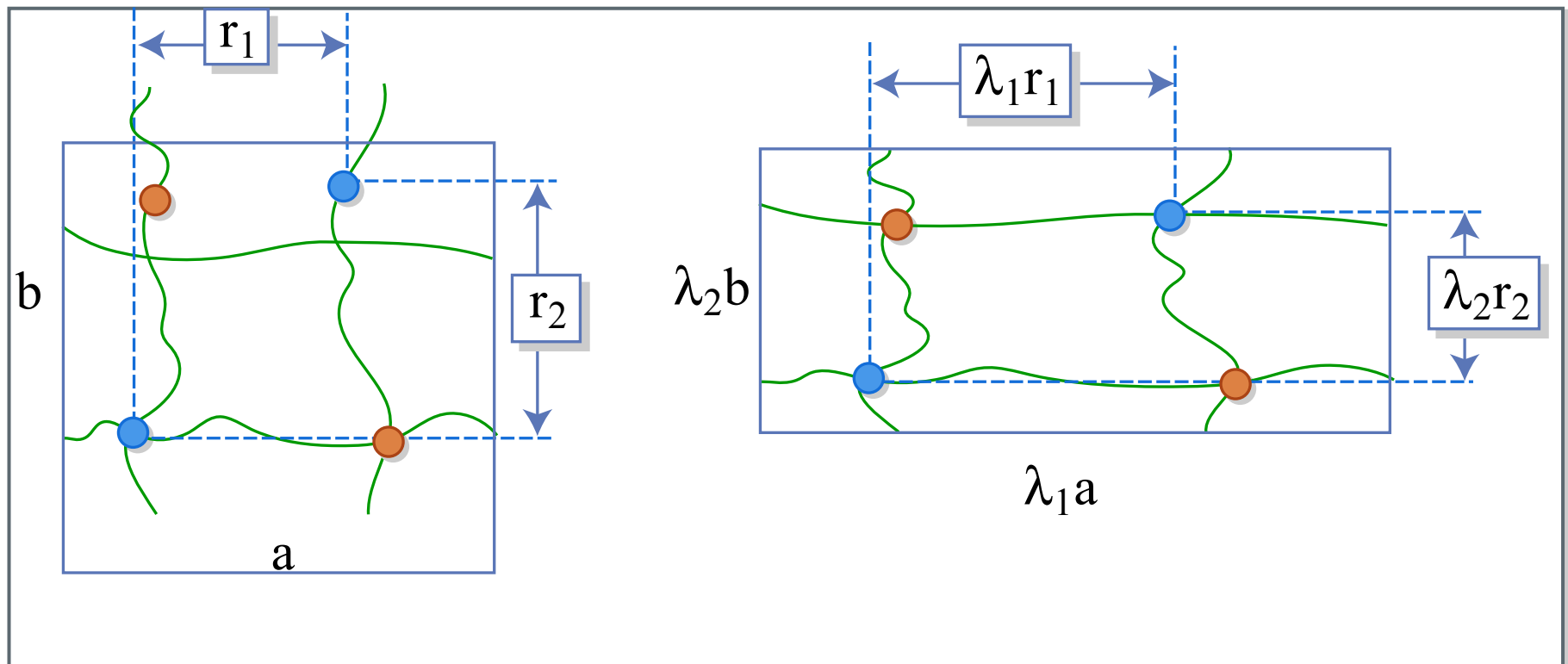


Figure by MIT OCW.



$$\Delta S = -kb^2 \sum_{N_b} (\lambda_1^2 - 1)x^2 + (\lambda_2^2 - 1)y^2 + (\lambda_3^2 - 1)z^2$$

$$\Delta S = -kb^2 N_b \left[(\lambda_1^2 - 1) \langle x^2 \rangle + (\lambda_2^2 - 1) \langle y^2 \rangle + (\lambda_3^2 - 1) \langle z^2 \rangle \right]$$

$\langle \dots \rangle$ Average values over all N_b chains
– need multiply by N_b to get total energy

Isotropic solid: End-to-end distances of the N_b chains are directed equally in all directions; therefore

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3} \langle r_b^2 \rangle$$

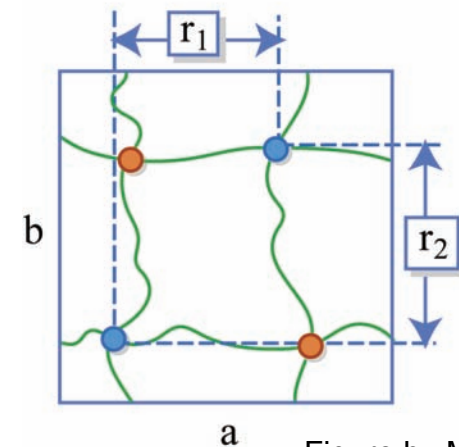


Figure by MIT OCW.



Entropic elasticity: Derivation



The length $\langle r_b^2 \rangle$ in the unstressed state is equal to the mean square length of totally free chains.

It can be shown that

$$r_{RMS} = \sqrt{n} \cdot l = \sqrt{\langle r_b^2 \rangle}$$
$$\langle r_b^2 \rangle = n \cdot l^2$$

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3} n \cdot l^2 = \frac{1}{2b^2}$$

$$\Delta S = -kN_b / 2 \left[(\lambda_1^2 - 1) + (\lambda_2^2 - 1) + (\lambda_3^2 - 1) \right] \quad \text{No explicit dep. on } b \text{ any more}$$

$$U = -T\Delta S = \frac{1}{2} N_b kT (\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3) \quad C = E / 6$$

$$U = C (\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3) \quad \sigma = (E / 3) (\lambda^2 - 1 / \lambda)$$



For SED: *Free energy density*

Young's modulus $U = -T\Delta S = \frac{1}{2} N_b kT (\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3)$

$C = E / 6$

Predictions:

$$E = 3N^*kT \quad N^* = N_b / V$$

Stiffness is proportional to temperature

$$E \sim T$$

Stiffness is proportional to degree of cross-linking (for ideal network, N^* equals twice the cross-link density)

$$E \sim N^*$$



Summary



- Developed rigorous link extension ratio and elastic properties of rubber-like materials
- Based on statistical theory and by considering changes in entropy due to deformation, arrived at an expression for the Neo-Hookeian solid
- This enables to link cross-linking density and temperature with Young's modulus

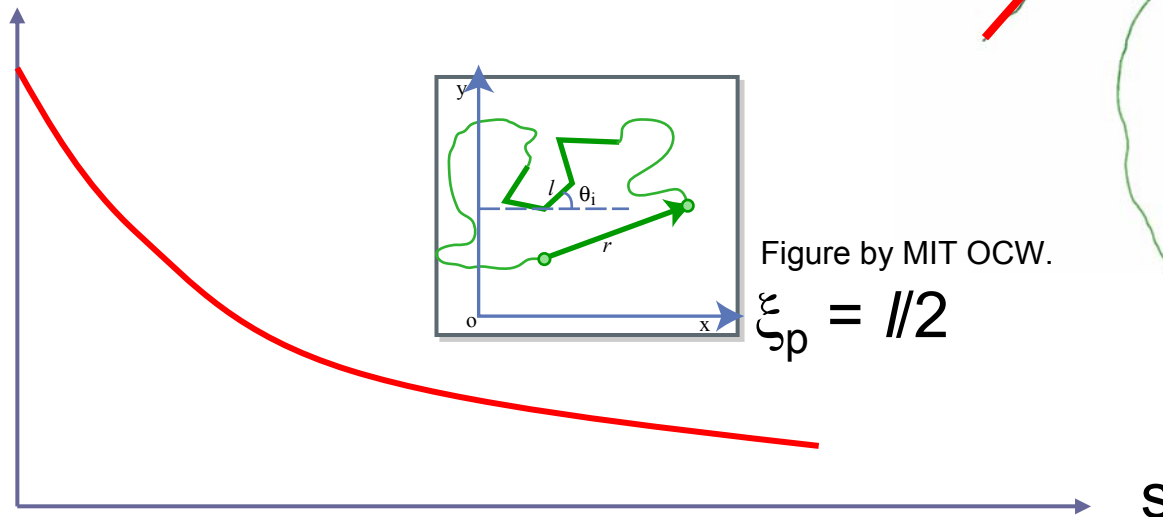


Persistence length



$$\langle \mathbf{t}(s) \cdot \mathbf{t}(s') \rangle = e^{-|s-s'| / \xi_p}$$

$\mathbf{t}(s)$ tangent slope



The length at which a filament is capable of bending significantly in independent directions, at a given temperature.

This is defined by a autocorrelation function which gives the characteristic distance along the contour over which the tangent vectors $\mathbf{t}(s)$ become uncorrelated

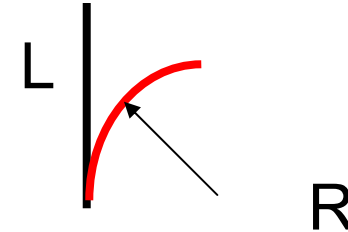


Persistence length: Illustration



- Bending deformation (R=radius, EI=flexural rigidity of the rod)
- energy

$$E_{bend} = EI \frac{L}{2R^2}$$



- Thermal (kinetic) energy per molecule (kinetic theory of gases)
- energy

$$E_{kin,mol} = \frac{3}{2} kT$$

- Example: $kT \sim 4E-21$ J at room temperature

- Persistence length is defined as $\xi_p = \frac{EI}{kT}$

(unit: length)



Contour length of molecules



- The contour length of a molecule is the total length in the stretched configuration, denoted as L

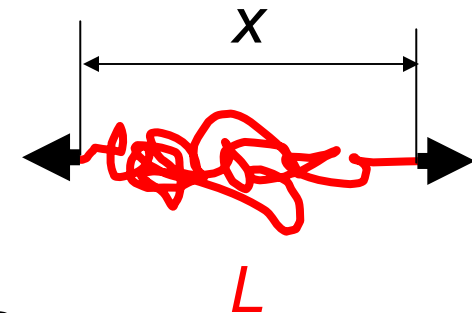
- When $L \ll \xi_p$

a filament appears relatively straight.

- When $L \gg \xi_p$

a filament adopts more convoluted shapes

No energetic interactions!



- To pull a highly convoluted molecule apart ($L \gg \xi_p$), a force is necessary; define effective spring constant

$$k_{sp} = \frac{3kT}{2L\xi_p}$$

$$F \sim k_{sp}x$$

$$x \ll L$$



Worm-like chain model



Freely-jointed rigid rods

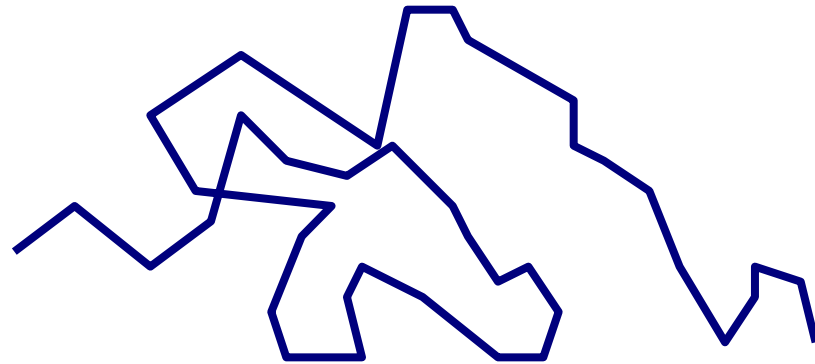
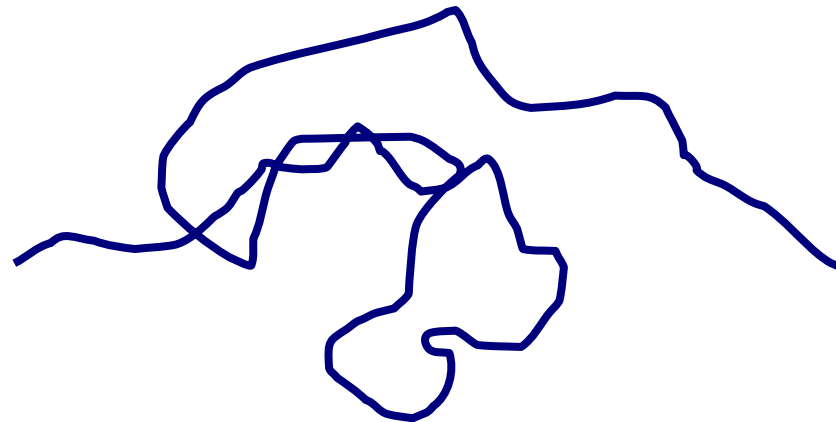


Image removed due to copyright restrictions.

Continuously flexible ropes



Worm like chain model



Worm-like chain model



- This spring constant is only valid for small deformations from a highly convoluted molecule, with length far from its contour length

$$x \ll L$$

- A more accurate model (without derivation) is the Worm-like chain model (WLC) that can be derived from the Kratky-Porod energy expression (see D. Boal, Ch. 2)
- A numerical, approximate solution of the WLC model:

$$F = \frac{kT}{\xi_p} \left(\frac{1}{4} \frac{1}{(1 - x/L)^2} - \frac{1}{4} + x/L \right)$$



Proteins



- An important building block in biological systems are proteins
- Proteins are made up of amino acids
- 20 amino acids carrying different side groups (R)
- Amino acids linked by the amide bond via condensation
- Proteins have four levels of structural organization: primary, secondary, tertiary and quaternary



Protein structure



- **Primary structure:** Sequence of amino acids

A A S X D X S L V E
V H X X

- **Secondary structure:** Protein secondary structure refers to certain common repeating structures found in proteins. There are two types of secondary structures: alpha-helix and beta-pleated sheet.

- **Tertiary structure:** Tertiary structure is the full 3-dimensional folded structure of the polypeptide chain.

Images removed due to copyright restrictions.

- **Quaternary Structure:** Quaternary structure is only present if there is more than one polypeptide chain. With multiple polypeptide chains, quaternary structure is their interconnections and organization.



20 natural amino acids



Images removed due to copyright restrictions.

Table of amino acid chemical structures.

See similar image:

<http://web.mit.edu/esgbio/www/lm/proteins/aa/aminoacids.gif>.



Hierarchical structure of collagen



Images removed due to copyright restrictions.

Collagen features
hierarchical structure

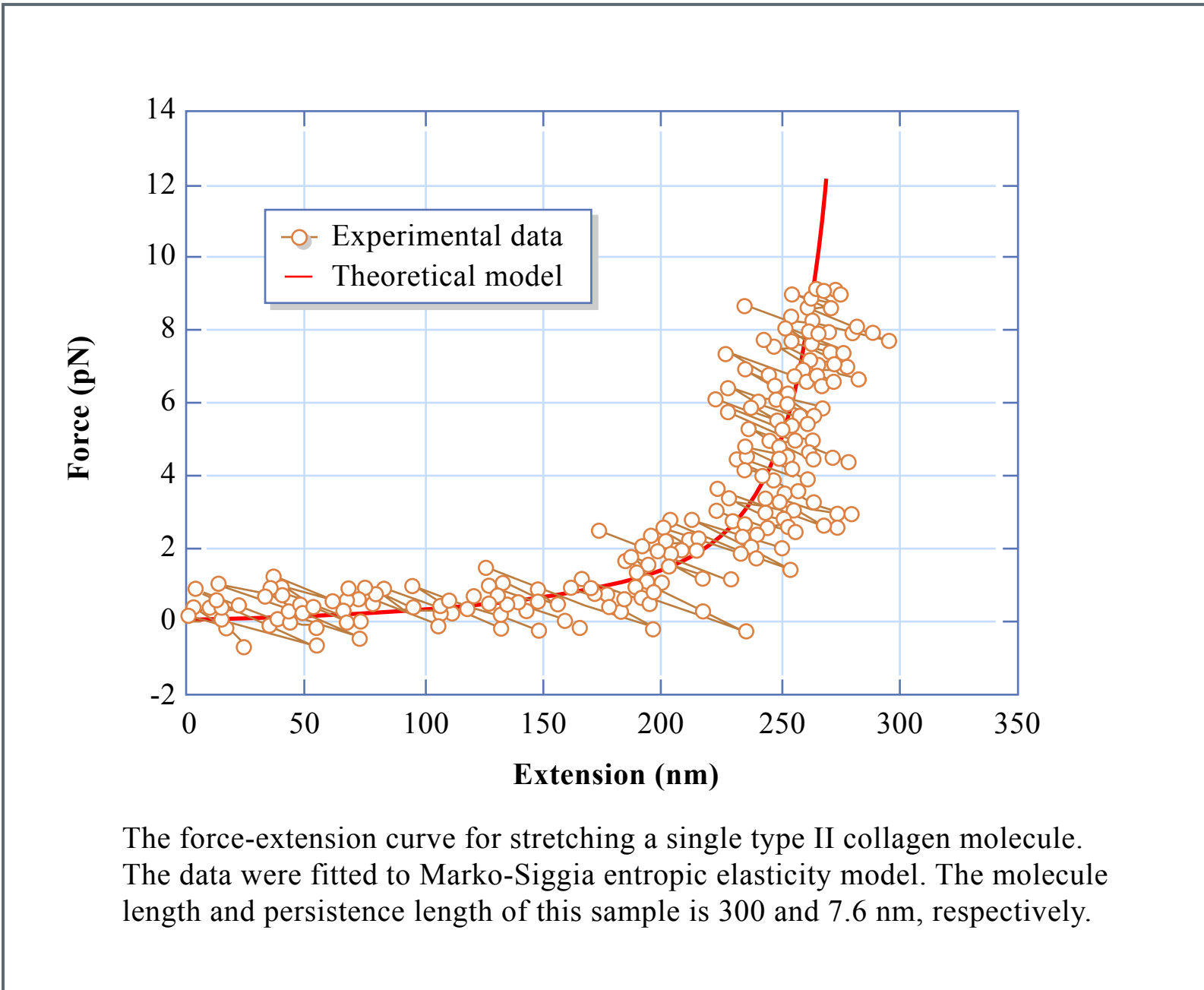
Goal: Understand the
scale-specific
properties and *cross-*
scale interactions

Macroscopic
properties of collagen
depend on the finer
scales

**Material properties
are scale-dependent**



Elasticity of tropocollagen molecules





Modeling organic chemistry



Covalent bonds (directional)
Electrostatic interactions
H-bonds
vdW interactions

Images removed due to copyright restrictions.



Model for covalent bonds

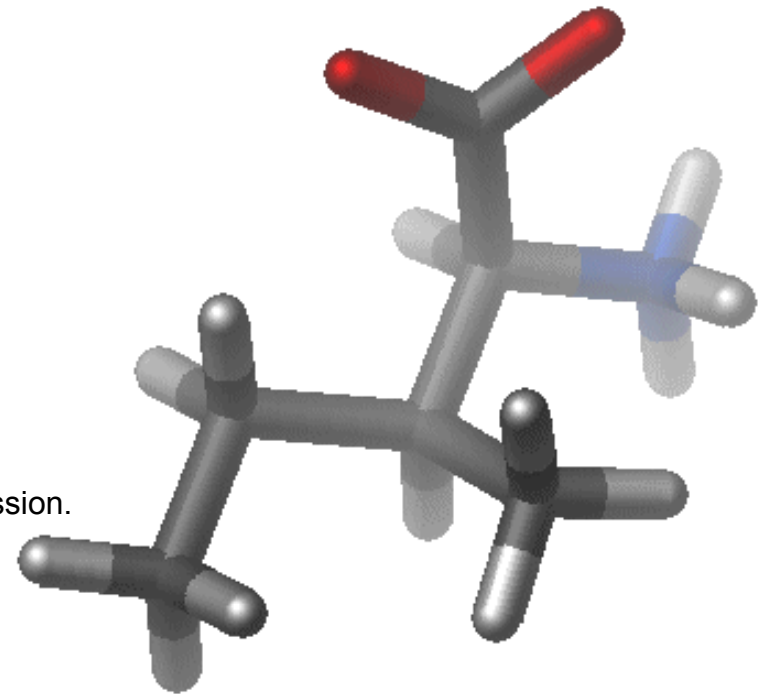


$$V(R) = E_{\text{bonded}} + E_{\text{non-bonded}}$$

$$E_{\text{bonded}} = E_{\text{bond-stretch}} + E_{\text{angle-bend}} + E_{\text{rotate-along-bond}}$$

Bonding between atoms described as combination of various terms, describing the angular, stretching etc. contributions

Courtesy of the EMBnet Education & Training Committee. Used with permission. Images created for the CHARMM tutorial by Dr. Dmitry Kuznetsov (Swiss Institute of Bioinformatics) for the EMBnet Education & Training committee (<http://www.embnet.org>)

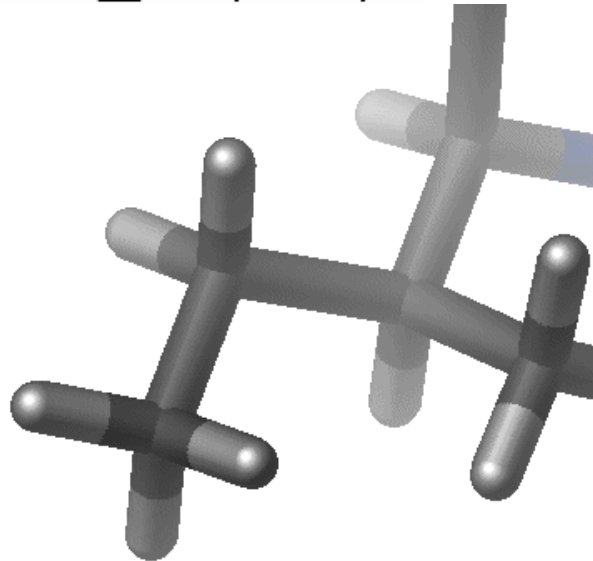




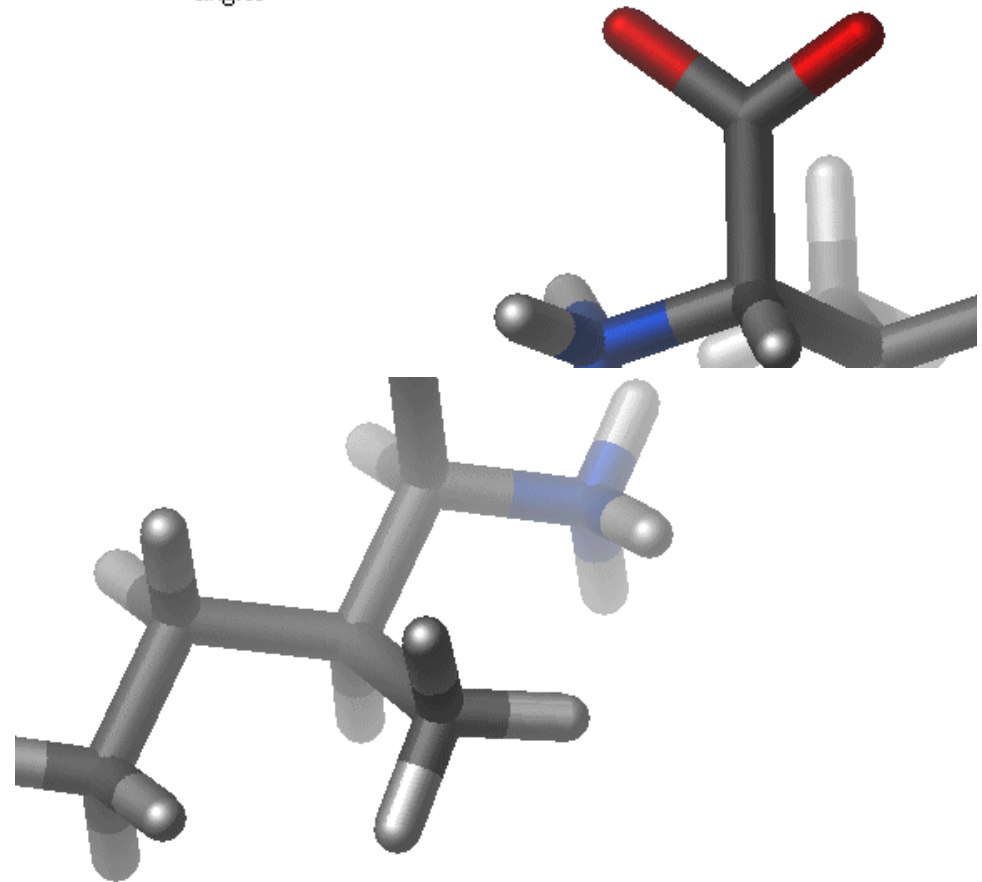
Model for covalent bonds



$$E_{bond-stretch} = \sum K_b (b - b_0)^2$$



$$E_{bond-bend} = \sum_{angles} K_\theta (\theta - \theta_0)^2$$



$$E_{rotate-along-bond} = \sum_{1,4\ pairs} K_\phi (1 - \cos(n\phi))$$

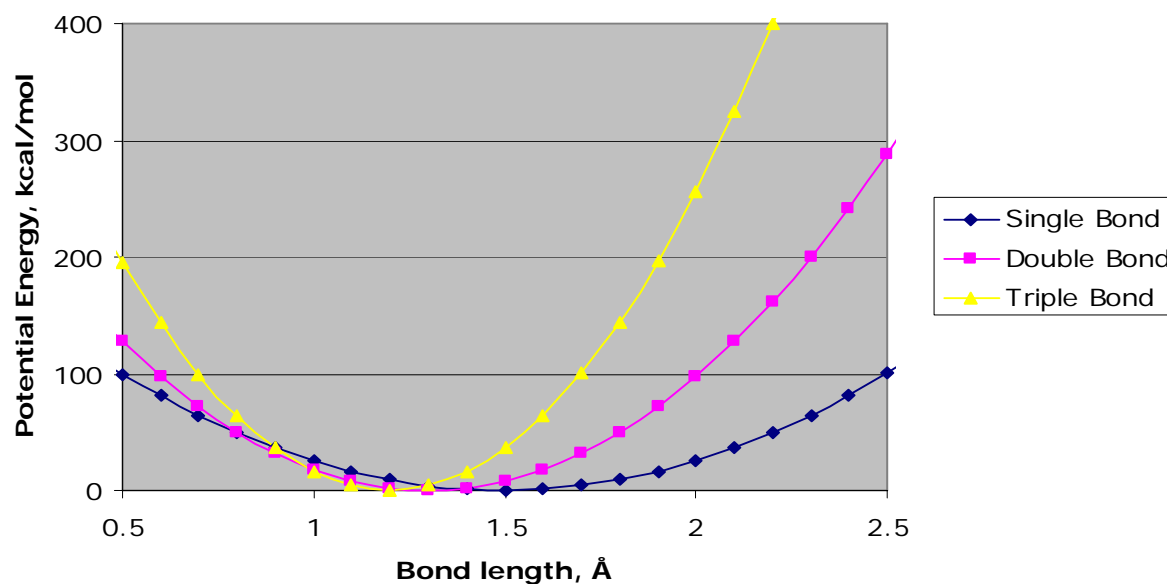


Review: CHARMM potential



Chemical type	K_{bond}	b_0
C-C	100 kcal/mole/Å ²	1.5 Å
C=C	200 kcal/mole/Å ²	1.3 Å
C≡C	400 kcal/mole/Å ²	1.2 Å

Bond Energy versus Bond length



Different types of C-C bonding represented by different choices of b_0 and k_b ;

Need to retype when chemical environment changes

$$V_{\text{bond}} = K_b (b - b_0)^2$$



Review: CHARMM potential



$$E_{non-bonded} = E_{van-der-Waals} + E_{electrostatic}$$

$$E_{van-der-Waals} = \sum_{\substack{nonbonded \\ pairs}} \left(\frac{A_{ik}}{r_{ik}^{12}} - \frac{C_{ik}}{r_{ik}^6} \right)$$

$$E_{electrostatic} = \sum_{\substack{nonbonded \\ pairs}} \frac{q_i q_k}{Dr_{ik}}$$

Image removed for copyright restrictions. □

See the graph on this page:

http://www.ch.embnet.org/MD_tutorial/pages/MD.Part2.html

Nonbonding interactions

vdW (dispersive)

Coulomb (electrostatic)

H-bonding



UFF “Universal Force Field”



- Can handle complete periodic table
- Force constants derived using general rules of element, hybridization and connectivity

$$E_R = \frac{1}{2}k_{IJ}(r - r_{IJ})^2$$

$$r_{IJ} = r_I + r_J + r_{BO} + r_{EN}$$

Features:

- Atom types=elements
- Chemistry based rules for determination of force constants

Pauling-type bond order correction

$$r_{BO} = -\lambda(r_I + r_J) \ln(n)$$

$$r_{EN} = r_I r_J (\sqrt{\chi_I} - \sqrt{\chi_J})^2 / (\chi_I r_I + \chi_J r_J)$$

$$k_{IJ} = \left(\frac{\partial^2 E_r}{\partial R^2} \right)_0 = 2G \frac{Z_I^* Z_J^*}{R^3} = 664.12 \frac{Z_I^* Z_J^*}{r_{IJ}^3}$$



Common empirical force fields



Class I (experiment derived, simple form)

- CHARMM
- CHARMM (Accelrys)
- AMBER
- OPLS/AMBER/Schrödinger
- ECEPP (free energy force field)
- GROMOS

Harmonic terms;
Derived from
vibrational
spectroscopy, gas-
phase molecular
structures
Very system-specific

Class II (more complex, derived from QM)

- CFF95 (Biosym/Accelrys)
- MM3
- MMFF94 (CHARMM, Macromodel...)
- UFF, DREIDING

Include anharmonic terms
Derived from QM, more
general

Image removed due to copyright restrictions.

http://www.ch.embnet.org/MD_tutorial/pages/MD.Part2.html

http://www.pharmacy.umaryland.edu/faculty/amackere/force_fields.htm

<http://amber.scripps.edu/>



Alpha helix and beta sheets



Hydrogen bonding

e.g. between O and H in H₂O

Between N and O in proteins...

Images removed due to copyright restrictions.

Image removed due to copyright restrictions.

Image removed due to copyright restrictions.

See:

<http://www.columbia.edu/cu/biology/courses/c2005/images/3levelpro.4.p.jpg>



Unfolding of alpha helix structure

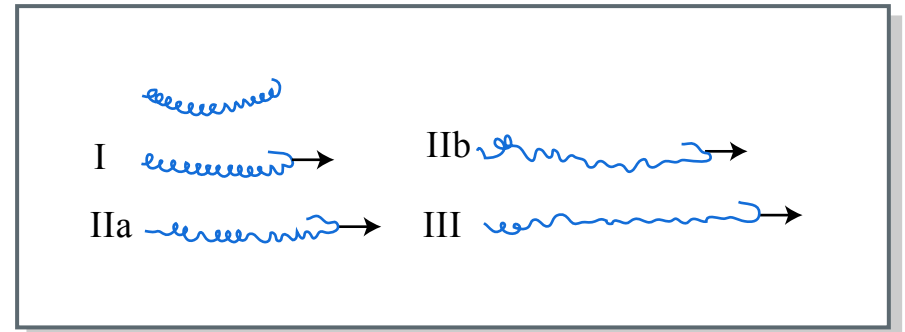


Figure by MIT OCW.

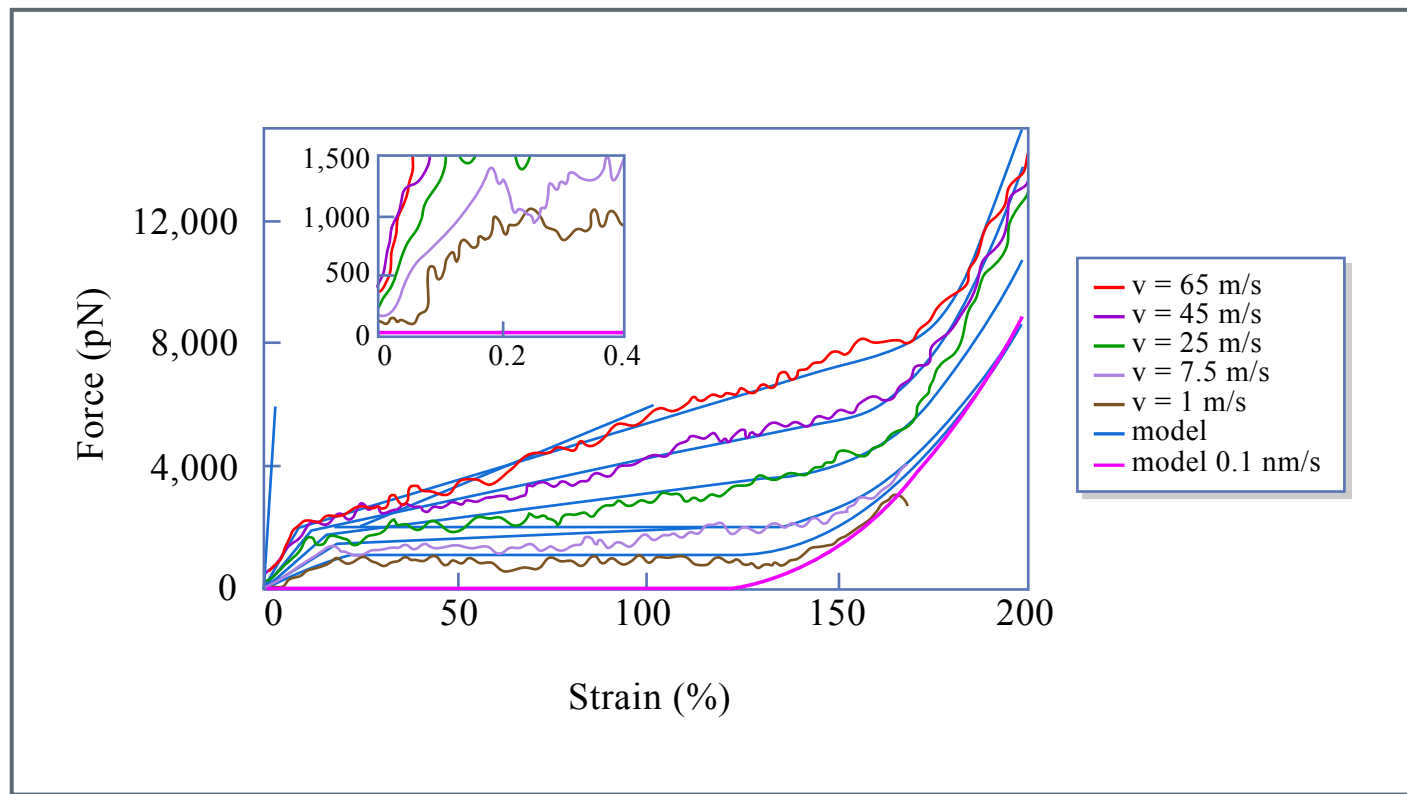
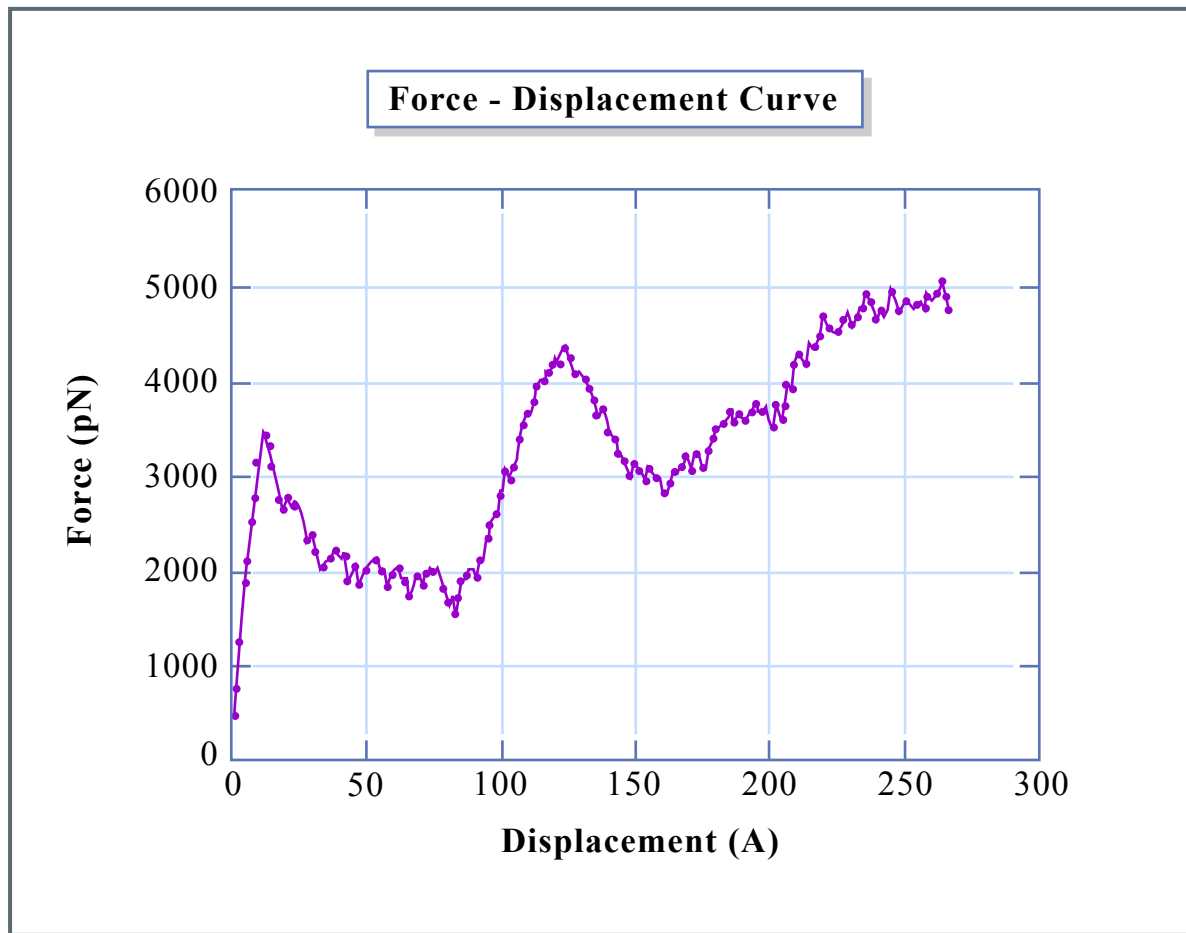


Figure by MIT OCW. After Ackbarow and Buehler, 2007.



Unfolding of beta sheet



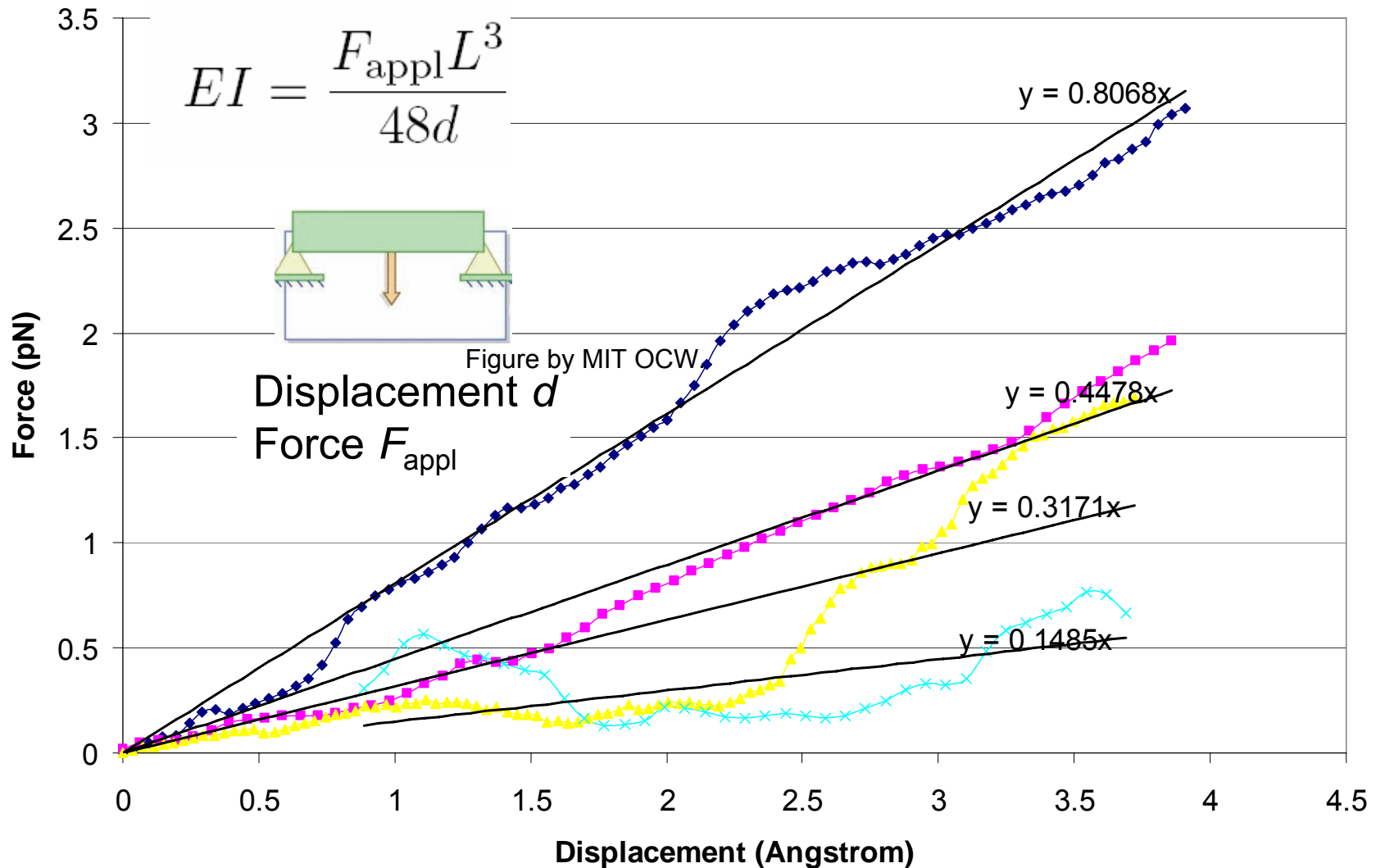
Titin I27 domain: Very resistant to unfolding due to parallel H-bonded strands

Figure by MIT OCW.

Image removed due to copyright restrictions.



Three-point bending test: Tropocollagen molecule



© 2007 Markus J. Buehler, CEE/MIT

Source: Buehler, M. J., and S. Y. Wong. "Entropic Elasticity Controls Nanomechanics of Single Tropocollagen Molecules." *Biophys J* 93 (2007): 37-43.



Three-point bending test: Tropocollagen molecule

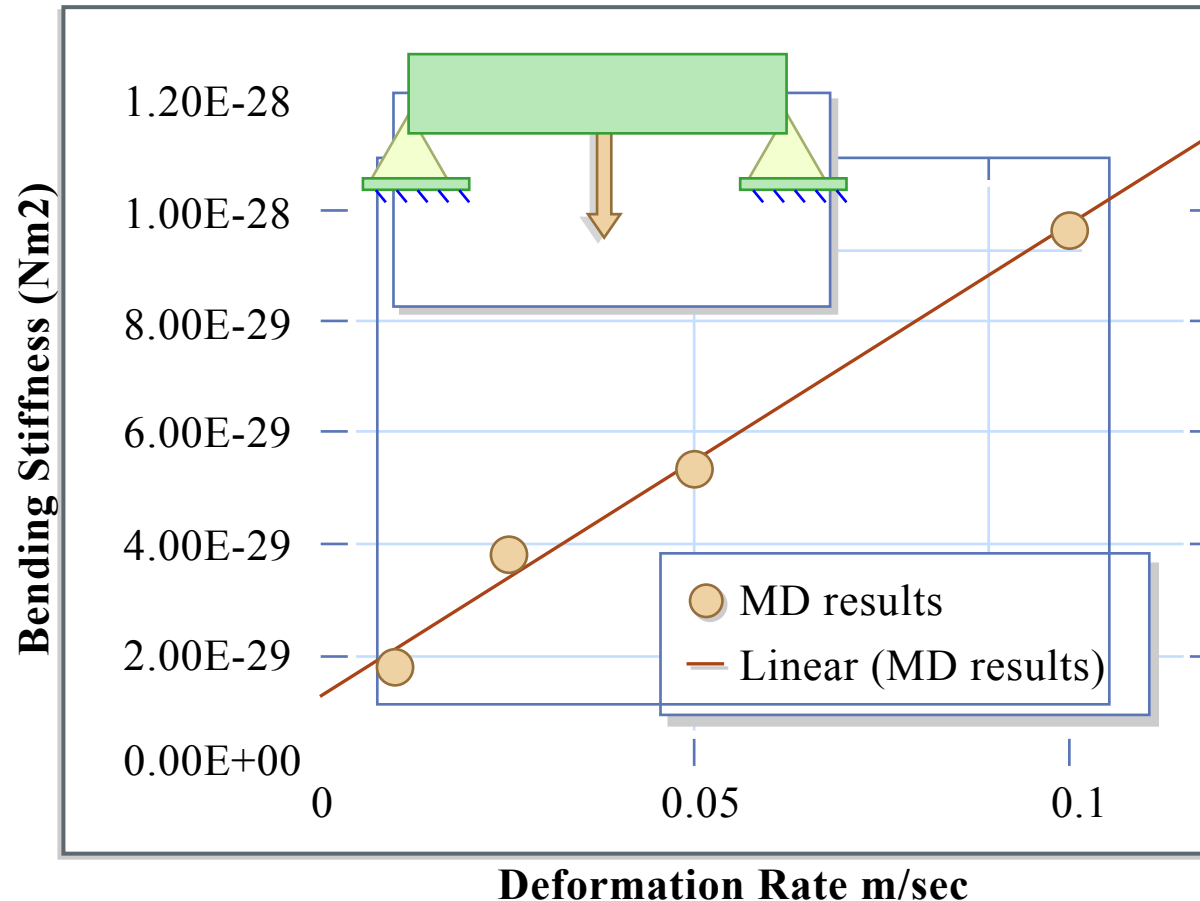


Figure by MIT OCW.

MD: Calculate bending stiffness; consider different deformation rates

Result: Bending stiffness at zero deformation rate (extrapolation)

Yields: Persistence length – between **3 nm** and **25 nm** (experiment: **7 nm**)



Stretching experiment: Tropocollagen molecule

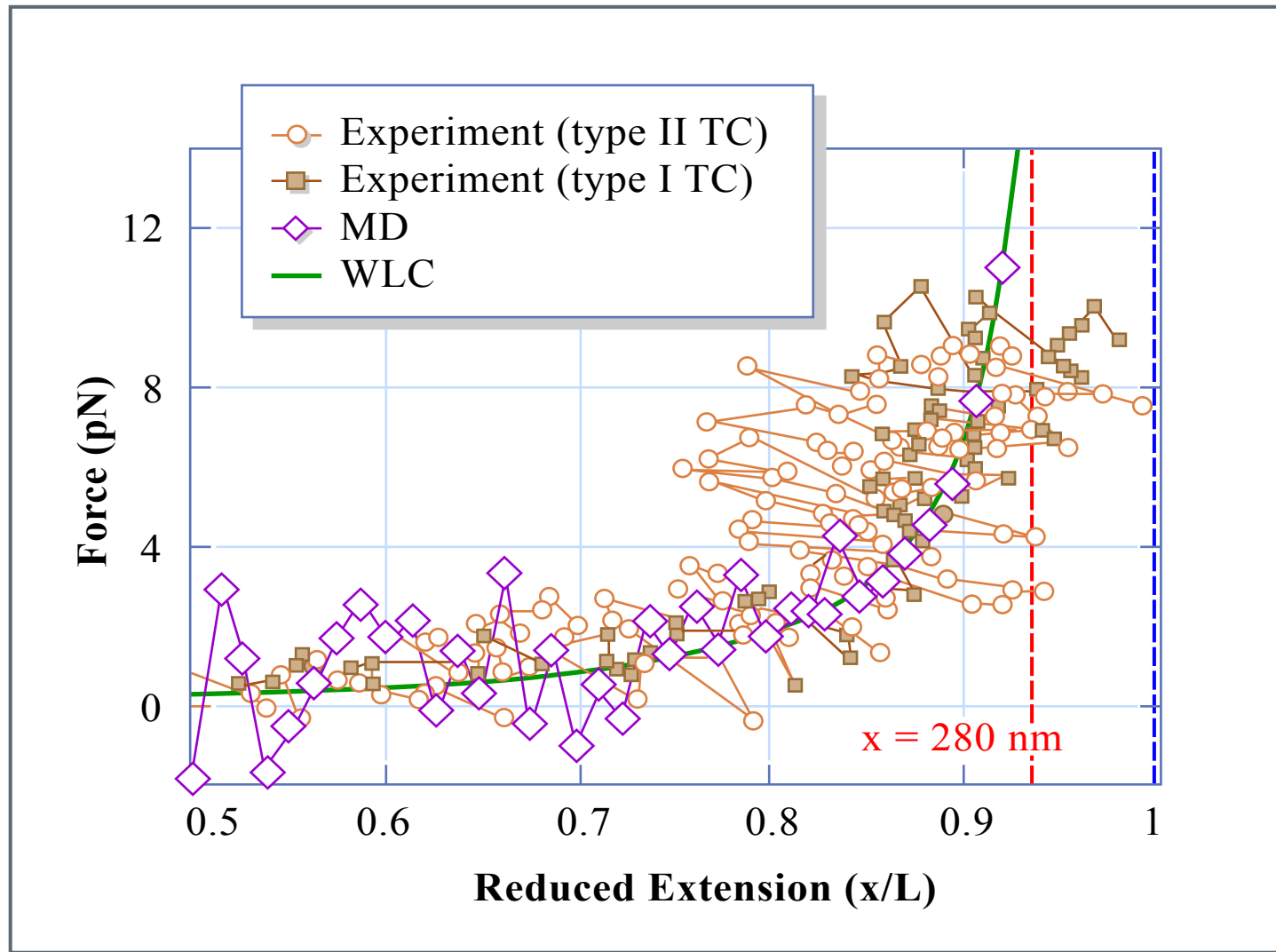


Figure by MIT OCW. Source: Buehler, M. J., and S. Y. Wong. "Entropic Elasticity Controls Nanomechanics of Single Tropocollagen Molecules." *Biophys J* 93 (2007): 37-43.