From nano to macro: Introduction to atomistic modeling techniques

IAP 2007

Nanomechanics of hierarchical biological materials

Lecture 6

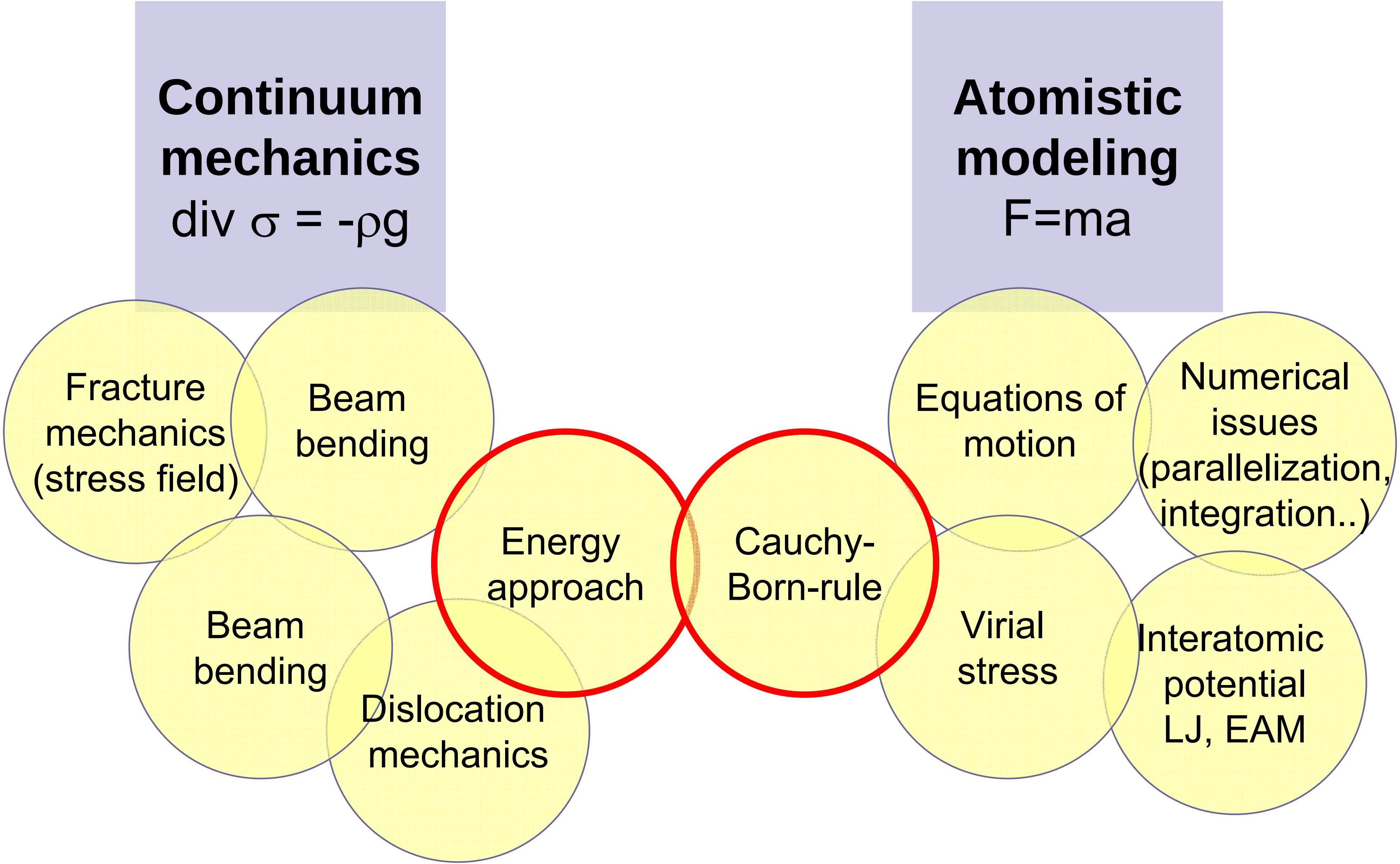
Department of
Civil & Environmental Engineering
Massachusetts Institute of Technology

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

Review



Continuum mechanics
div $\sigma = -\rho g$

Fracture mechanics (stress field)

Beam bending

Beam bending

Dislocation mechanics

Energy approach

Cauchy-Born-rule

Atomistic modeling
$F=ma$

Equations of motion

Numerical issues (parallelization, integration..)

Virial stress

Interatomic potential LJ, EAM

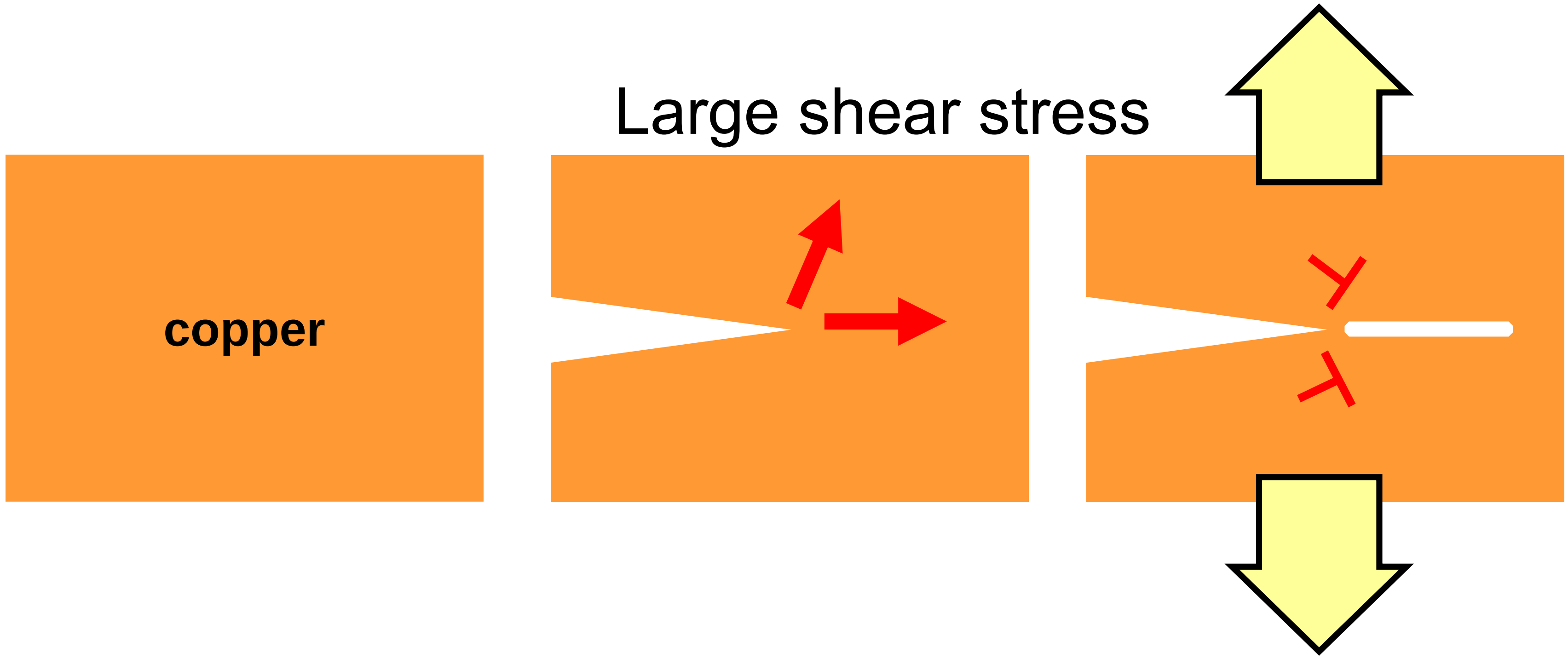
Outline and content (Lecture 5)

- **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:**

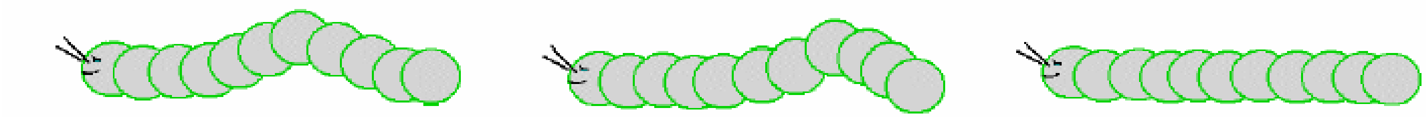
  Material covered in last 2-3 lectures

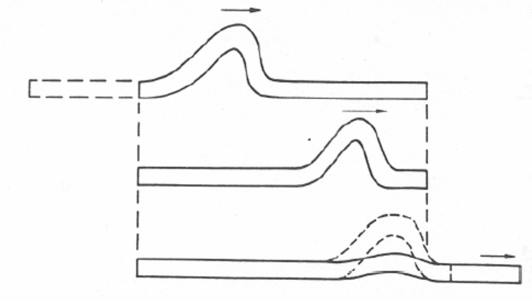
Dislocation nucleation from a crack tip

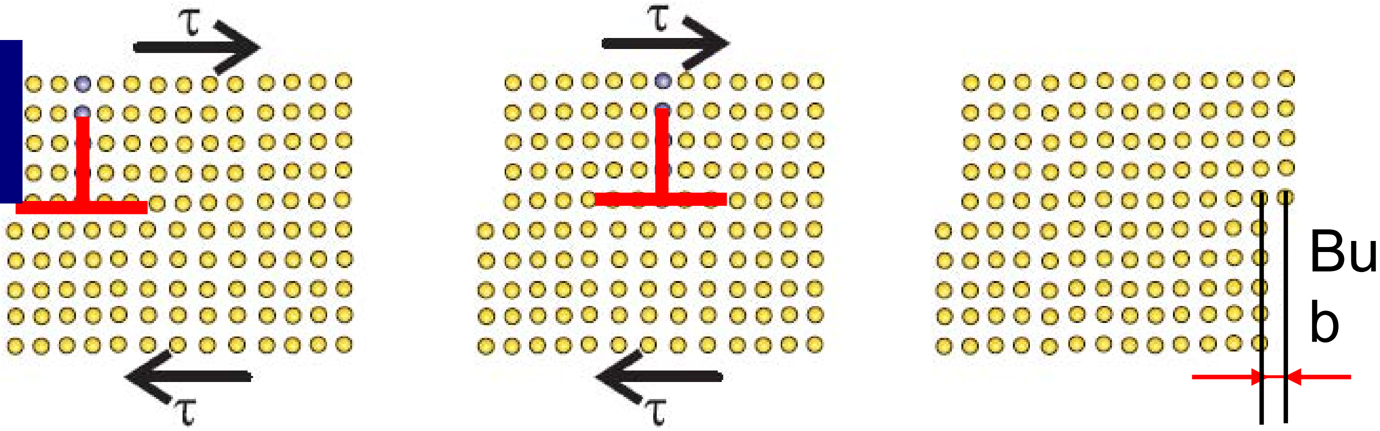


Ductile
vs. brittle
Depends on atomic
behavior at crack tip

Ductile materials are governed by the motion of dislocations: Introduction







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

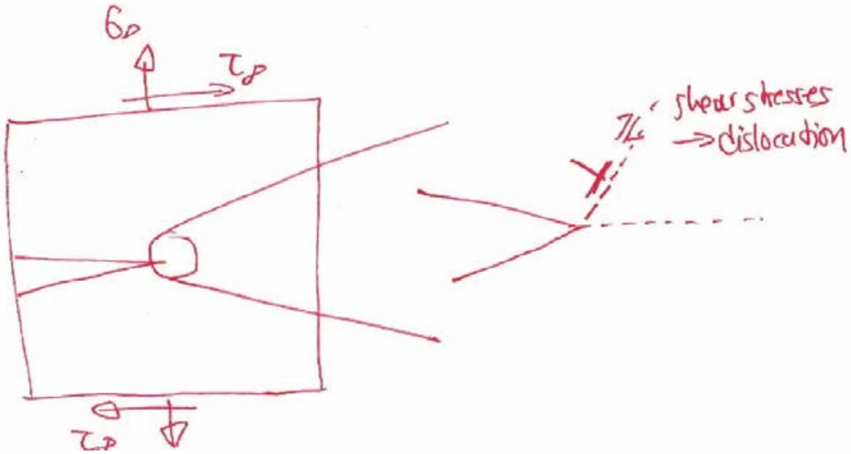
http://www.people.virginia.edu/~lz2n/mse209/Chapter7.pdf

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

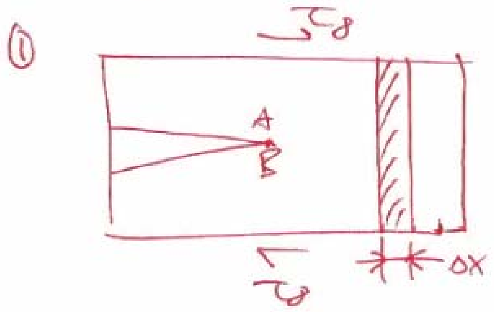
Rice-Thomson model

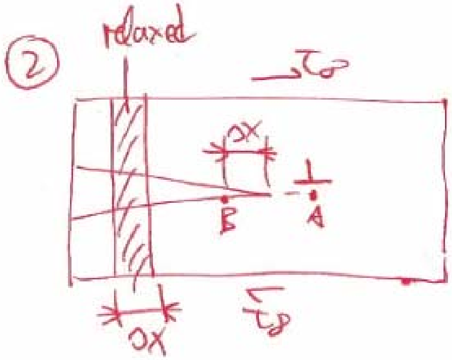


$$\sigma_\infty = \sqrt{\frac{2b}{a}} \frac{1}{f(\theta)} \frac{\mu}{4\pi(1-\nu)}$$

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

Rice-Peirls model



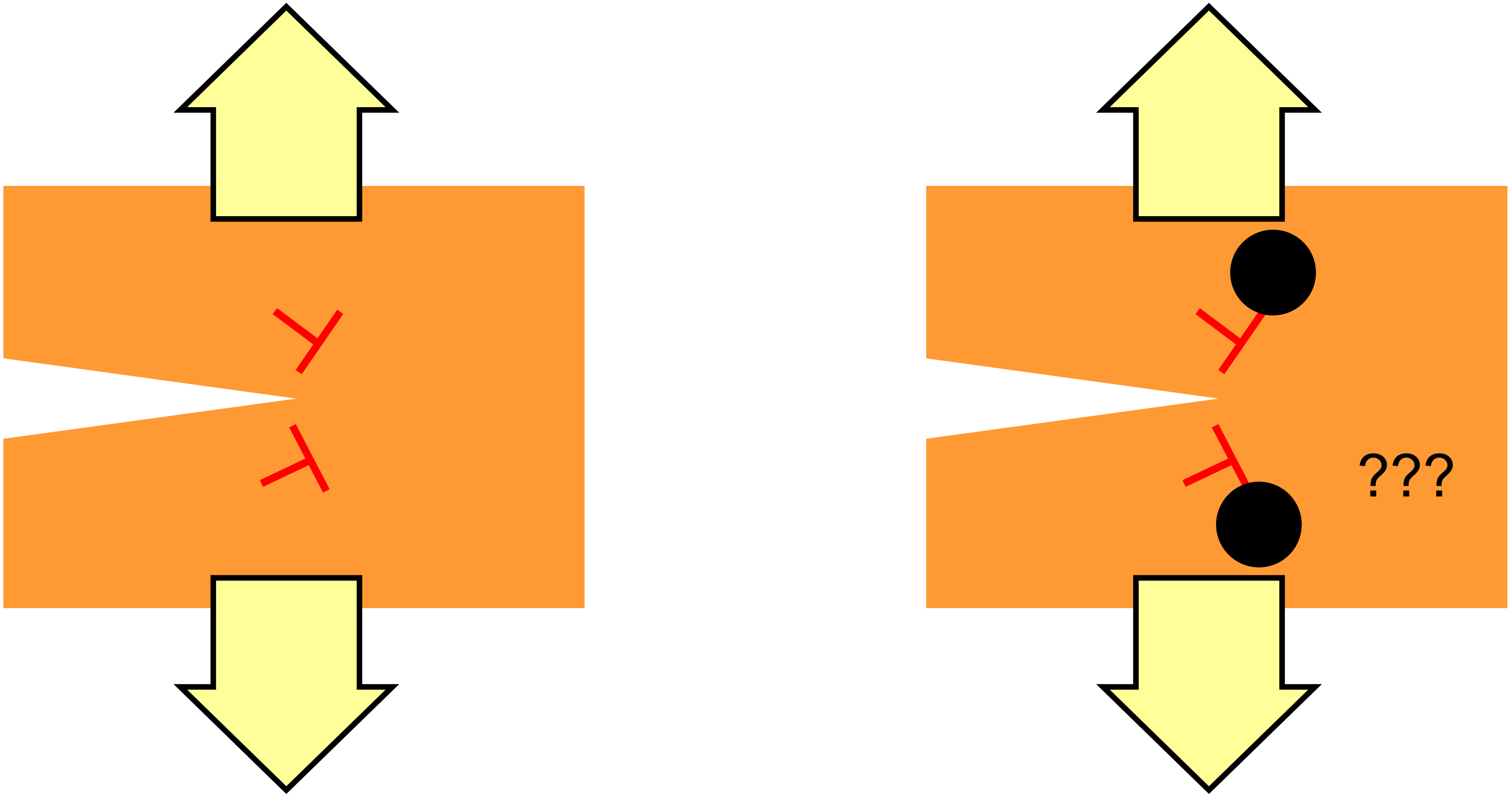


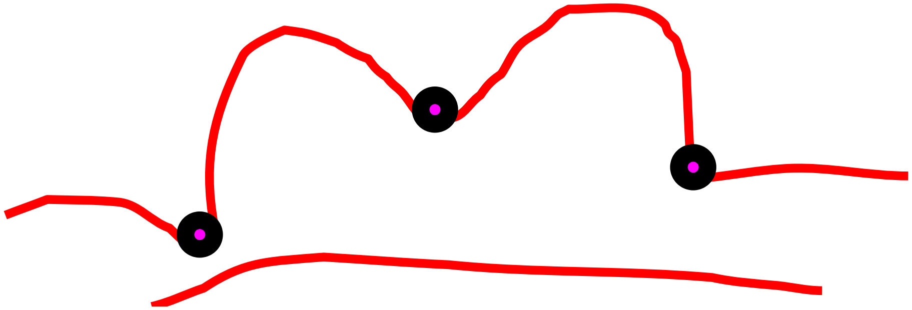
$$\tau_{\infty,\text{disl}} = \sqrt{\frac{2\gamma_{\text{us}}\mu}{H}}.$$

$$\tau_{\infty,\text{surf}} = \sqrt{\frac{4\gamma_{\text{s}}\mu}{H}}.$$

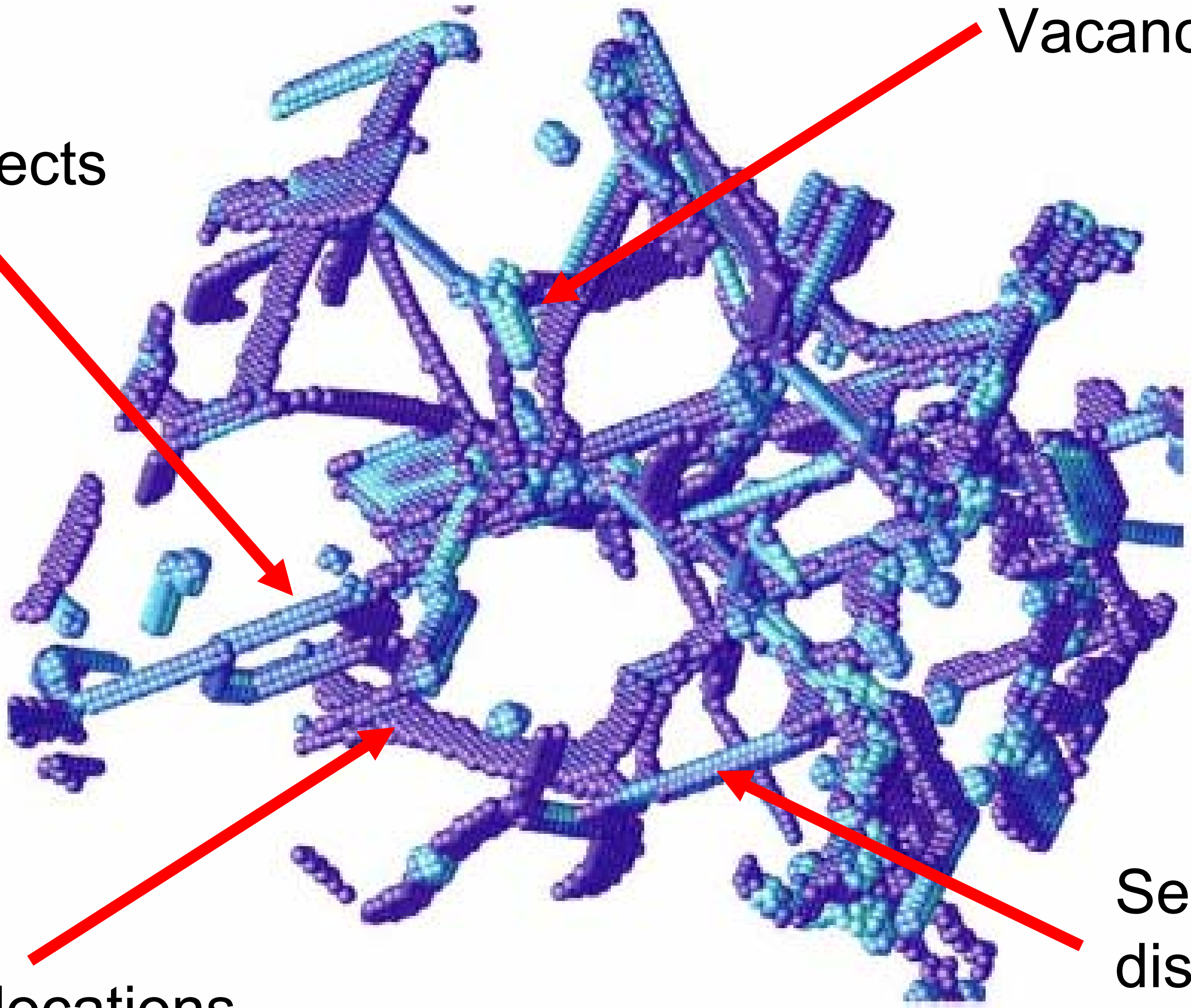
$$\alpha = \frac{\gamma_{\text{us}}}{2\gamma_{\text{s}}}$$

Strengthening mechanisms





Final sessile structure



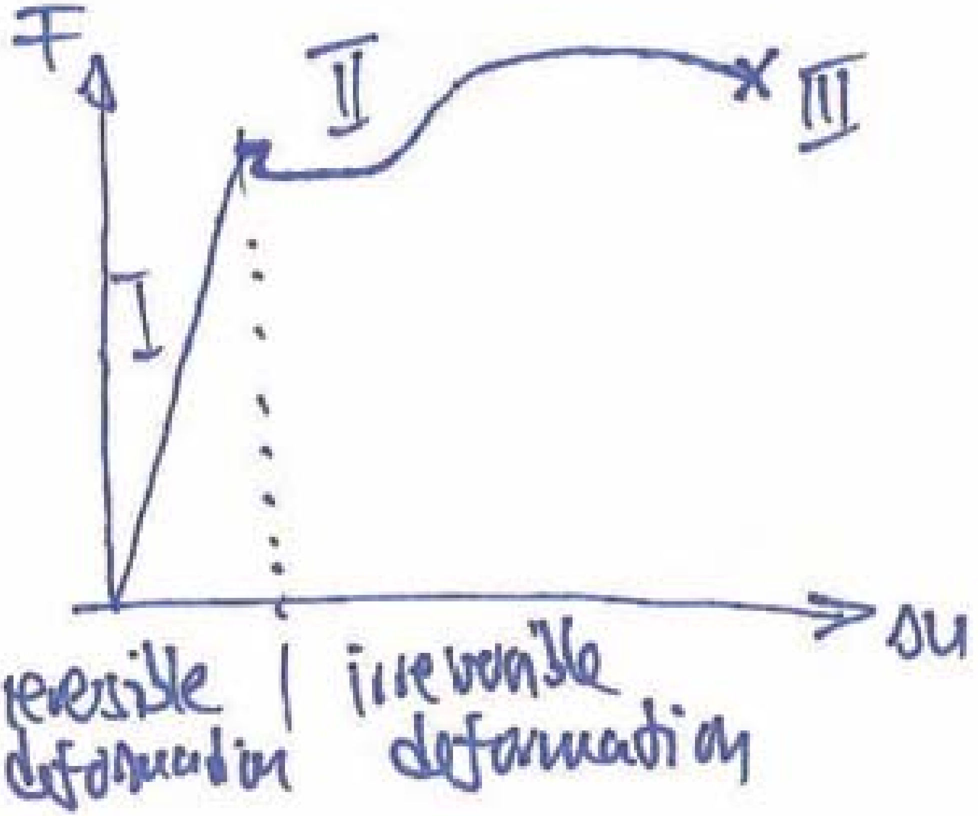
Partial
point defects

Vacancy tubes

Partial dislocations

Sessile
dislocations

Energy approach to elasticity



$$F = k_s \Delta u$$

Energy approach to elasticity

1st law of TD

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \delta W + \delta Q.$$

External work rate

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

Applied force

2nd law

$$\frac{\mathrm{d}S}{\mathrm{d}t} \geq \frac{\delta Q}{T}$$

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

$$\frac{\mathrm{d}D}{\mathrm{d}t} = T\frac{\mathrm{d}S}{\mathrm{d}t} - \delta Q \geq 0$$

Dissipation rate

$$\delta Q = \mathrm{d}U/\mathrm{d}t - \delta W$$

Dissipation rate after consider 1st law of TD:

$$\frac{\mathrm{d}D}{\mathrm{d}t} = \delta W - \frac{\mathrm{d}}{\mathrm{d}t}(U - TS)$$

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):

$$\frac{\mathrm{d}D}{\mathrm{d}t} = 0$$

$$\delta W - \frac{\mathrm{d}F}{\mathrm{d}t} = 0$$

Assume only internal energy change

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

$$\dot{x}\left(F_e - \frac{\mathrm{d}F}{\mathrm{d}x}\right) = 0.$$

Expand equation
dU/dt = dU/dx dx/dt

$$\dot{x} F_e - \frac{\mathrm{d}F}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}t} = 0$$

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

$$F_e = \frac{\mathrm{d}F}{\mathrm{d}x} \qquad F_e = \frac{\mathrm{d}U}{\mathrm{d}x}$$

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

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

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

$$\Phi = \frac{1}{\Omega_0} \int_{\Omega_0^*} U(l)\, D_\Omega\, d\Omega$$

U(l) a function of deformation gradient

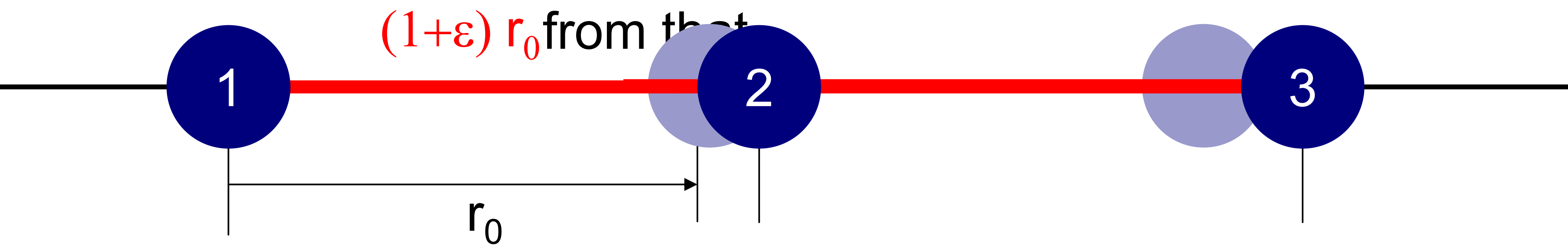
- D_Ω: Mapping function, e.g. $D(l_0, \theta, \phi) = \delta_D(l_0 - l_0^*) D_{\theta\phi}(\theta, \phi)$

- 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 $\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$



$$\Phi(\varepsilon) = \frac{1}{r_0 \cdot D}\phi(r) = \frac{1}{r_0 \cdot D}\phi((1+\varepsilon)\cdot r_0)$$

Strain energy density function

$r_0 \cdot D$ Atomic volume

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

- Mechanics of biological materials

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Example: Stretching of proteins

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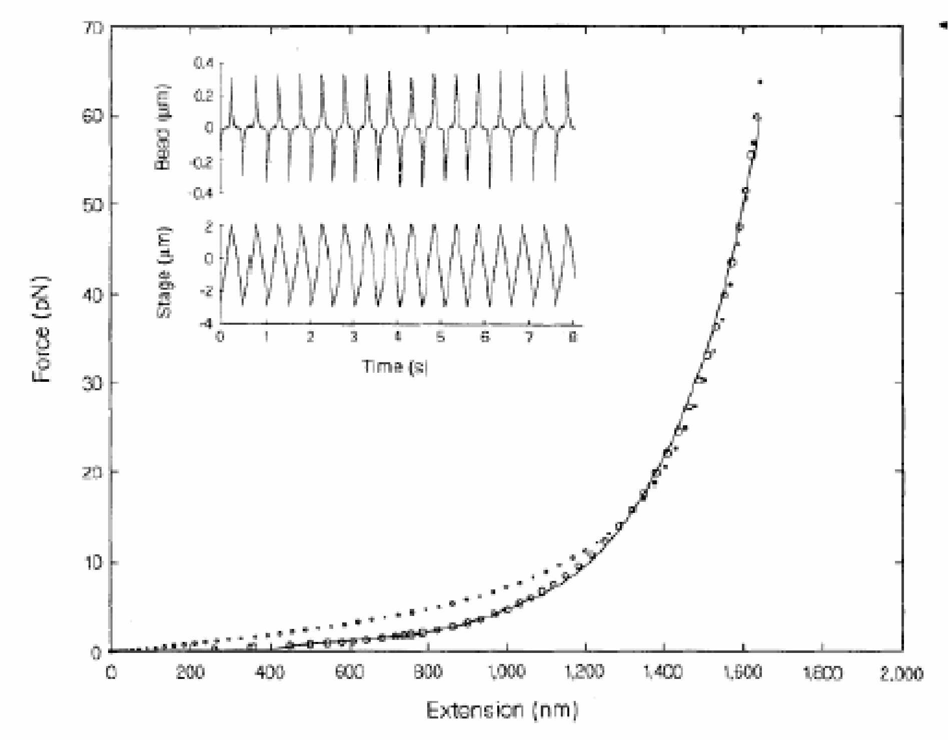


Physical origin?
Soft matter
Nonlinear
Viscoelastic (time dependent)
…

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)

Physical fundamentals of elasticity

- 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

$$\boxed{F(T,V) = U - TS}$$

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

Extension ratios: Large-strain deformation

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

Extension ratio

$$\lambda = l / l_0$$

$$\lambda_i = 1 + \Delta_i$$

$$\varepsilon_{ii} = \varepsilon_i = \Delta_i$$

In small-strain elasticity

$$\lambda_i^2 = 1 + 2\Delta_i + \cancelto{0}{\Delta_i^2}$$

$\Delta_i \rightarrow 0$ 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

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

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

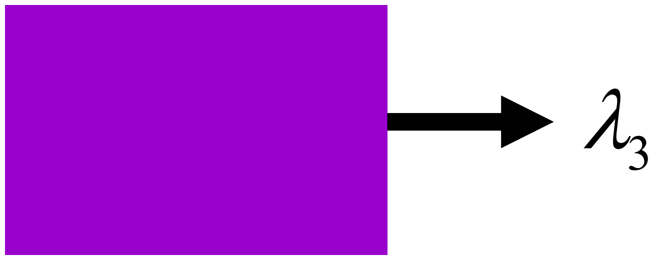
Incompressible (retain volume during deformation)

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

Orthogonal to pulling direction:

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

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



$$\boxed{\begin{aligned} &U = C\left(\lambda^2 + 2/\lambda\ - 3\right) \quad \text{for uniaxial tension} \\ &dU/d\lambda = 2C(\lambda - 1/\lambda^2) = \sigma \end{aligned}}$$

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:

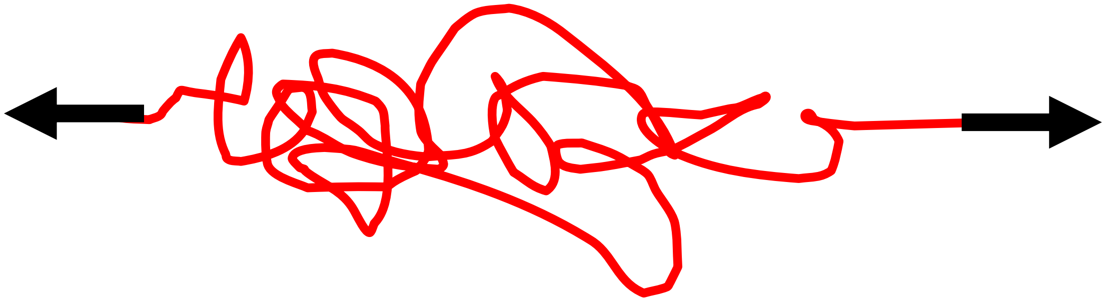
$$\sigma = 2C(\lambda \ - 1/\lambda^2)$$

For small strains: $\lambda_i = 1 + \varepsilon_i$

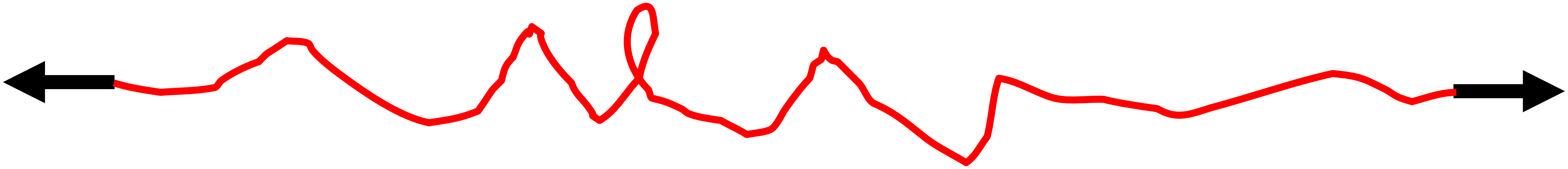
$$\sigma = 2C((1+\varepsilon)^2 - 1/(1+\varepsilon)) \approx 2C[\cancel{1} + \overset{3}{\cancel{2}}\varepsilon - (\cancel{1} - \cancel{\varepsilon}) + O(0)]$$

$\boxed{\sigma = 6C\varepsilon = E\varepsilon}$ Hooke's law (*linear* elasticity) $\boxed{C = E/6}$

Entropic change as a function of stretch



High entropy

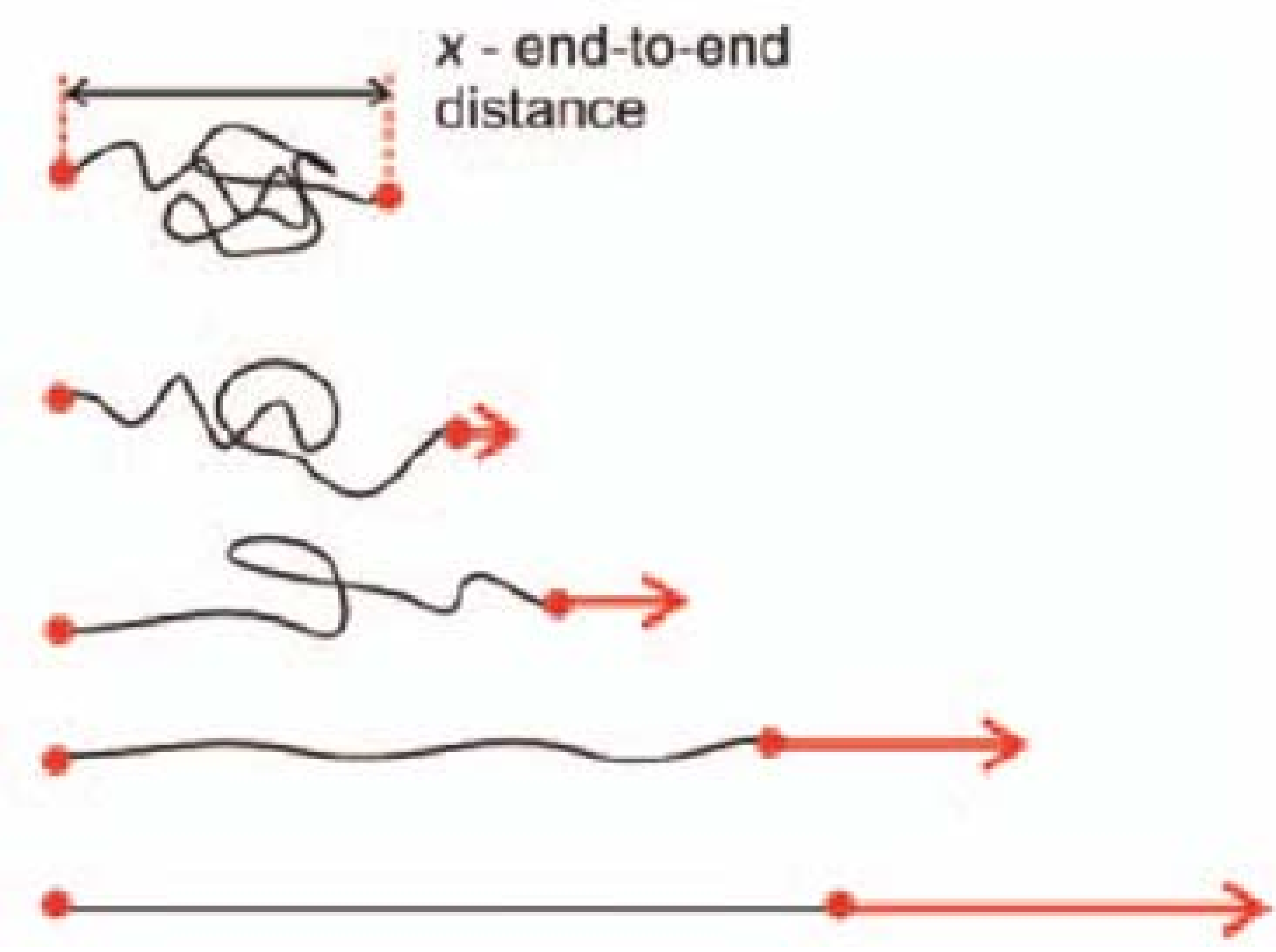


Low entropy

Entropic change as a function of stretch

Entropic regime

Energetic regime



Statistical theory of rubber elasticity

- 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

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

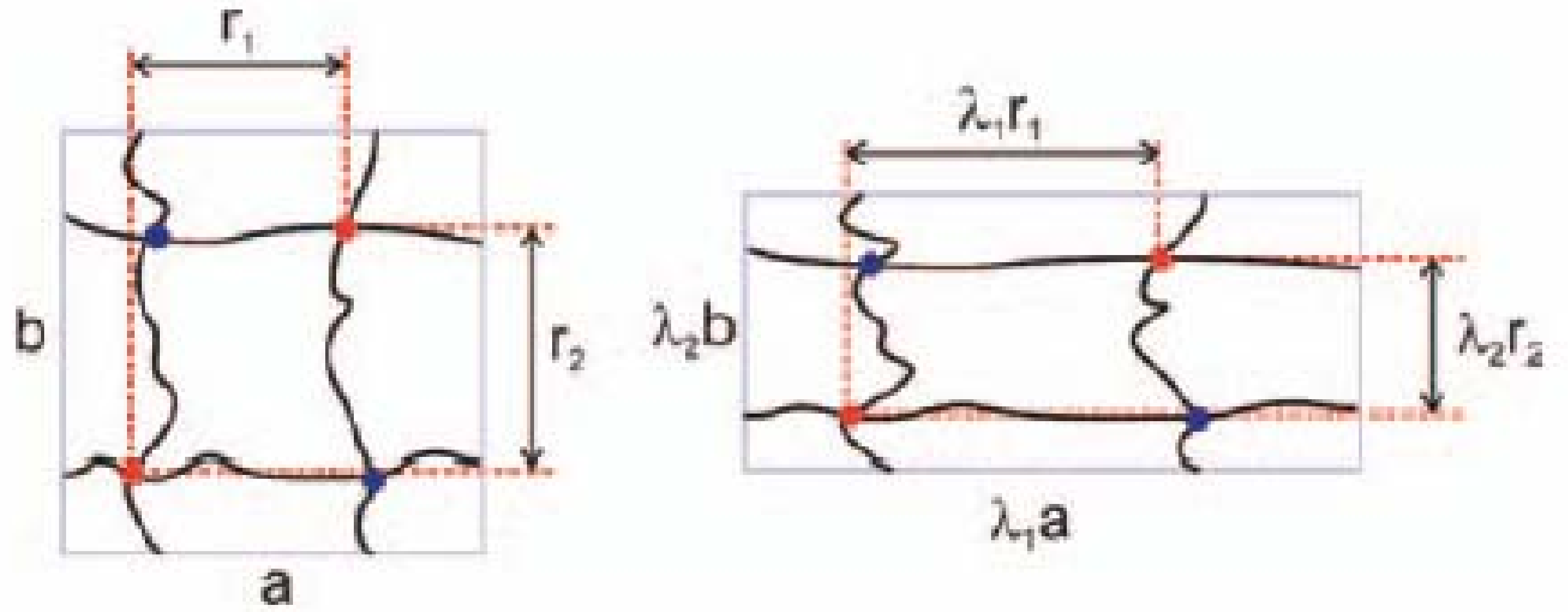
$$\sigma_n = C(\lambda - 1/\lambda^2)$$

This is the result for a neo-Hookean solid

(see Courtney, p. 64)

Statistical theory of rubber elasticity

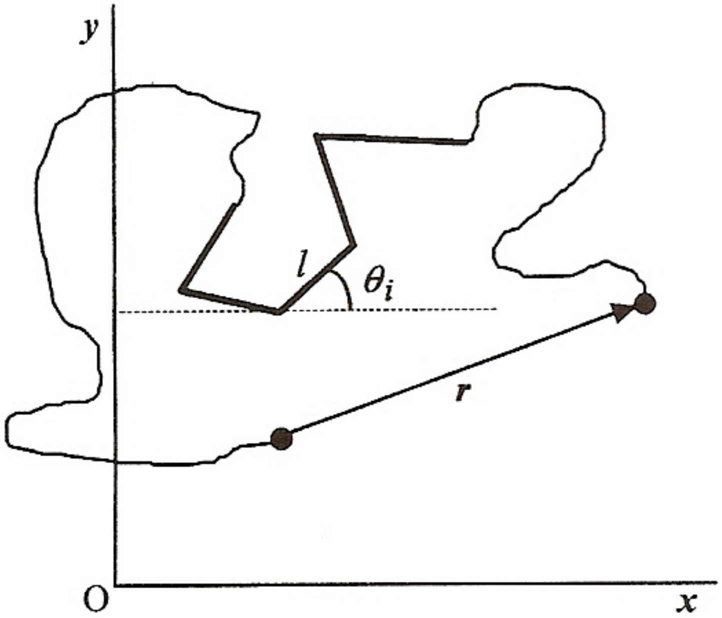
Note: No change in elastic energy of molecules



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



$$\boxed{S = c - kb^2 r^2}$$

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

Total length: *nl=L*

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

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

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

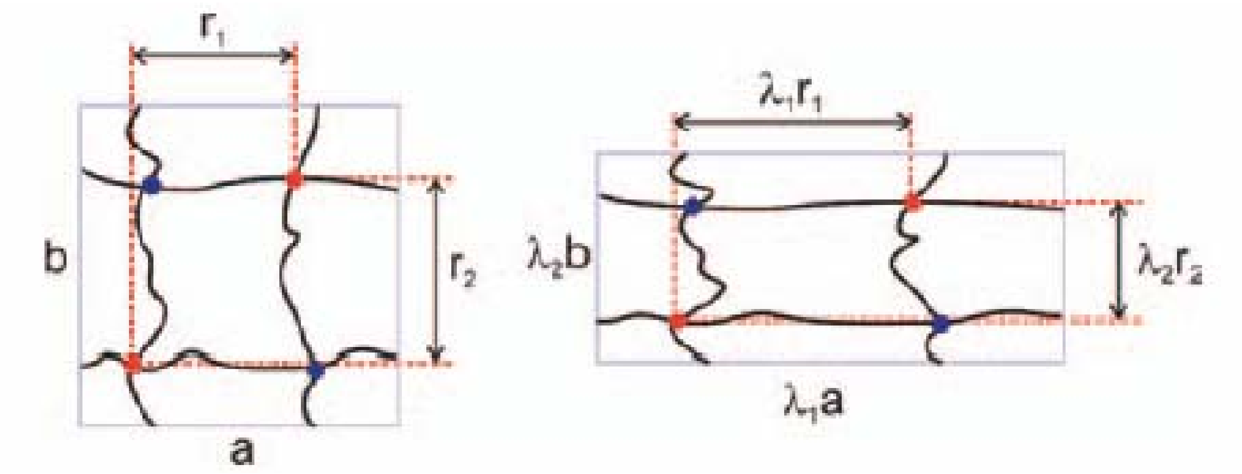
Entropic elasticity: Derivation

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

$$S = c - kb^2 r^2$$ where $$b^2 = \frac{3}{2nl^2}$$

r end-to-end distance of chain

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



Entropic elasticity: Derivation

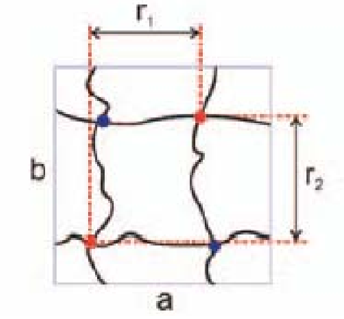
$$\Delta S = -kb^2 \sum_{N_b} \left(\lambda_1^2 - 1\right)x^2 + \left(\lambda_2^2 - 1\right)y^2 + \left(\lambda_3^2 - 1\right)z^2$$

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

$< .. >$ Average values over all N_b chains
– need multiply by N_b to get total energy

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

$$< x^2 > = < y^2 > = < z^2 > = \tfrac{1}{3} < r_b^2 >$$



Entropic elasticity: Derivation

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

It can be shown that

$$r_{RMS} = \sqrt{n} \cdot l =< \sqrt{< r_b^2 >}$$

$$< r_b^2 >= n \cdot l^2$$

$$< x^2 >=< y^2 >=< z^2 >= \tfrac{1}{3} n \cdot l^2 = \frac{1}{2b^2}$$

$$\Delta S = -kN_b / 2\left[\left(\lambda_1^2 - 1\right) + \left(\lambda_2^2 - 1\right) + \left(\lambda_3^2 - 1\right)\right]$$

No explicit dep. on *b* any more

$$U = -T\Delta S = \tfrac{1}{2} N_b kT\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3\right)$$

$$C = E / 6$$

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

$$\sigma = (E / 3)(\lambda^2 - 1 / \lambda)$$

Entropic elasticity

For SED: *Free energy density*

Young's modulus

$$U = -T\Delta S = \underbrace{\tfrac{1}{2} N_b kT}_{C = E/6}\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3\right)$$

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)

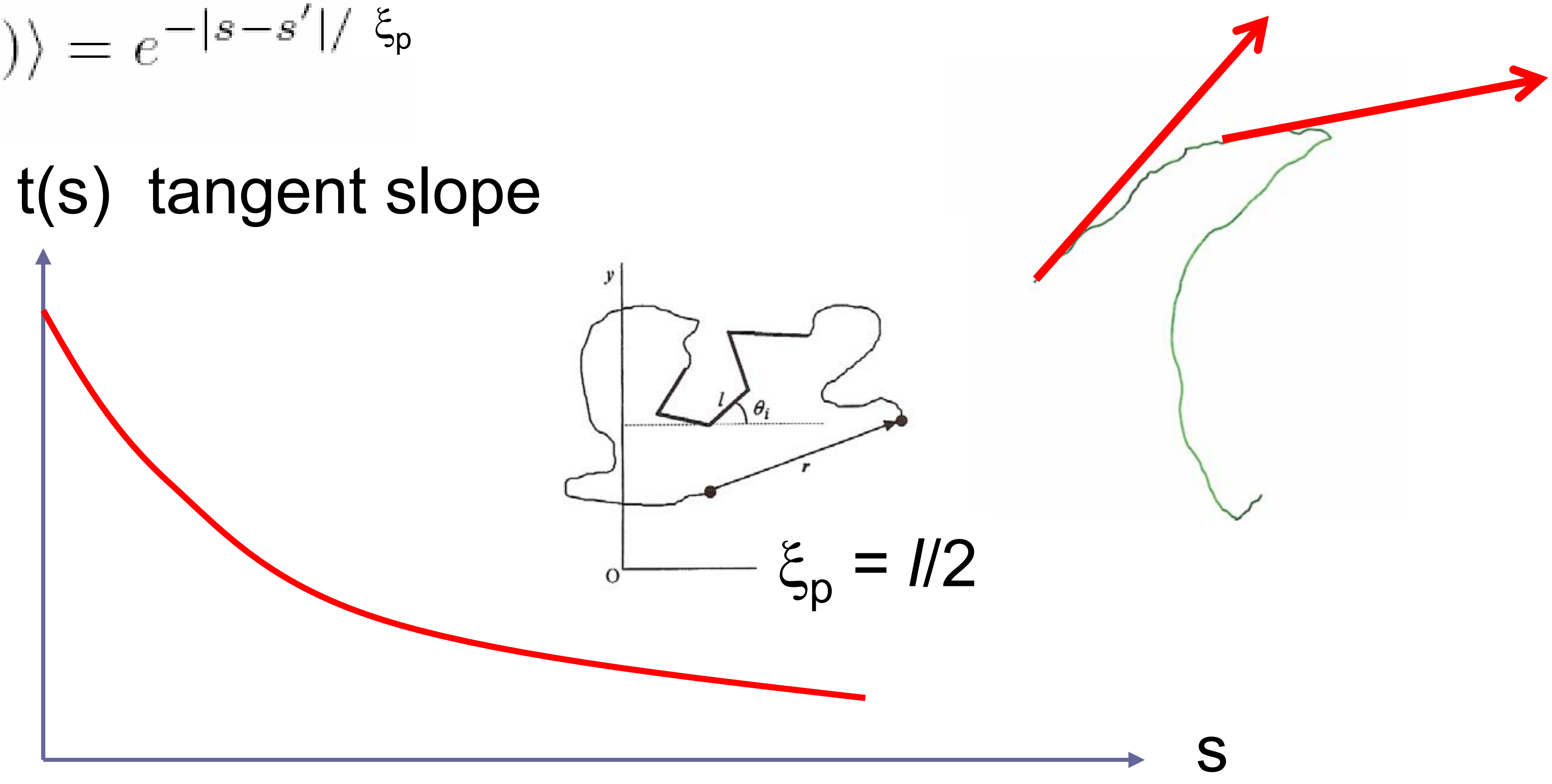
$$E \sim N^*$$

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

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

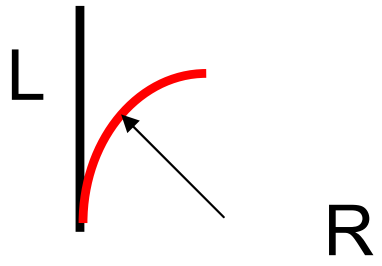


The length at which a filament is capable of bending significantly in independent directions, at a given temperature.
This is defined by a autocorrelation function which gives the characteristic distance along the contour over which the tangent vectors **t(s)** become uncorrelated

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*~4E-21 J at room temperature

- Persistence length is defined as $\xi_p = \dfrac{EI}{k\,T}$

(unit: length)

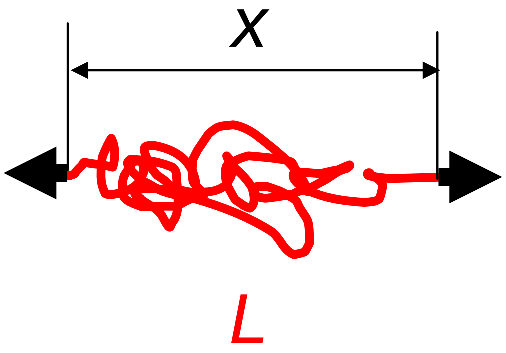
Contour length of molecules

- 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

$$k_{sp} = \frac{3kT}{2L\xi_p} \qquad F \sim k_{sp} x \qquad x \ll L$$

Worm-like chain model

Freely-jointed rigid rods

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DNA 4-plat electron micrograph
(Cozzarelli, Berkeley)

Continuously flexible ropes

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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

$$x << L$$

- 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.

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

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

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20 natural amino acids

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Table of amino acid chemical structures.

See similar image: http://web.mit.edu/esgbio/www/lm/proteins/aa/aminoacids.gif.

Hierarchical structure of collagen

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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

(Buehler, JMR, 2006)

Elasticity of tropocollagen molecules

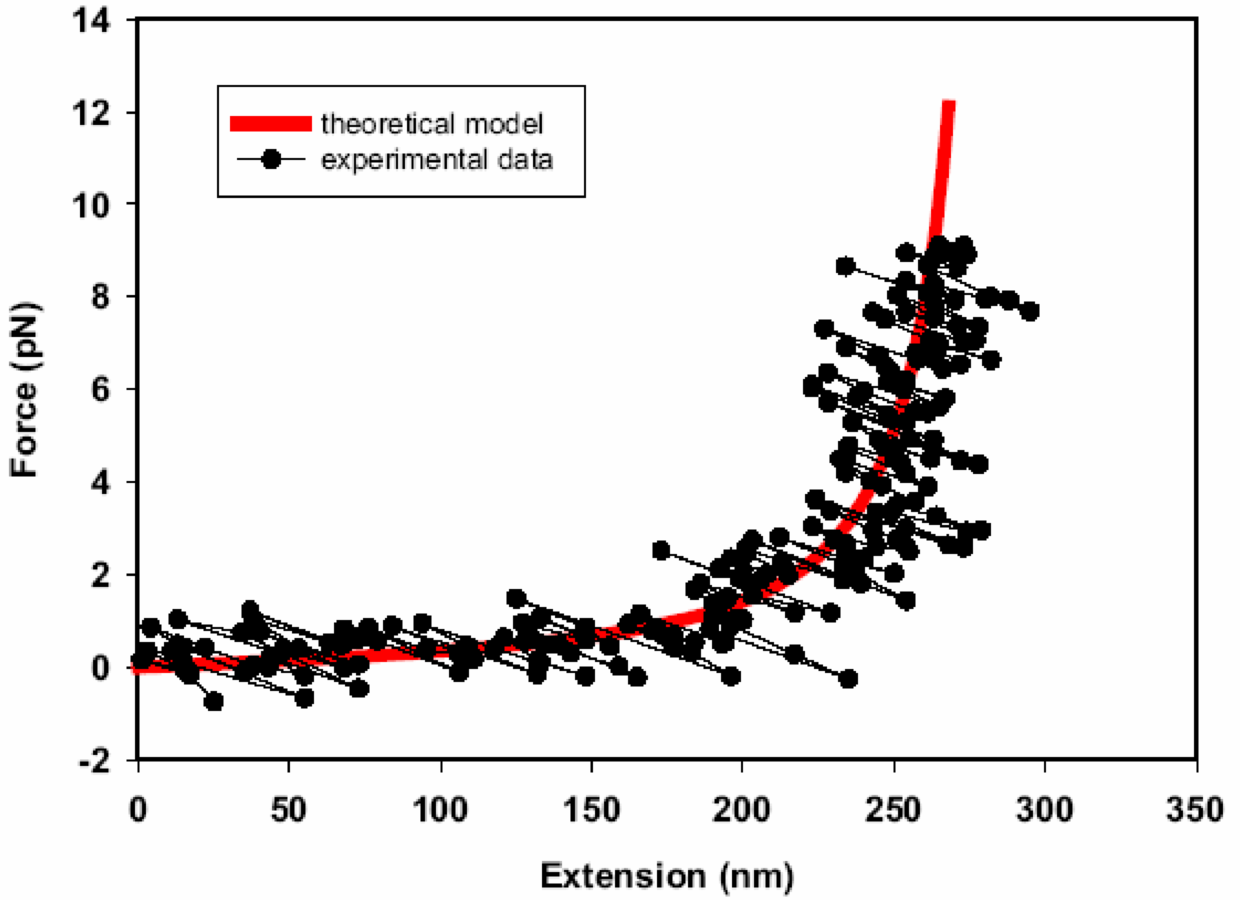

Fig. 2. The force-extension curve for stretching a single type II collagen molecule. The data were fitted to Marko–Siggia entropic elasticity model. The molecule length and persistence length of this sample is 300 and 7.6 nm, respectively.

Sun, 2004

Modeling organic chemistry

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

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Common empirical force fields

Class I (<u>experiment derived</u>, 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, <u>derived from QM</u>)

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

Include anharmonic terms
Derived from QM, more general

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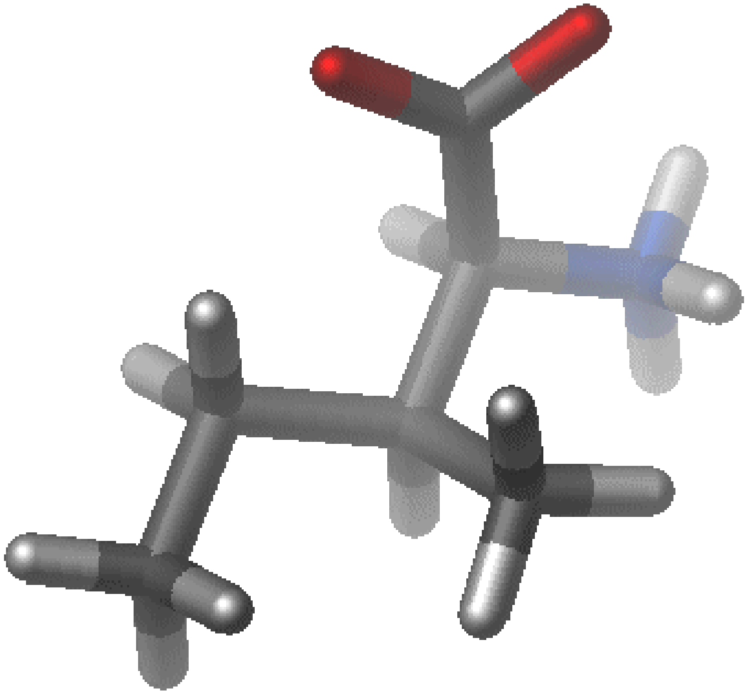
http://www.ch.embnet.org/MD_tutorial/pages/MD.Part2.html
http://www.pharmacy.umaryland.edu/faculty/amackere/force_fields.htm
http://amber.scripps.edu/

Model for covalent bonds

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

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

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



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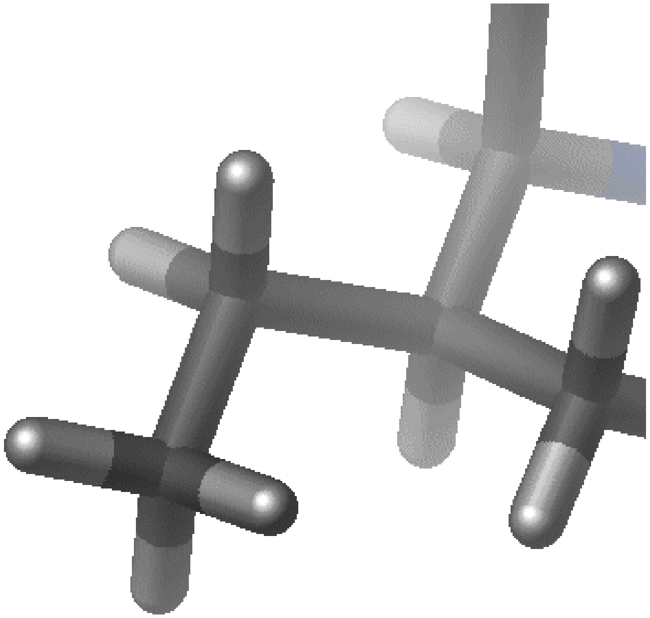
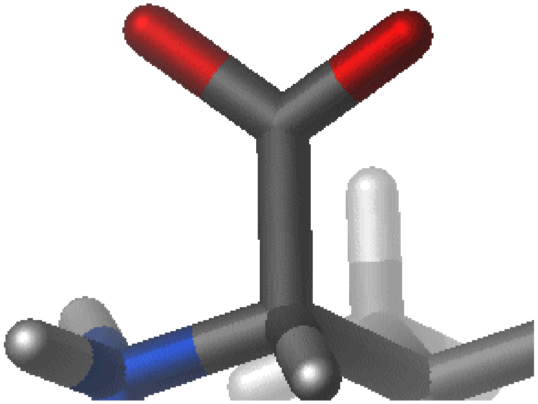
http://www.ch.embnet.org/MD_tutorial/pages/MD.Part2.html
http://www.pharmacy.umaryland.edu/faculty/amackere/force_fields.htm

Model for covalent bonds

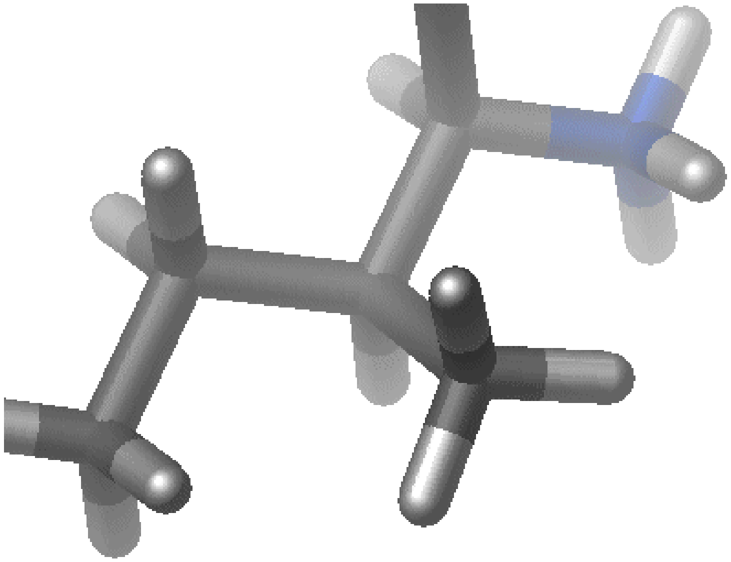
$$E_{bond-stretch} = \sum K_b (b - b_0)^2$$



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



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



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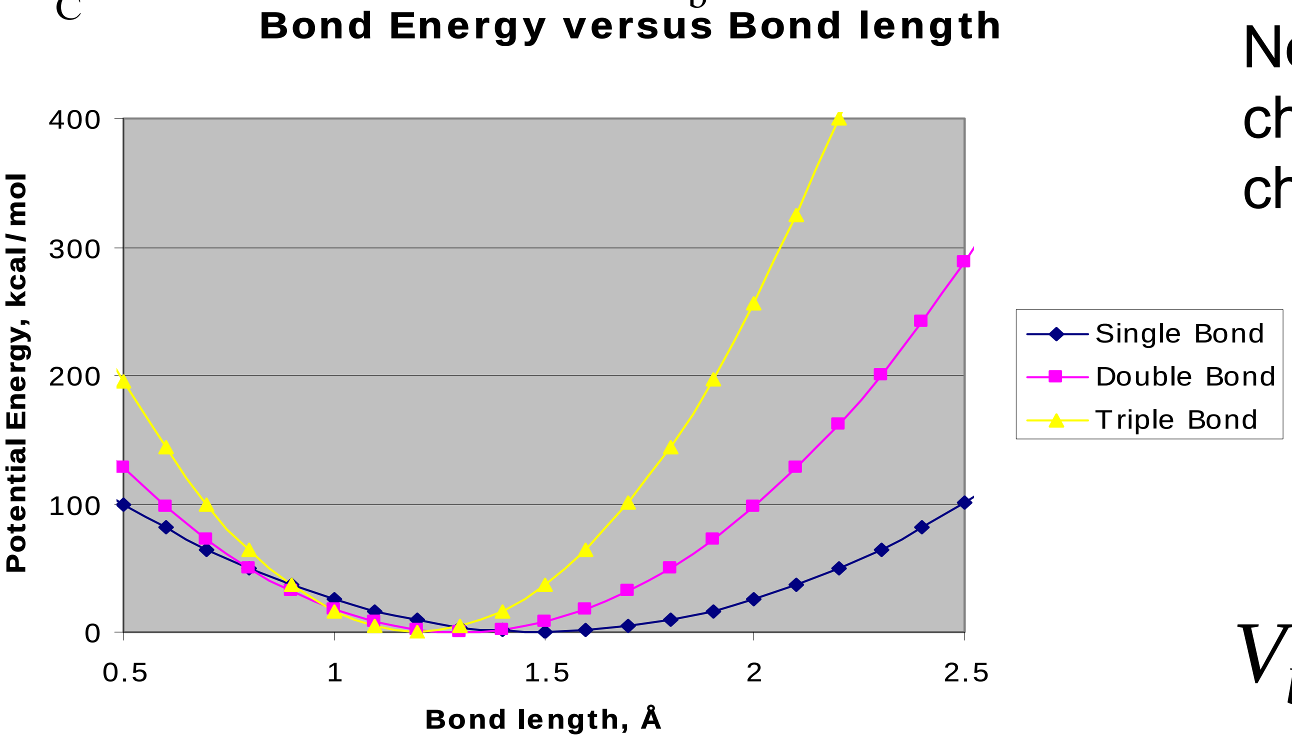
http://www.ch.embnet.org/MD_tutorial/pages/MD.Part2.html

Review: CHARMM potential

Chemical type	K_{bond}	o
−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

C b



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

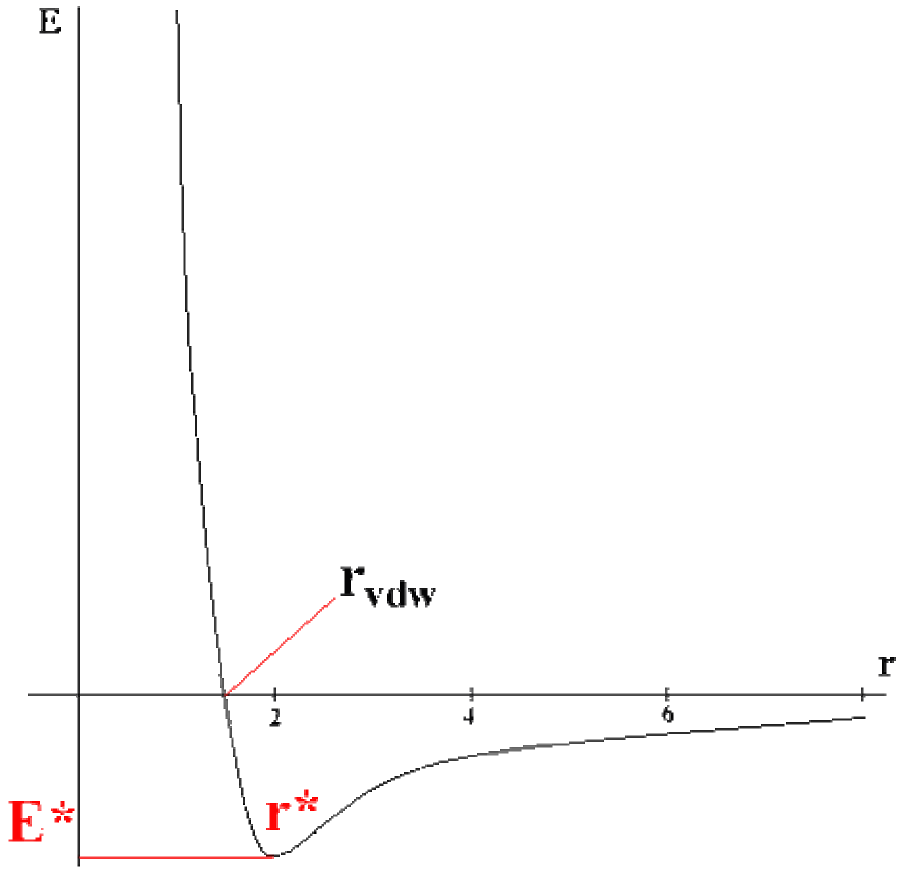
Need to retype when chemical environment changes

$$V_{bond} = K_b \left(b - b_o\right)^2$$

http://www.ch.embnet.org/MD_tutorial/pages/MD.Part2.html
http://www.pharmacy.umaryland.edu/faculty/amackere/force_fields.htm

Review: CHARMM potential

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



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

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

Nonbonding interactions

vdW (dispersive)

Coulomb (electrostatic)

H-bonding

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

UFF “Universal Force Field”

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

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

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

Features:

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

Pauling-type bond order correction

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

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

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

Rappé *et al.*

Alpha helix and beta sheets

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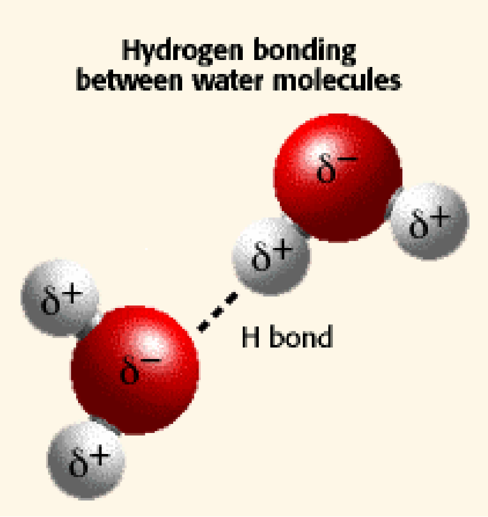
Hydrogen bonding
e.g. between O and H in H_2O
Between N and O in proteins…



Beta sheet

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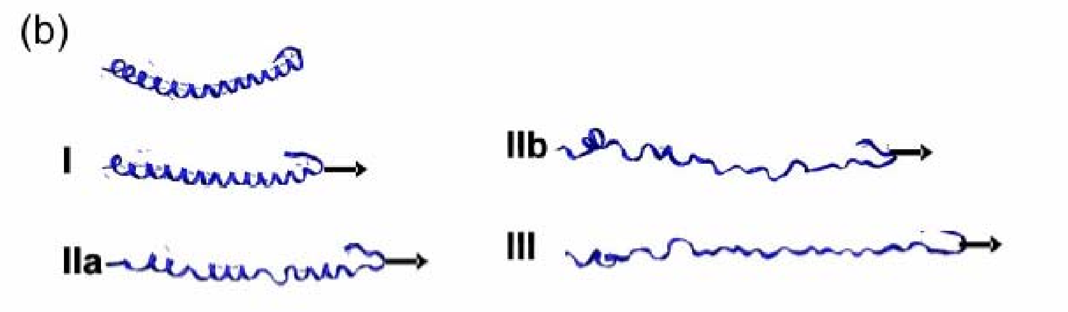
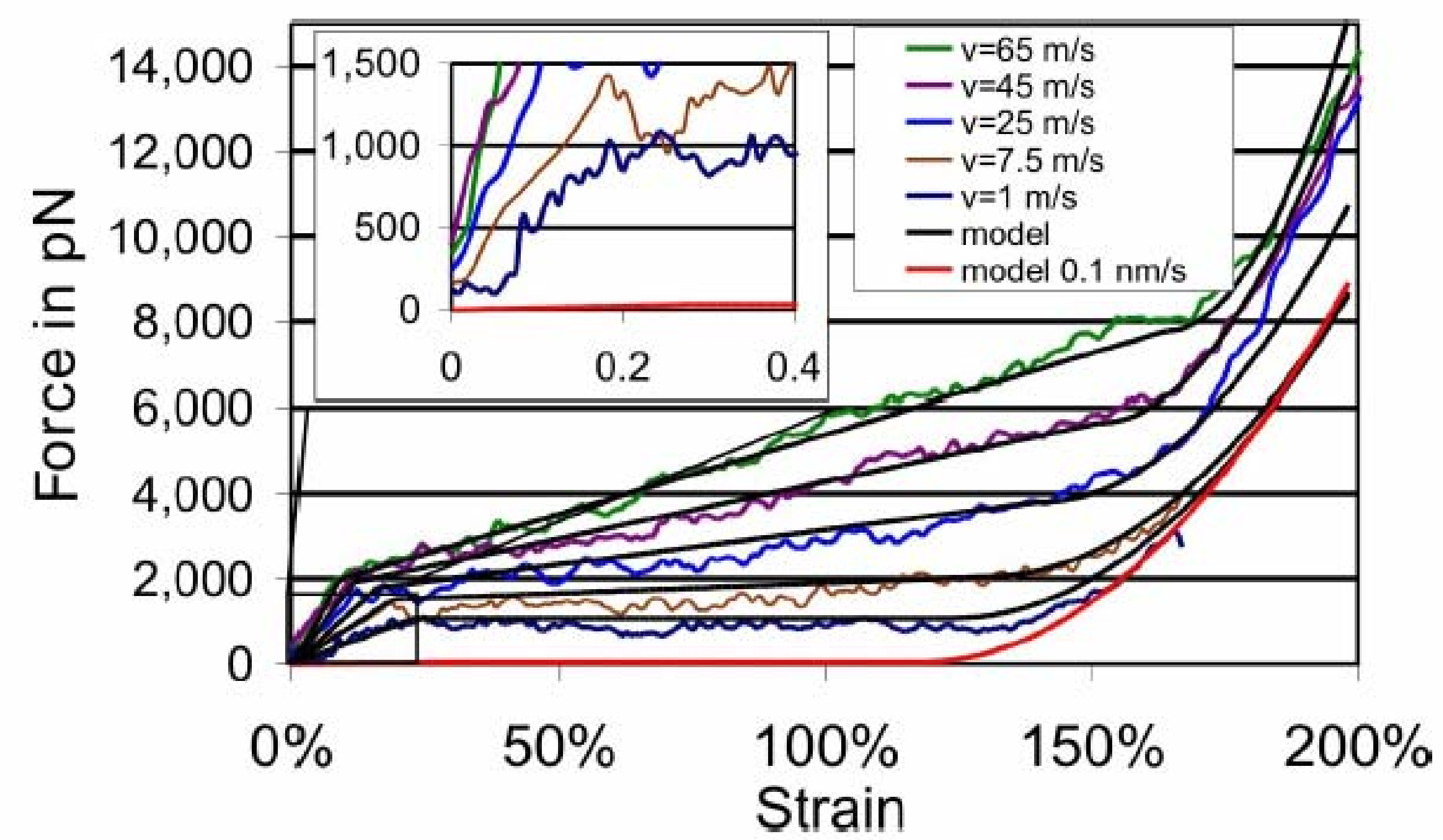
See: http://www.columbia.edu/cu/biology/courses/c2005/images/3levelpro.4.p.jpg

Alpha helix

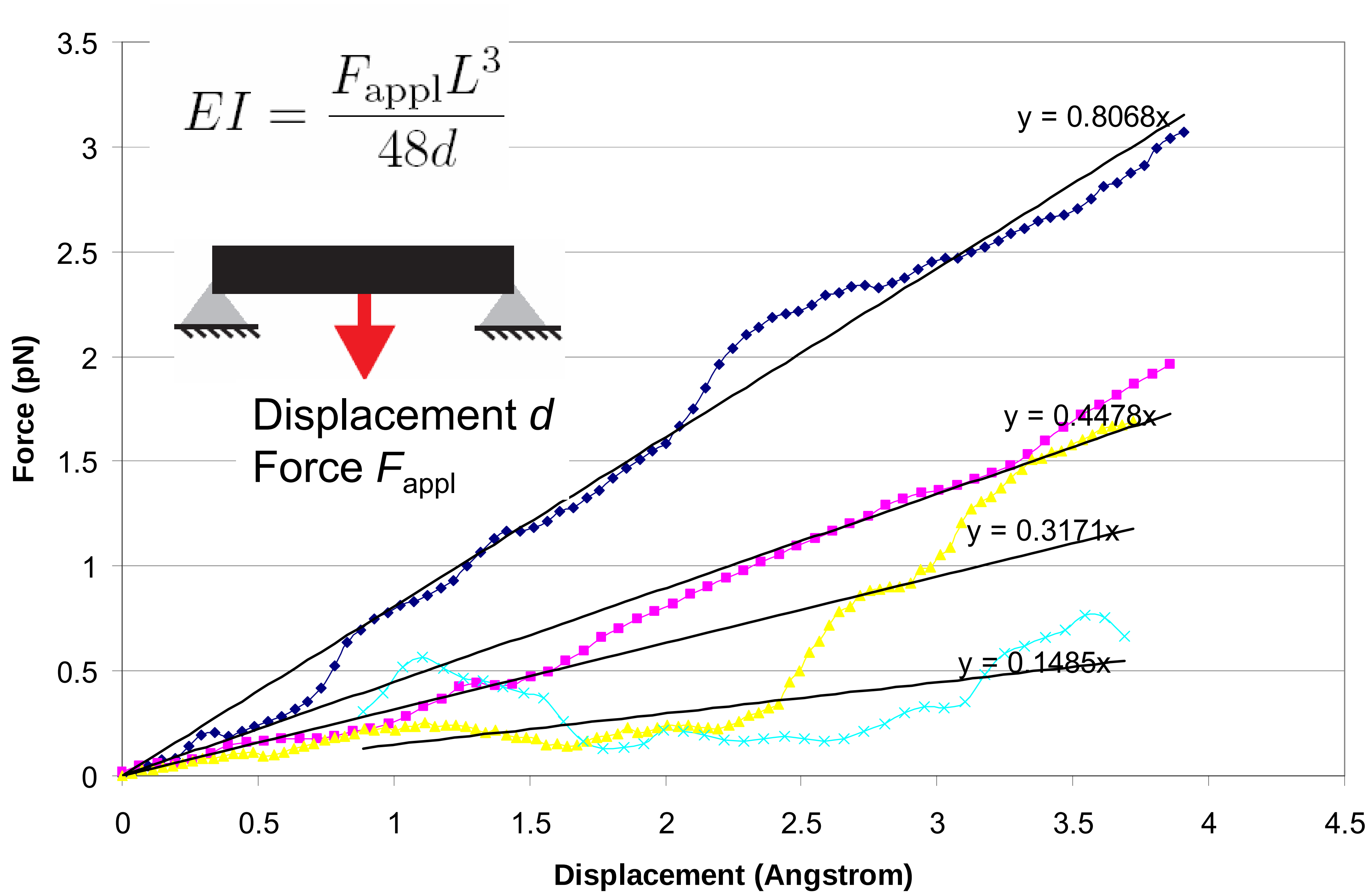
Unfolding of alpa helix structure





Ackbarow and Buehler, 2007

Three-point bending test: Tropocollagen molecule

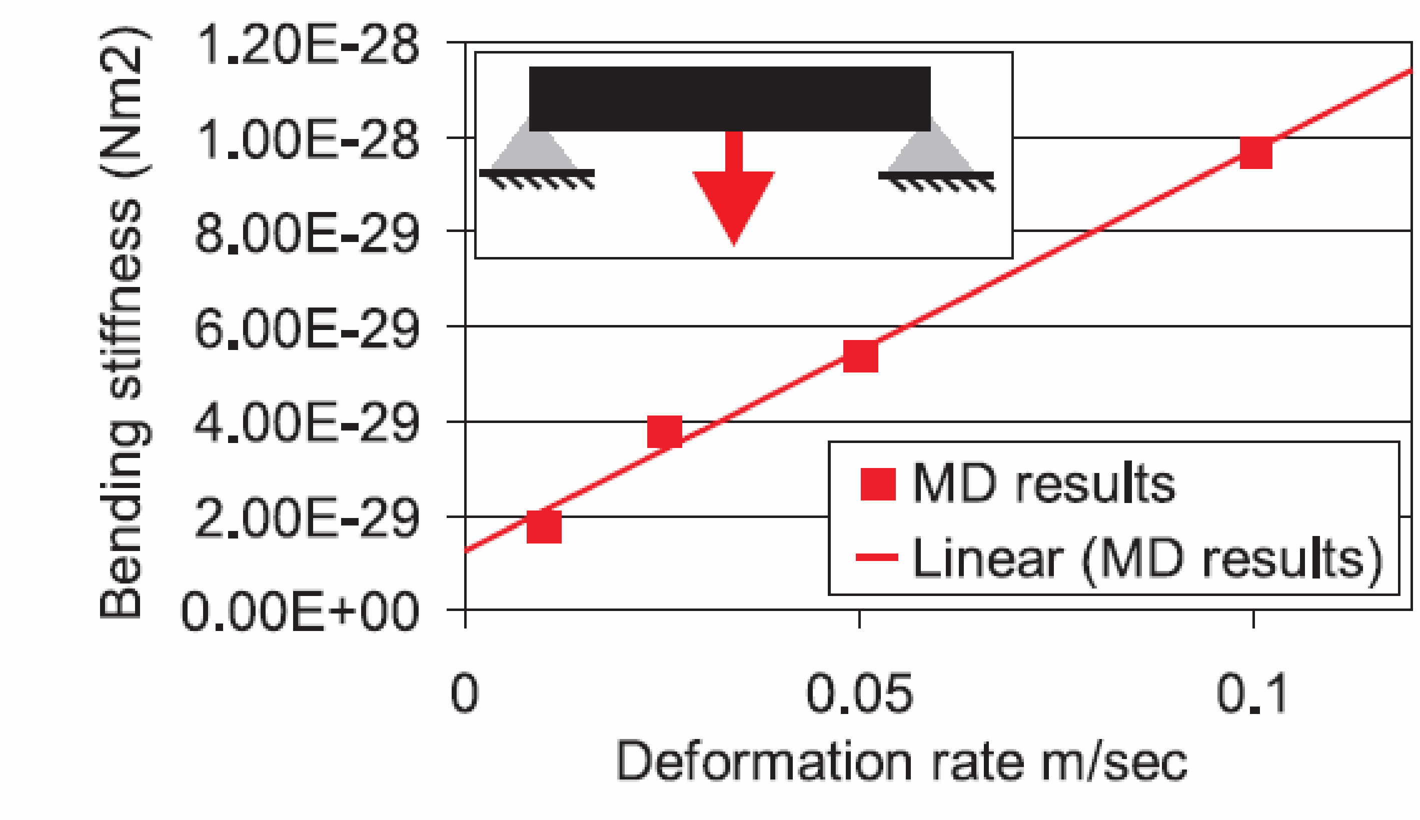


$$EI = \frac{F_{\mathrm{appl}} L^3}{48d}$$

Displacement d

Force F_{appl}

Three-point bending test: Tropocollagen molecule

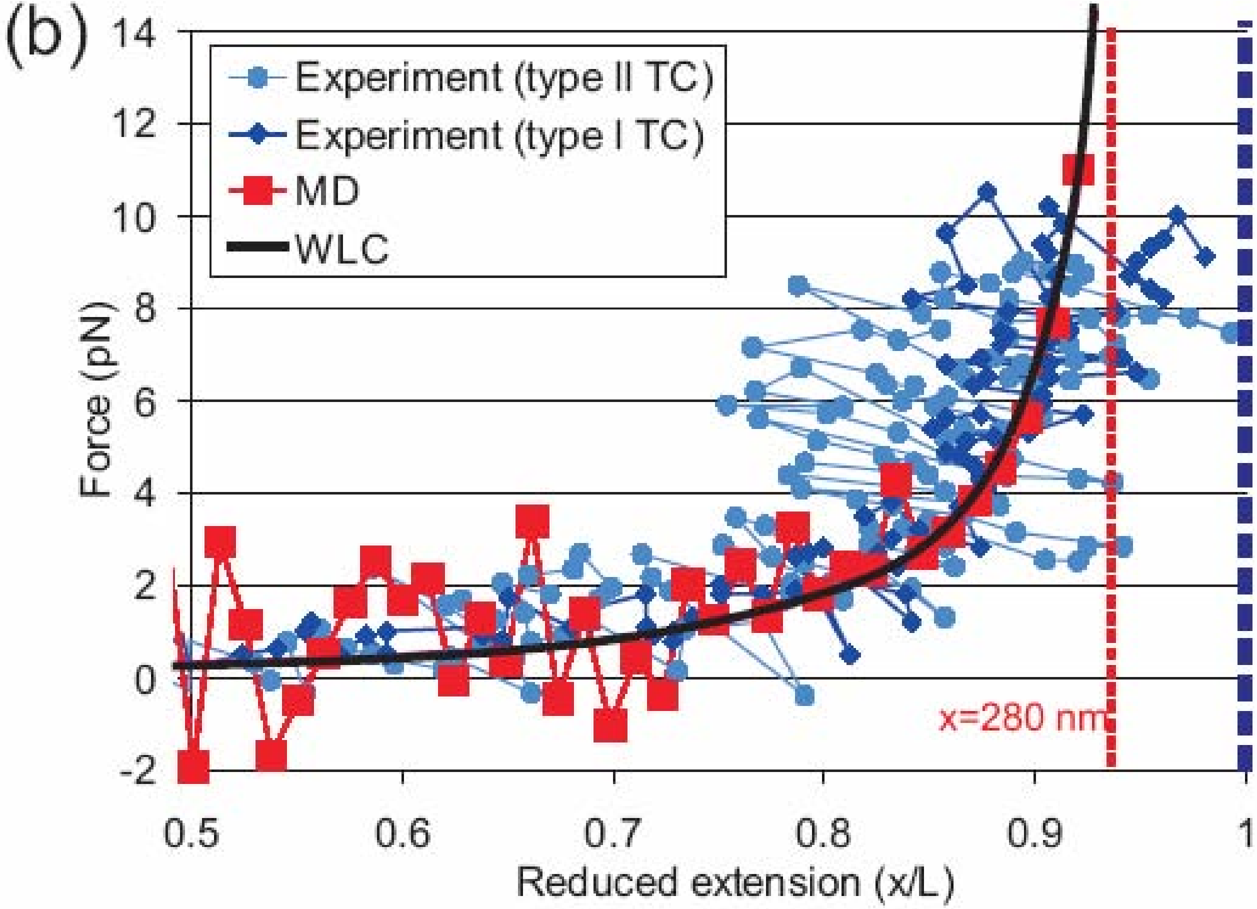


MD: Calculate bending stiffness; consider different deformation rates

Result: Bending stiffness at zero deformation rate (extrapolation)

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

Stretching experiment: Tropocollagen molecule



Buehler and Wong, 2007, unpublished