

**1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation**  
**Spring 2018**

# **How to model chemical interactions (cont'd)**

Lecture 7

Markus J. Buehler

**Laboratory for Atomistic and Molecular Mechanics**  
**Department of Civil and Environmental Engineering**  
**Massachusetts Institute of Technology**

E-mail: [mbuehler@MIT.EDU](mailto:mbuehler@MIT.EDU)

URL: <http://web.mit.edu/mbuehler/www/>



**Massachusetts Institute of Technology**

# Content overview

## I. Fundamentals of particle methods

1. Atoms, molecules, chemistry
2. Statistical mechanics
3. Molecular dynamics, Monte Carlo
4. Visualization and data analysis
5. Mechanical properties – application: how things fail (and how to prevent it)
6. Multi-scale modeling paradigm
7. Biological systems (simulation in biophysics) – how proteins work and how to model them

Lectures 1-12

February/March

## II. Advanced topics in particle methods

1. Quantum Weirdness: The Theory of Quantum Mechanics
2. The Many-Body Problem: From Many-Body to Single-Particle
3. Quantum modeling of materials
4. From Atoms to Solids
5. Basic properties of materials
6. Advanced properties of materials
7. Materials Informatics

Lectures 13-24

March/April/May

# Lecture 7: How to model chemical interactions

## Outline:

1. Review & closure: Model of fracture of brittle materials
2. Force fields for proteins (and polymers)

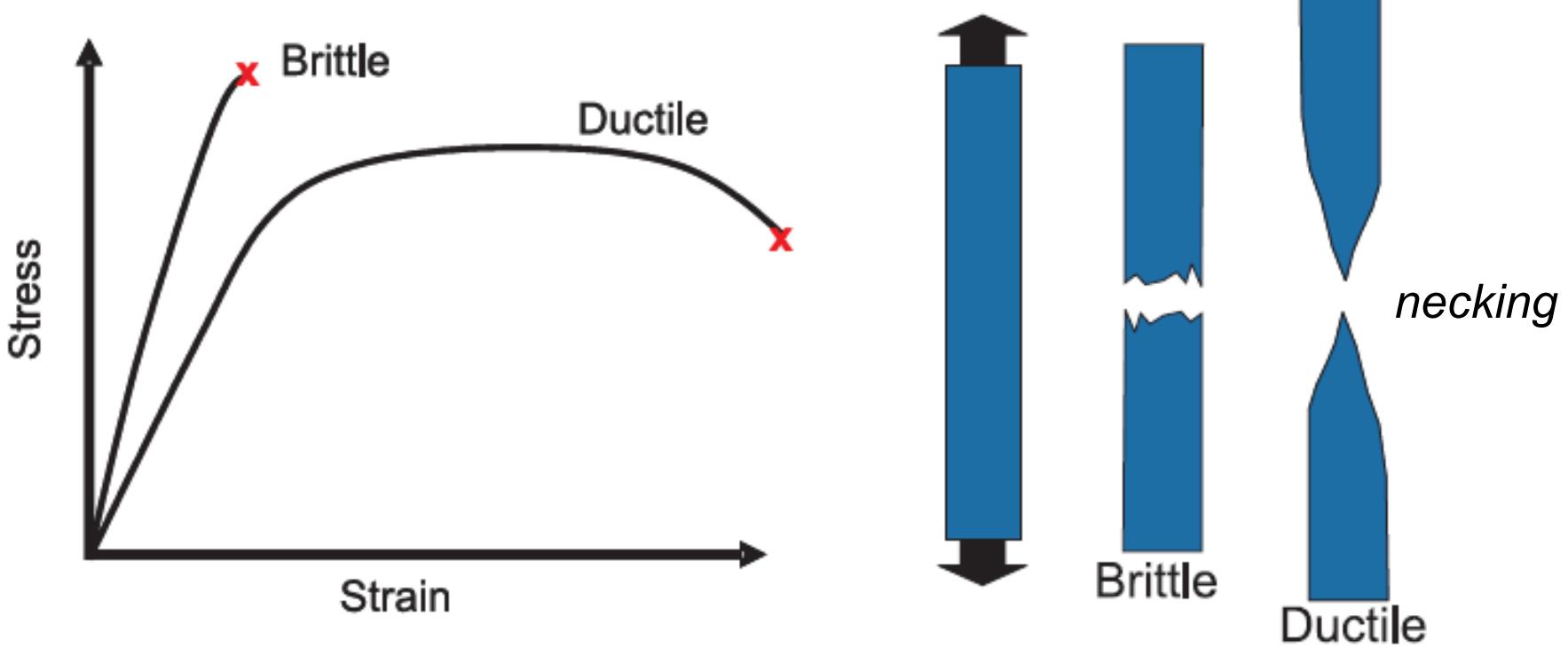
## Goal of today's lecture:

- Applications to model materials failure
- Learn about fracture (brittle fracture)
- Apply molecular dynamics to understand earthquake dynamics
- Learn how to develop force fields for proteins and similar materials

# **1. Review & closure: Model of fracture of brittle materials**

# Tensile test of a wire

copper nanowire? (pset #1)



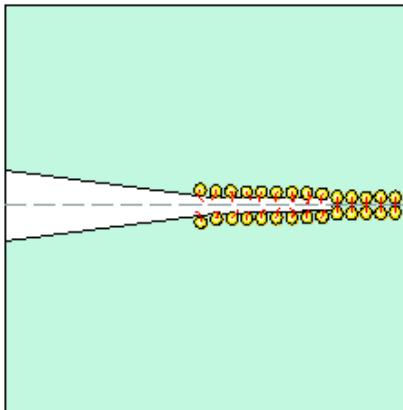
stress == applied force / cross-sectional area of specimen

# Ductile versus brittle materials

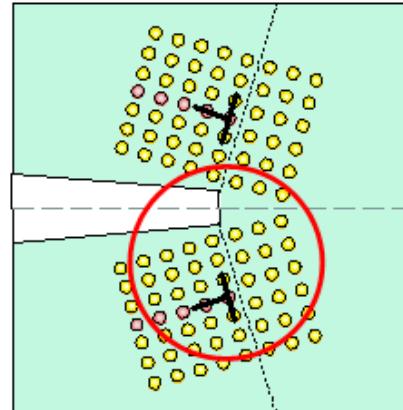
Glass  
Polymers  
Ice  
Silicon

***Difficult  
to deform,  
breaks easily***

**brittle**

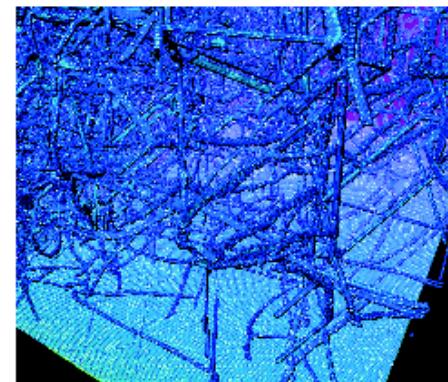
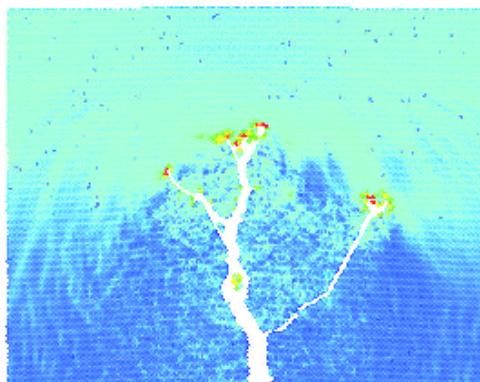


**ductile**



Copper,  
Gold,  
Nickel  
Platinum

***Easy to deform  
hard to break***



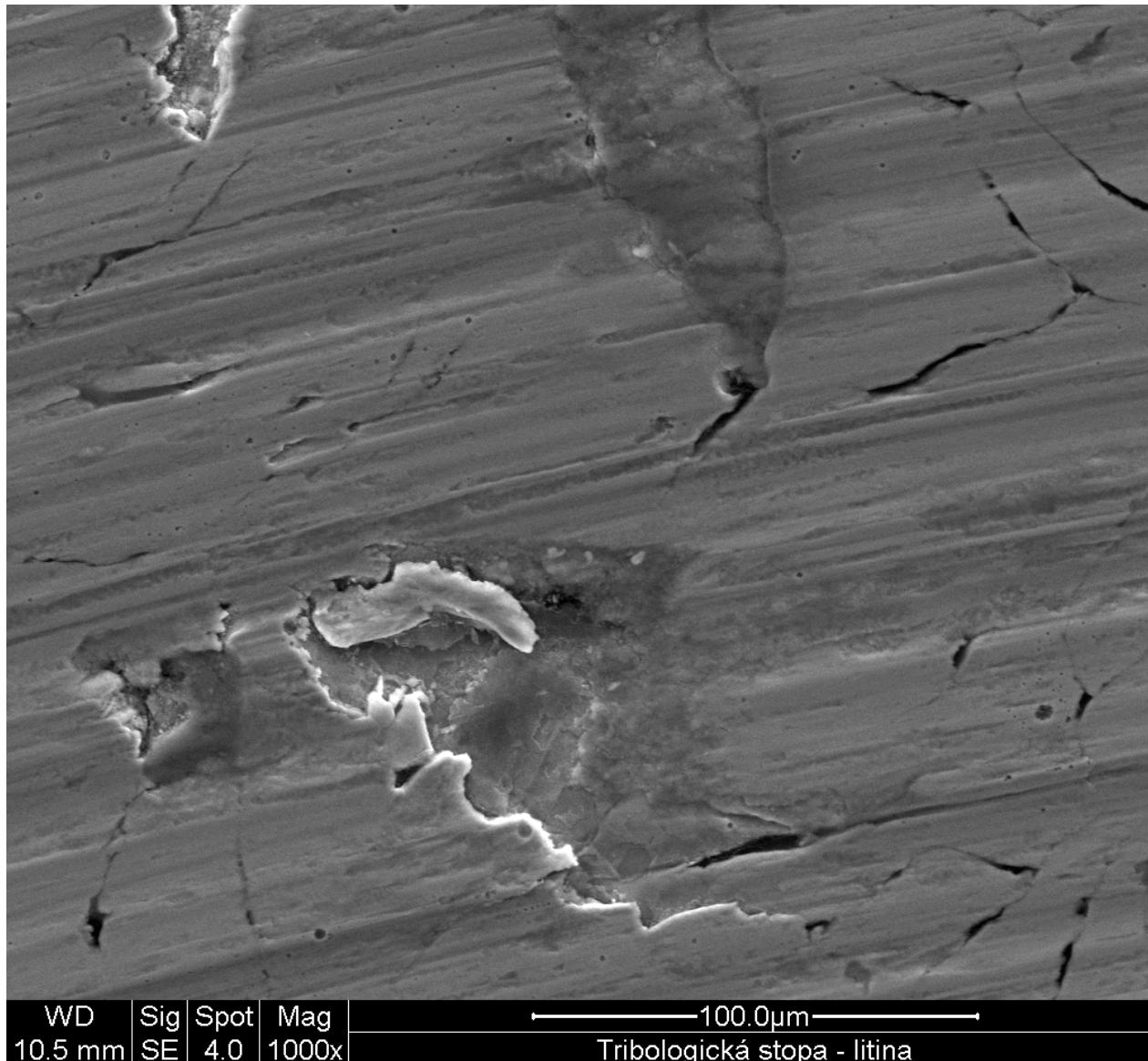
# Deformation of materials: Nothing is perfect, and flaws or cracks matter



**Failure of materials initiates at cracks**

**Griffith, Irwine** and others: Failure initiates at defects, such as cracks, or grain boundaries with reduced traction, nano-voids, other imperfections 7

# SEM picture of material: nothing is perfect



# Brittle fracture is catastrophic

- Materials: **glass, silicon, many ceramics, rocks**
- At large loads, rather than accommodating a shape change, materials break

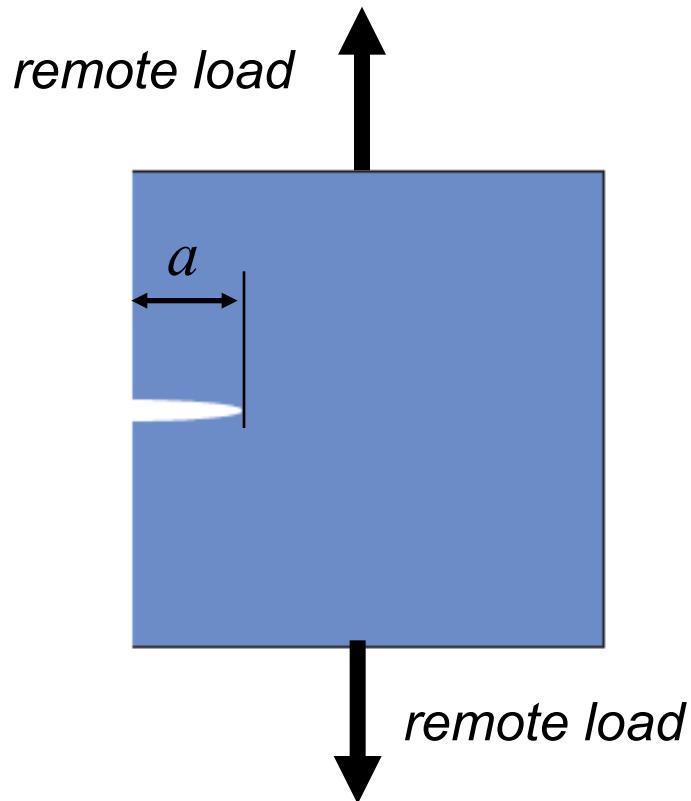




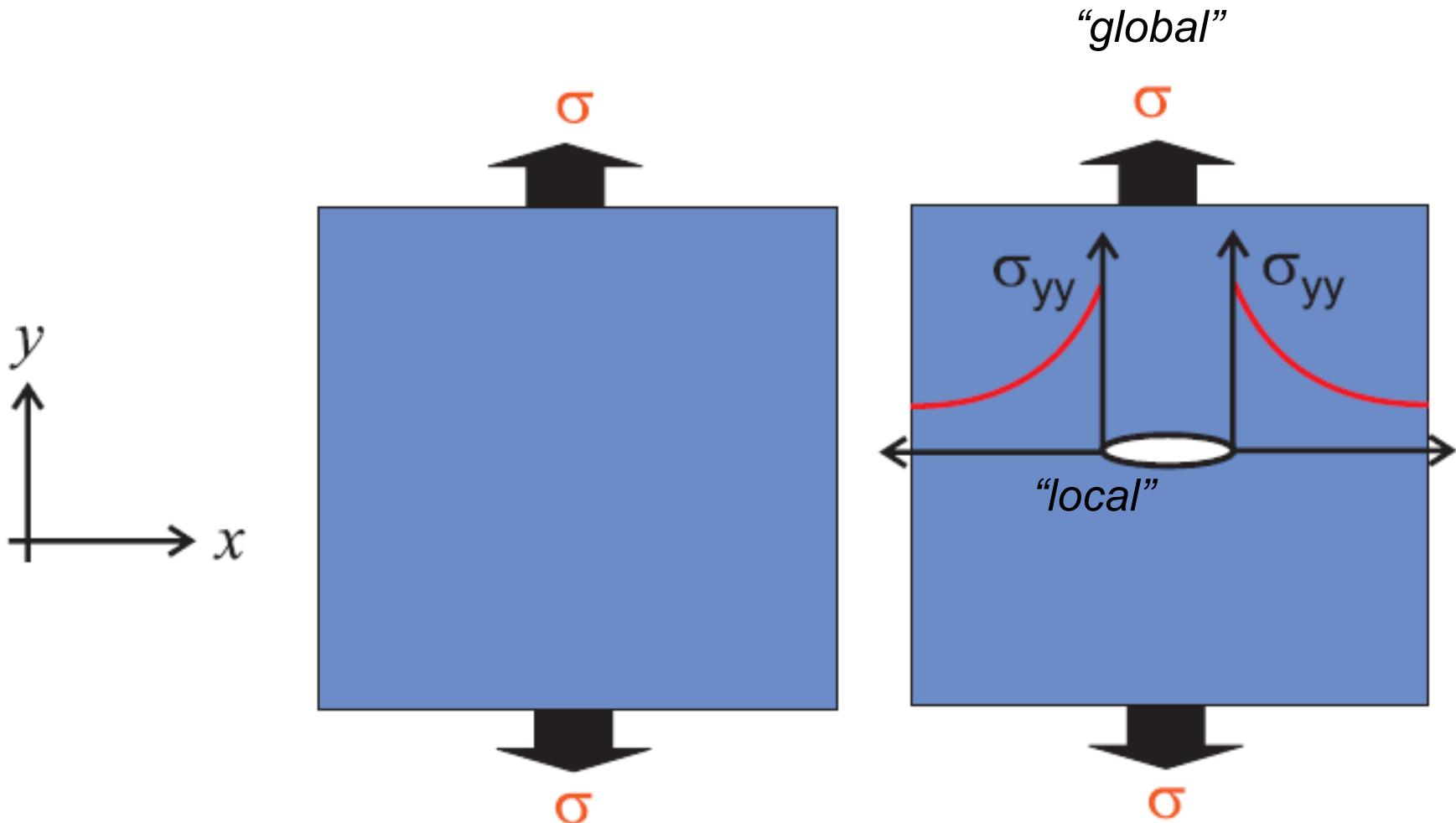


# Science of fracture: model geometry

- Typically consider a single crack in a crystal
- Remotely applied mechanical load
- Following discussion focused on single cracks and their behavior

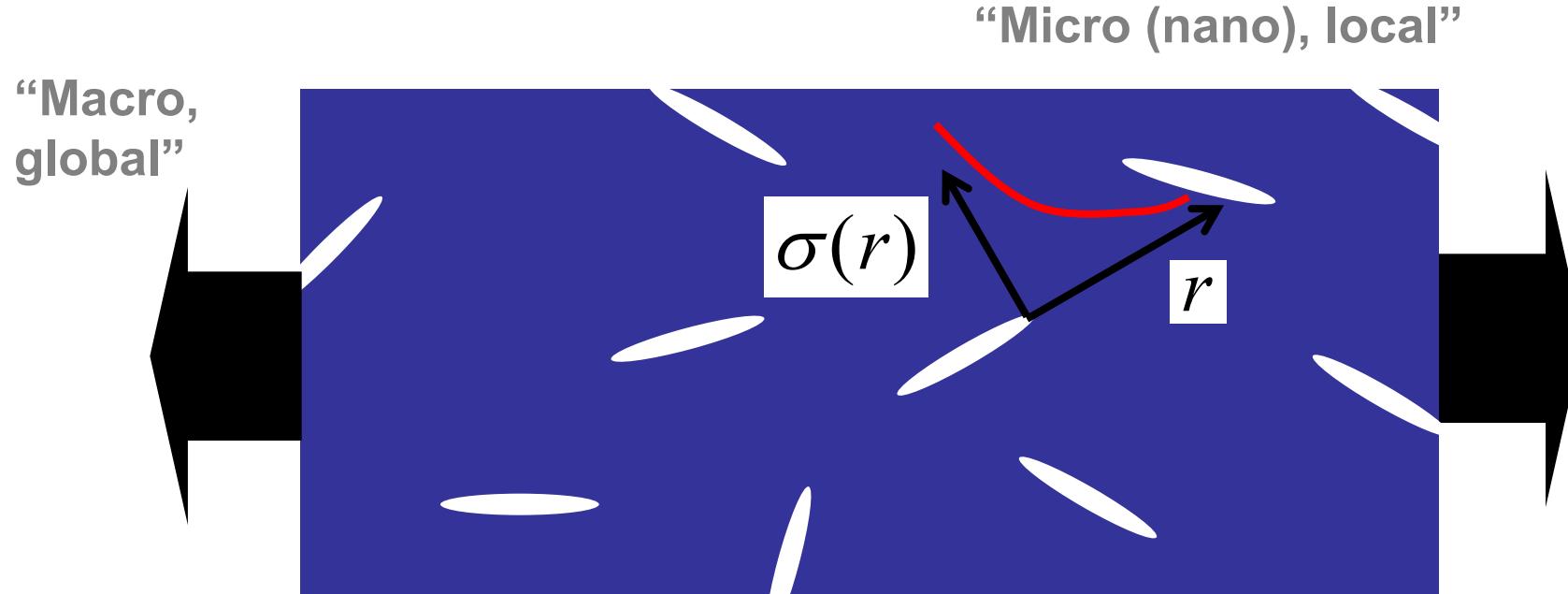


# Significance of material flaws



Stress concentrators: **local stress >> global stress** 13

# Deformation of materials: Nothing is perfect, and flaws or cracks matter



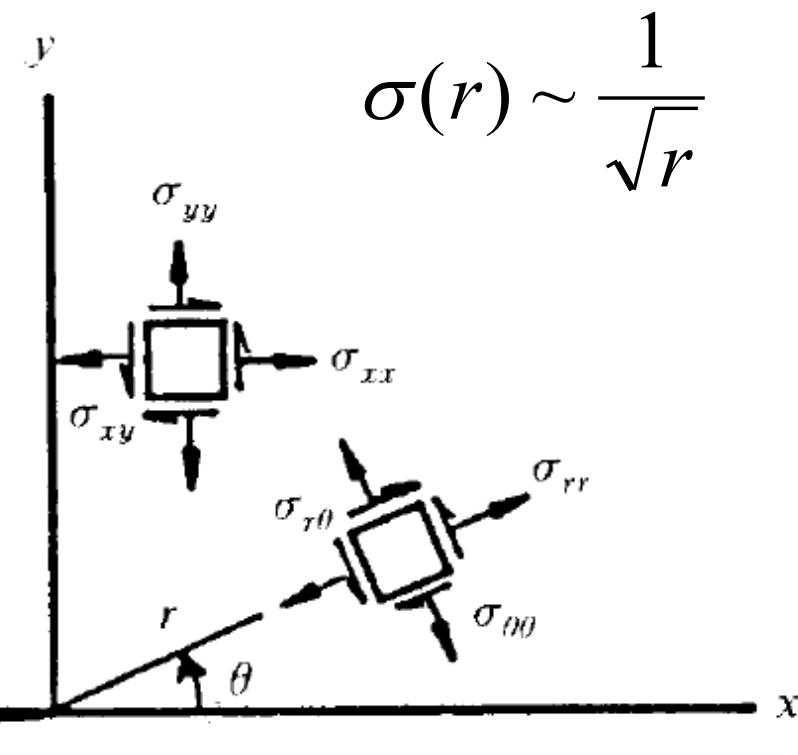
**Failure of materials initiates at cracks**

**Griffith, Irwine** and others: Failure initiates at defects, such as cracks, or grain boundaries with reduced traction, nano-voids, other imperfections 14

# Cracks feature a singular stress field, with singularity at the tip of the crack

stress tensor

$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{Bmatrix} = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \begin{Bmatrix} 1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \\ 1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \\ \sin \frac{\theta}{2} \cos \frac{3\theta}{2} \end{Bmatrix}$$

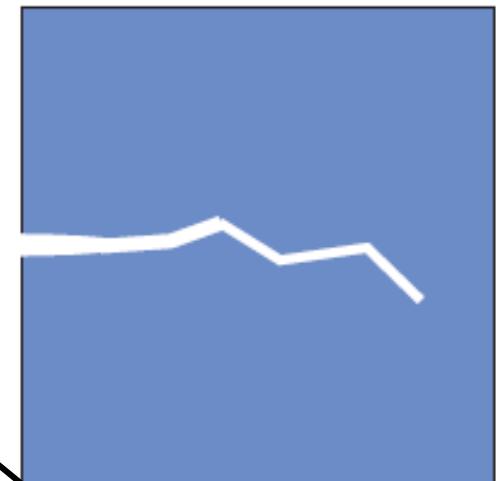
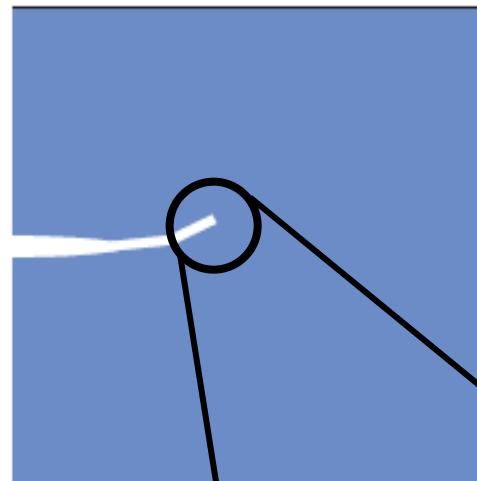
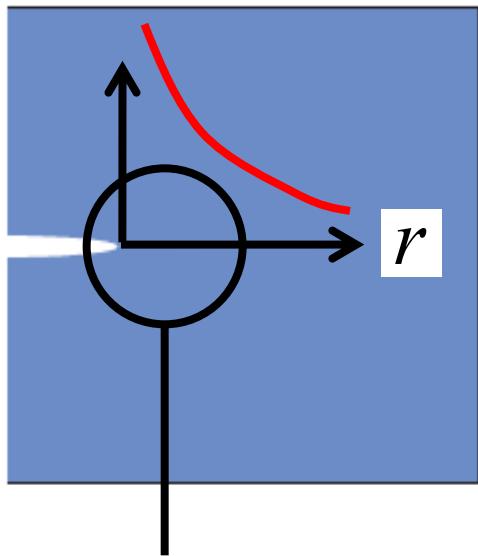


$$\sigma(r) \sim \frac{1}{\sqrt{r}}$$

$K_I$  : Stress intensity factor (function of geometry)

# Crack extension: brittle response

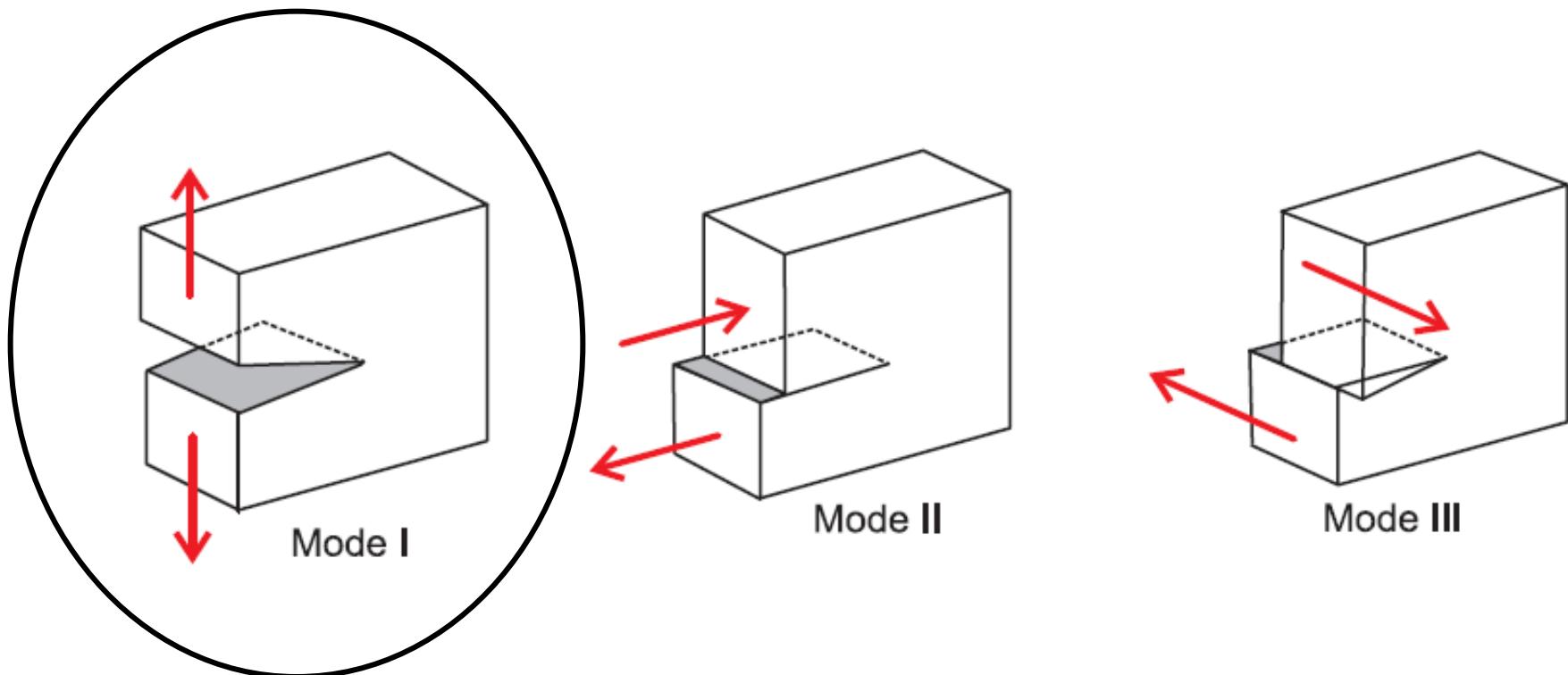
$$\sigma(r)$$



*Large stresses lead to  
rupture of chemical  
bonds between atoms  
Thus, crack extends*

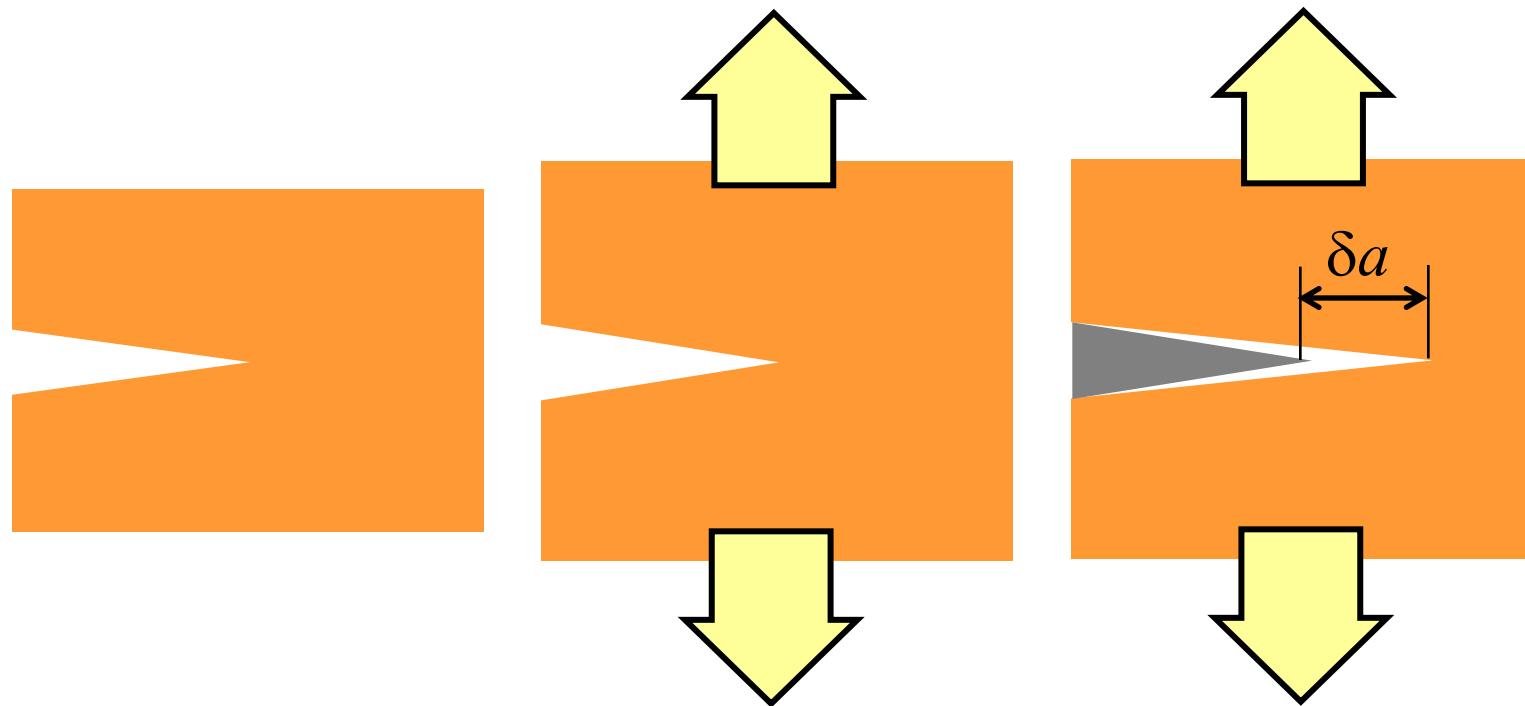
# Brittle fracture loading conditions

- Commonly consider a single crack in a material geometry, under three types of loading: mode I, mode II and mode III



*Tensile load, focus  
of this lecture*

# Basic fracture process: dissipation of elastic energy



Undeformed



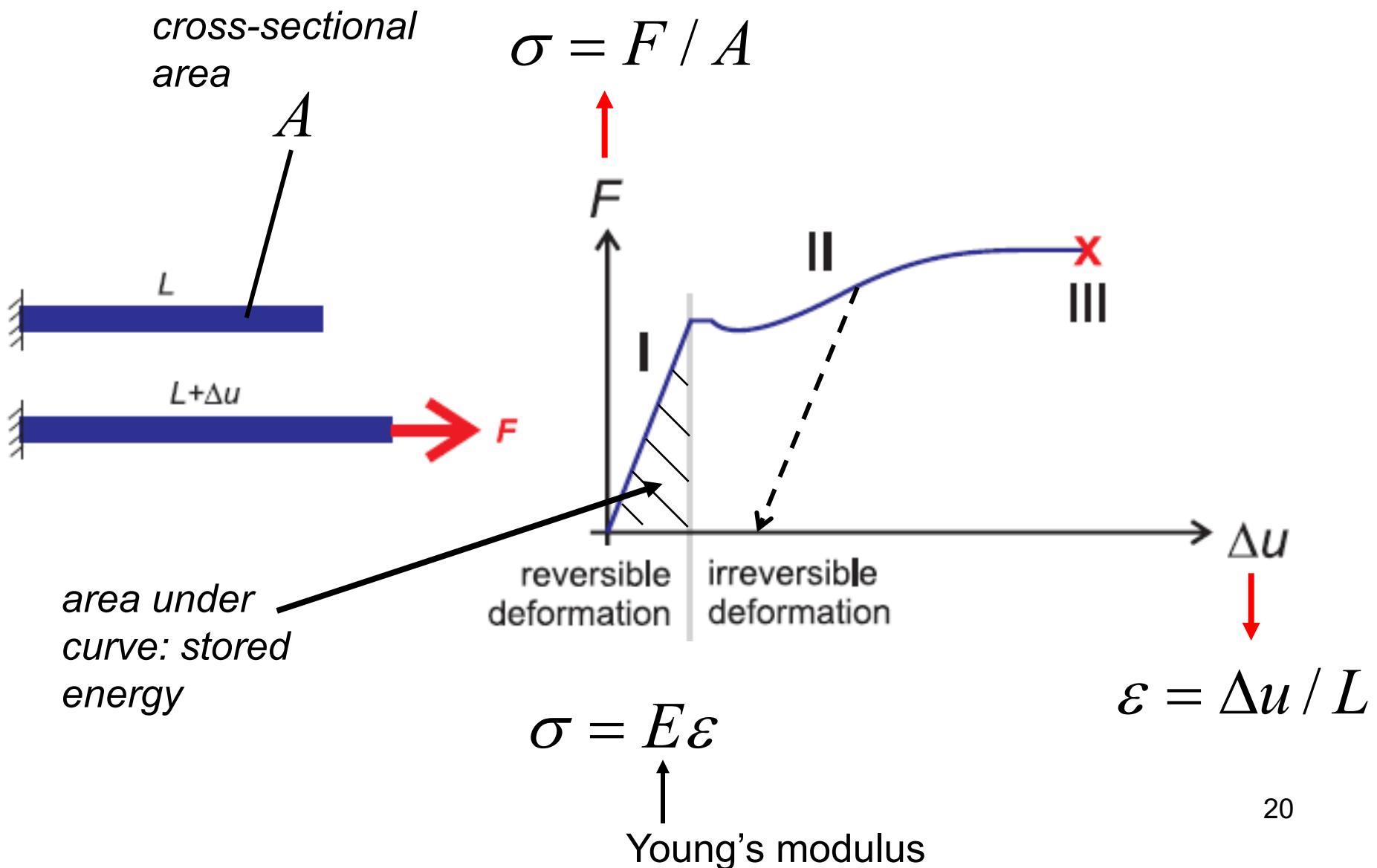
Stretching=store elastic energy



Release elastic energy  
dissipated into breaking  
chemical bonds  
---SURFACE ENERGY!

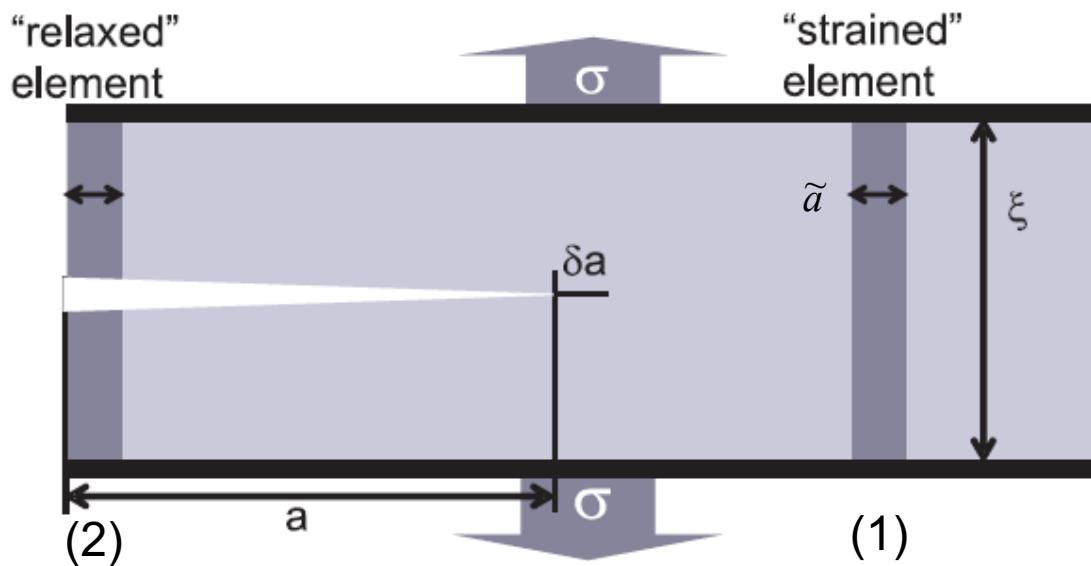
# *A theory to predict the onset of fracture*

# Elasticity = reversible deformation



# Continuum description of fracture

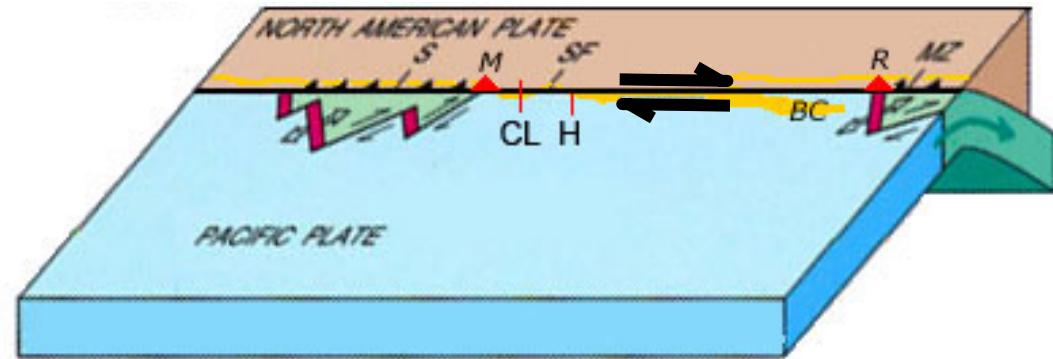
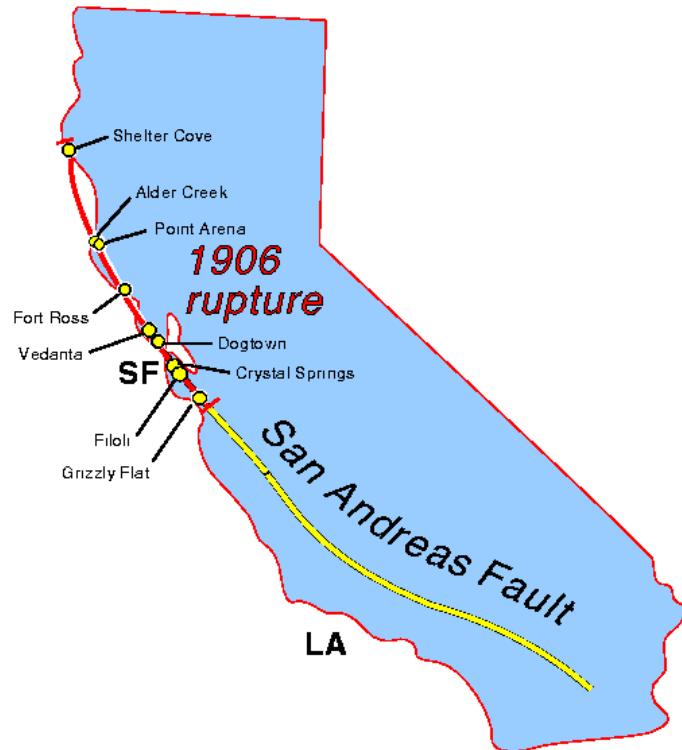
- Fracture is a dissipative process in which elastic energy is dissipated to break bonds (and to heat at large crack speeds)
- Energy to break bonds = surface energy  $\gamma_s$  (energy necessary to create new surface, dimensions: energy/area, Nm/m<sup>2</sup>)



$$\left. \begin{aligned} W_P(1) &= \frac{1}{2} \frac{\sigma^2}{E} V = \frac{1}{2} \frac{\sigma^2}{E} \xi \tilde{a} B \\ W_P(2) &= 0 \end{aligned} \right\} \quad \begin{aligned} W_P(2) - W_P(1) &= \underbrace{\frac{1}{2} \frac{\sigma^2}{E} \xi \tilde{a} B}_{\text{change of elastic (potential) energy}} \stackrel{!}{=} 2 \gamma_s \tilde{a} B \\ &\text{energy to create surfaces} \end{aligned}$$

$$\sigma = \sqrt{\frac{4 \gamma_s E}{\xi}}$$

# Earthquakes: “brittle” failure of the Earth



Once critical load exceeds, failure initiates

Critical condition given by “critical energy release rate”: Dissipation of recoverable (elastic) energy equals surface energy



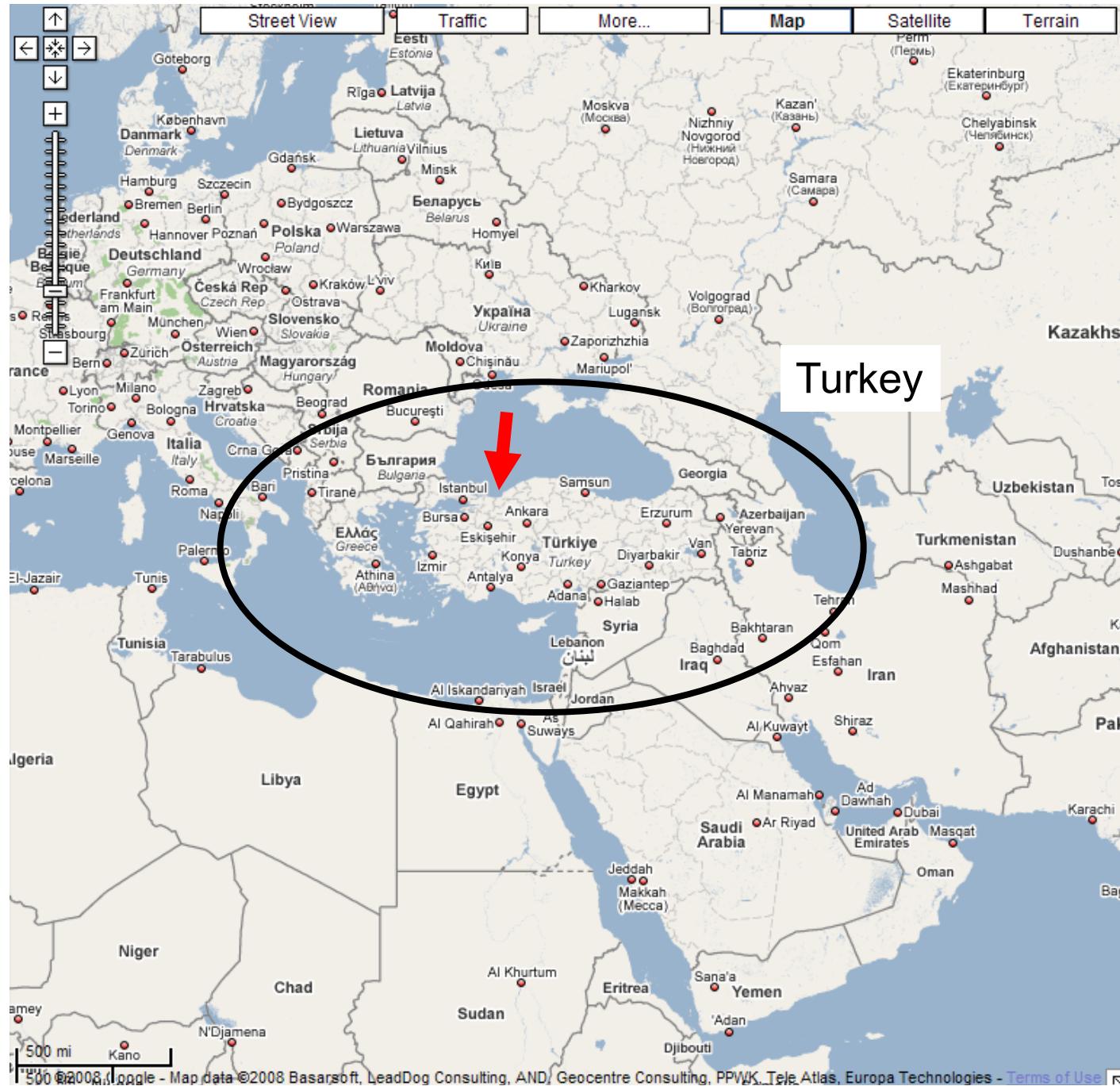
Undeformed



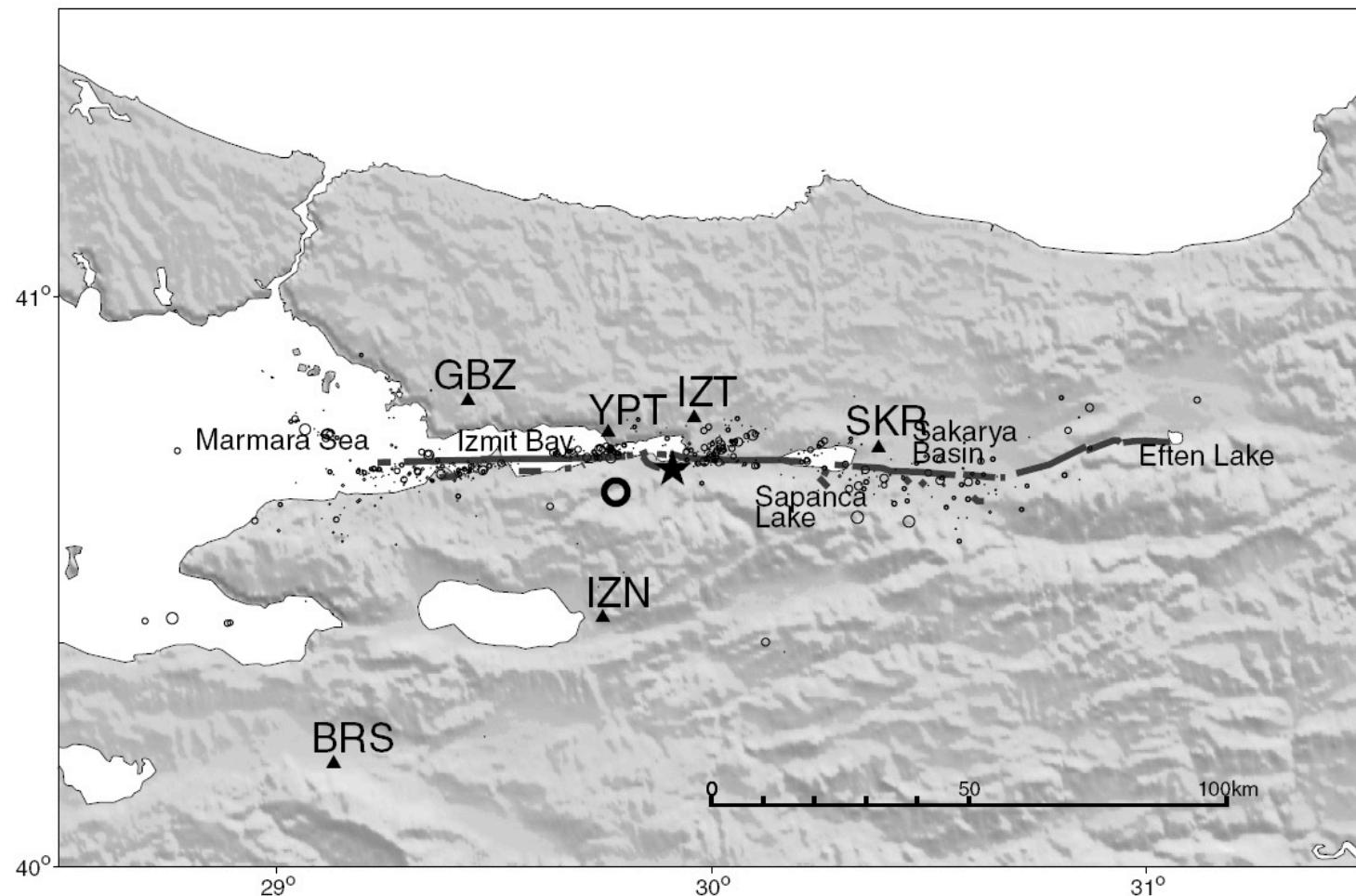
Stretching=store elastic energy



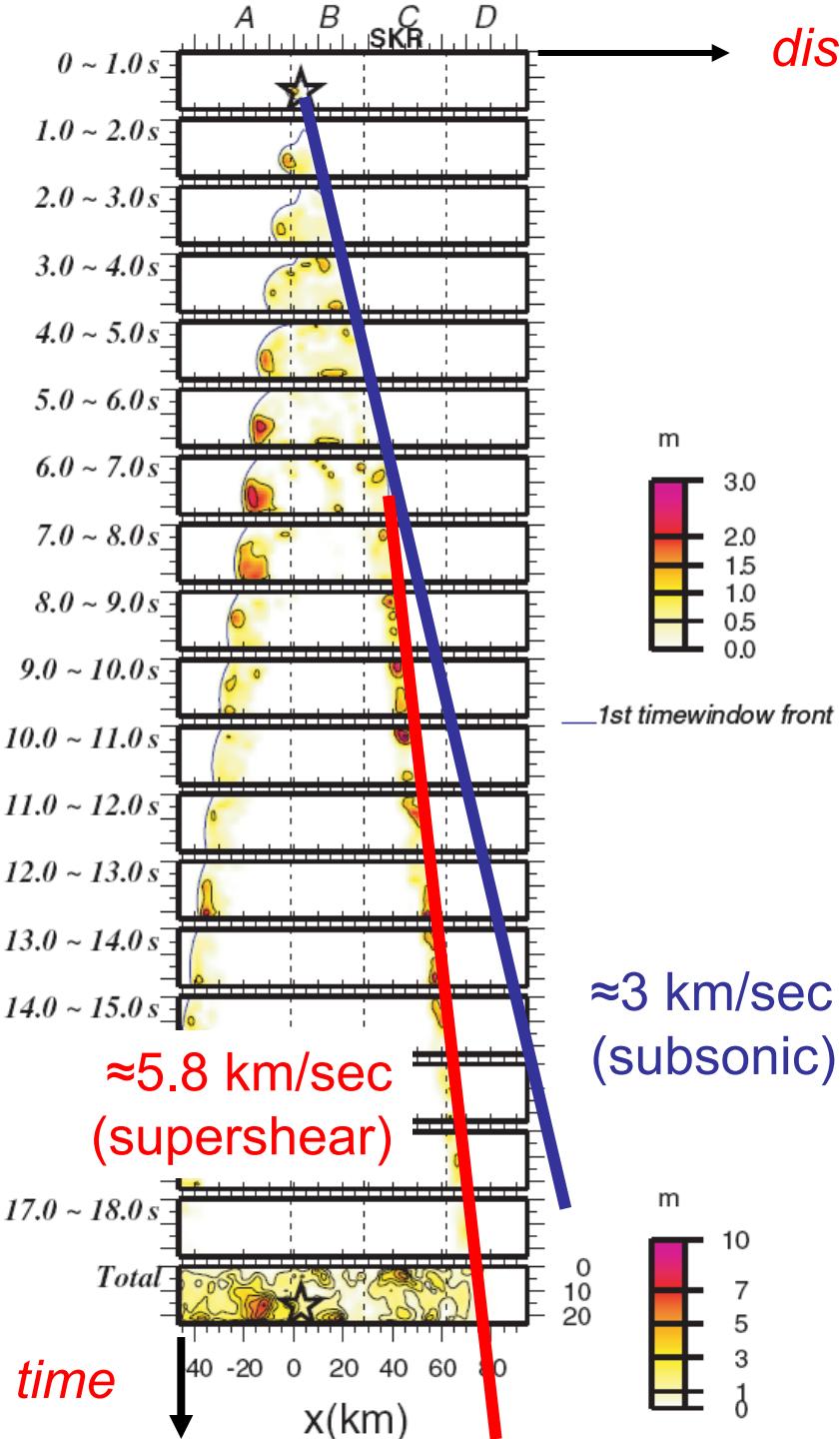
Release elastic energy  
dissipated into breaking  
chemical bonds



# Earthquake dynamics (1999 Kocaeli, Turkey)



Sekiguchi et al., *Bulletin of the Seismological Society of America*, 92, 1, pp. 300–311, February 2002

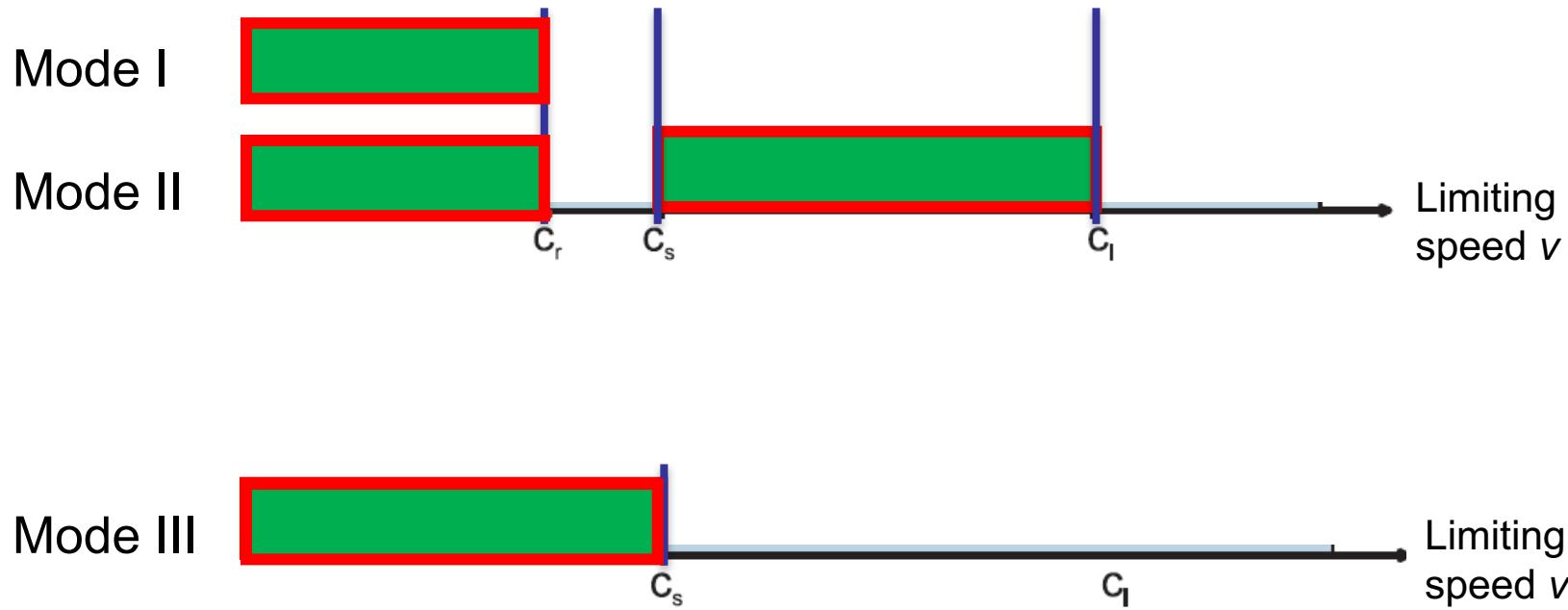


“Then about 7.0 sec after the origin time, a strong moment release is triggered just behind the first time-window front moving at 5.8 km/sec [...]”

***Significance: hints at intersonic fracture!***

Sekiguchi et al., *Bulletin of the Seismological Society of America*, 92, 1, pp. 300–311, February 2002

# Limiting speeds of cracks: linear elastic continuum theory



- Cracks **can not exceed** the limiting speed given by the corresponding wave speeds **unless material behavior is nonlinear**
- Cracks that exceed limiting speed would produce energy (physically impossible - ***linear elastic continuum theory***)

# Sound speeds in materials: overview

Material	$c_R$ (in m/s)	$c_s$ (in m/s)	$c_l$ (in m/s)
Steel	2,940	3,200	6,000
Al	2,850	3,100	6,300
Glass	3,030	3,300	5,800
PMMA	920	1,000	2,400

Wave speeds are calculated based on elastic properties of material

$$c_l = \sqrt{\frac{3\mu}{\rho}} \quad c_s = \sqrt{\frac{\mu}{\rho}} \quad c_R \approx \beta c_s \quad \beta \approx 0.923$$

$\mu$  = shear modulus

$$E = 8/3\mu$$

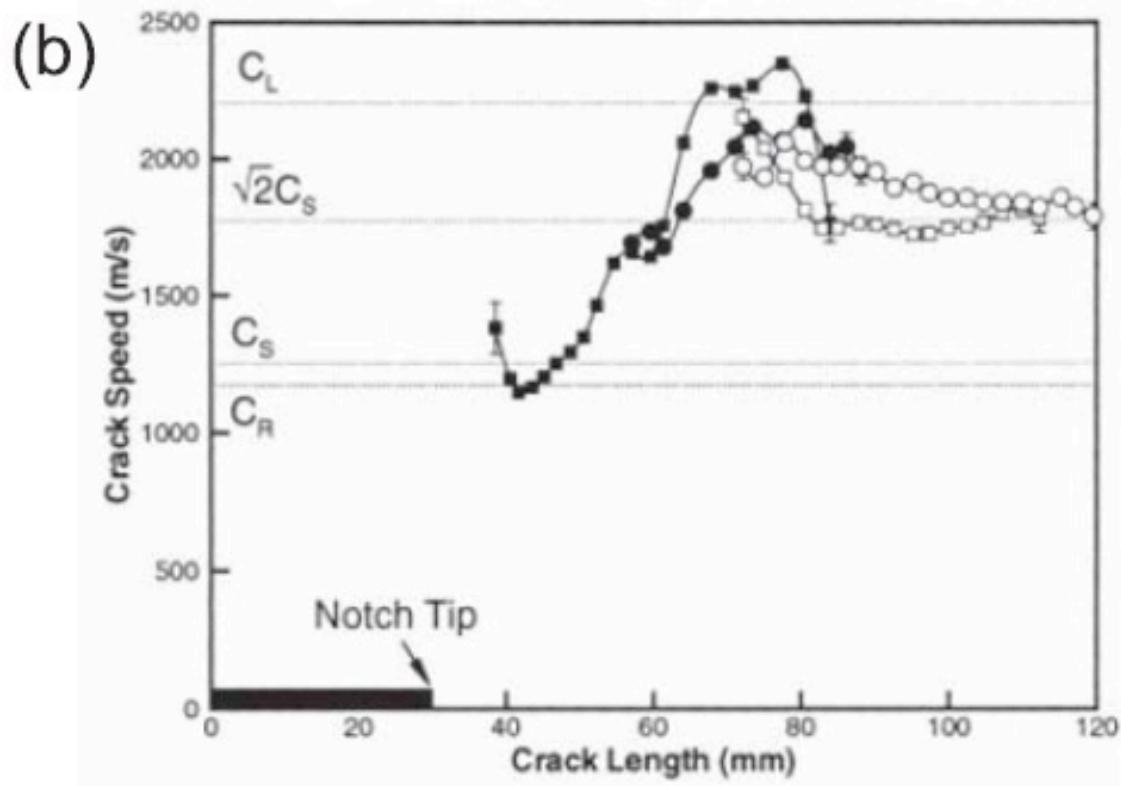
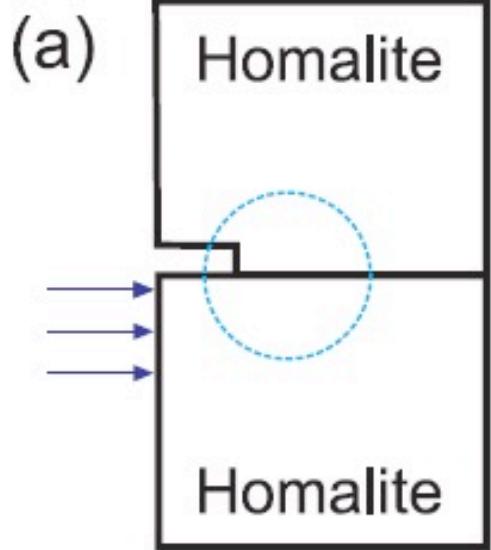
$$\mu = 3/8E$$

# *Experiment evidence (“laboratory earthquakes” at Caltech)*



Ares Rosakis

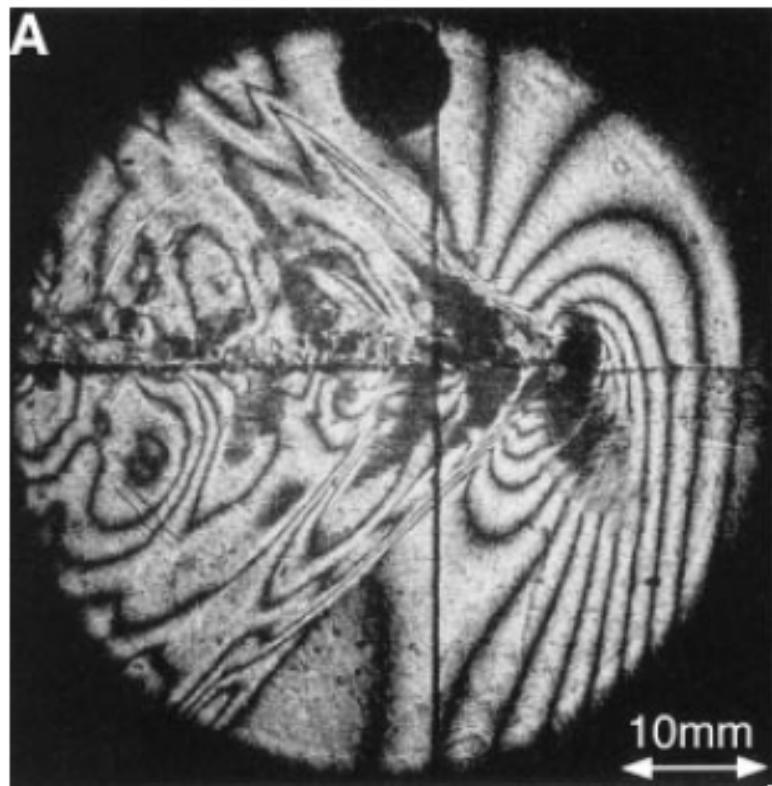
# Experiment: intersonic cracks



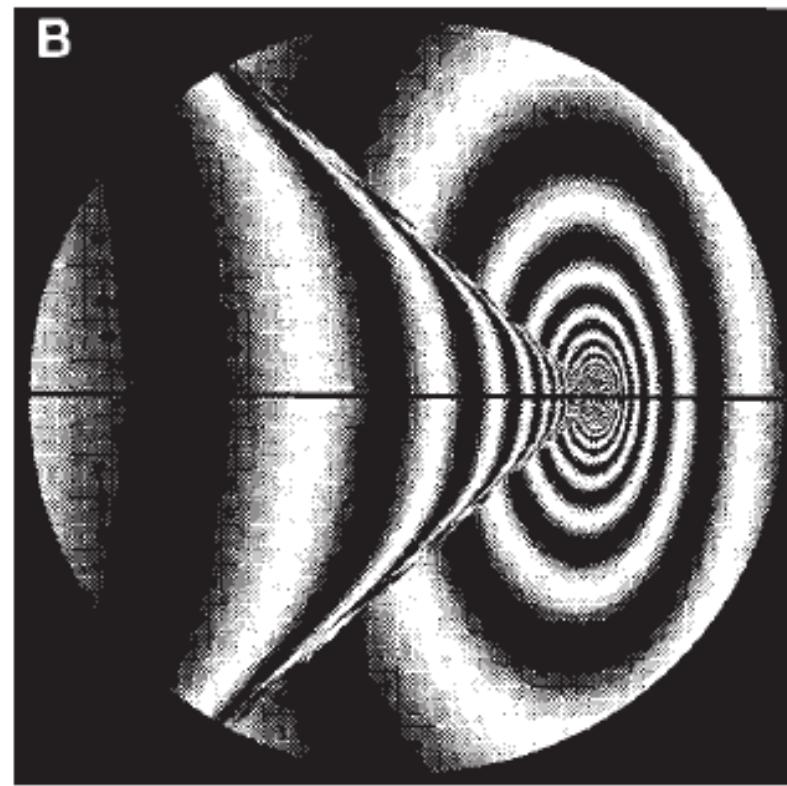
Rosakis et al., *Science*, 1999  
**Paper posted on Stellar**

# Experiment: intersonic cracks (47% faster than shear wave speed)

*Isochromatic fringe pattern around a steady-state mode II intersonic crack along a weak plane in Homalite-100*

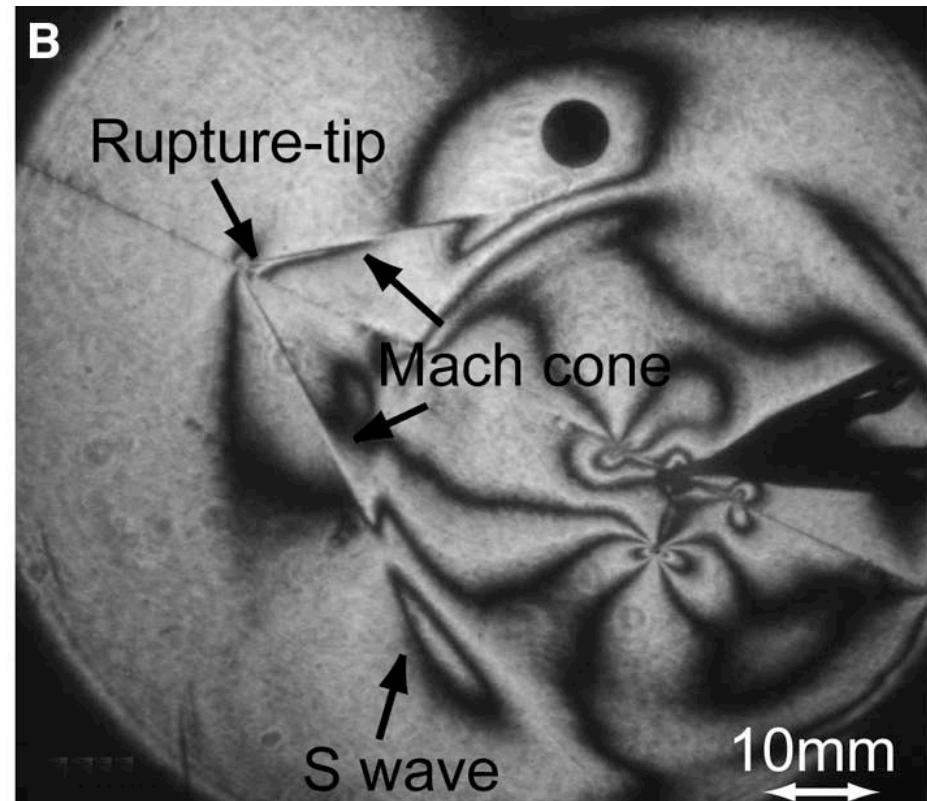
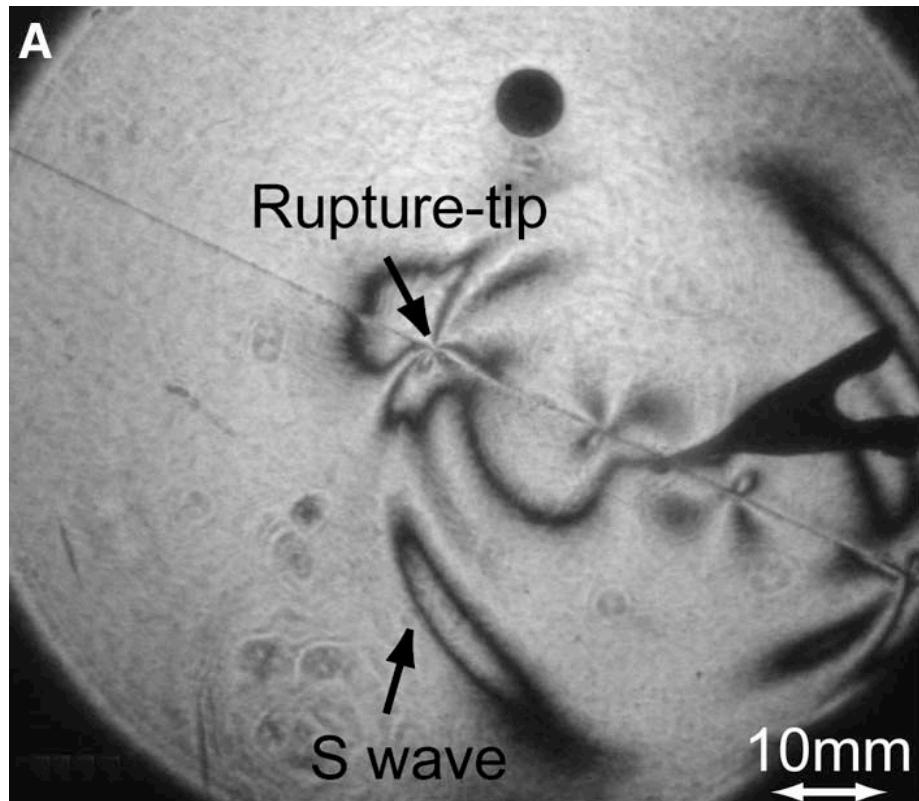


Experiment



Theory (L.B. Freund)

# Experiment: intersonic cracks



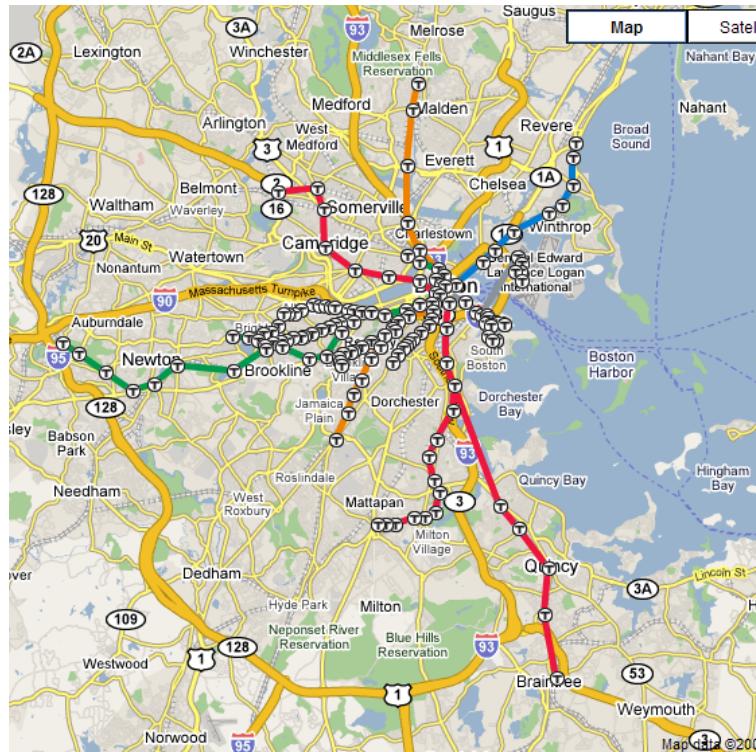
K. Xia, A. Rosakis et al., *Science*, 2004  
*Paper posted on Stellar*

*Building an atomistic model*

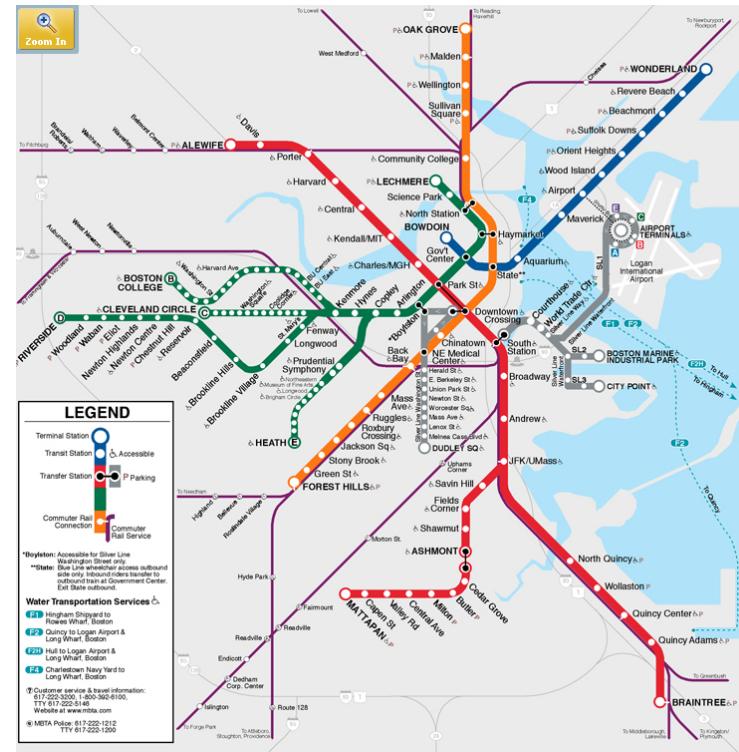
# Model building - review

Mike Ashby (Cambridge University):

- A model is an idealization. Its relationship to the real problem is like that of the map of the London tube trains to the real tube systems: a gross simplification, but one that captures certain essentials.



“Physical situation”



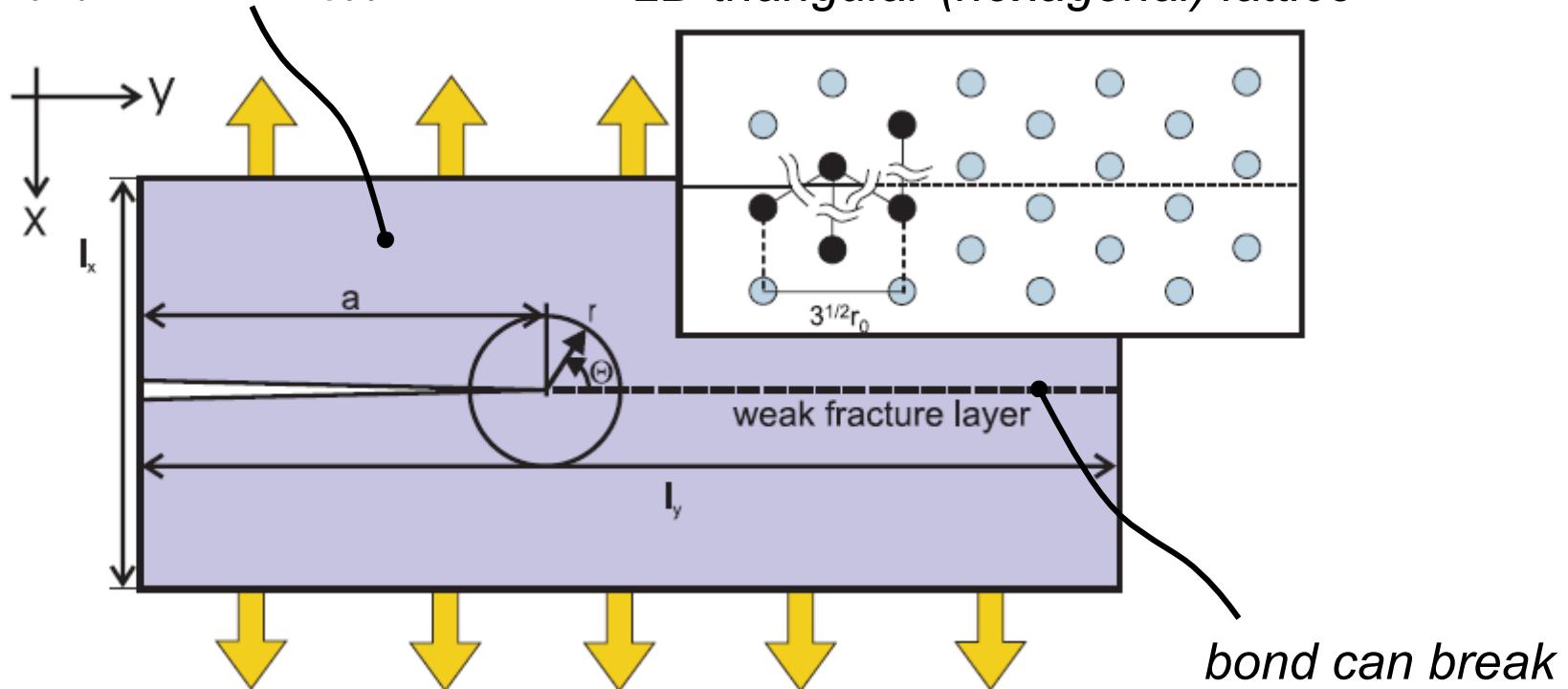
“Model”

# A “simple” atomistic model: geometry

$$\phi = \frac{1}{2} k_0 (r - r_0)^2$$

elasticity (store energy)

*stable configuration of pair potential*  
*2D triangular (hexagonal) lattice*



*bond can break*

*Pair potential to describe atomic interactions*

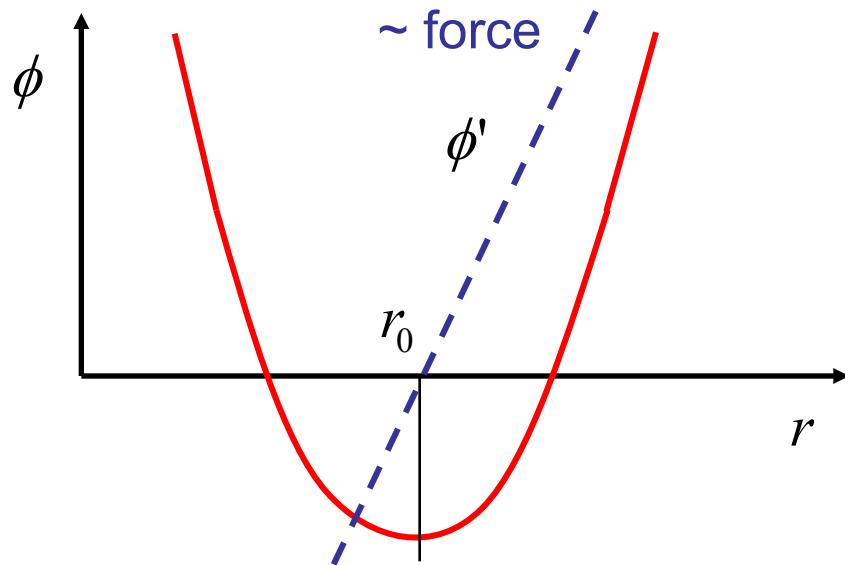
*Confine crack to a 1D path (weak fracture layer):*

*Define a pair potential*

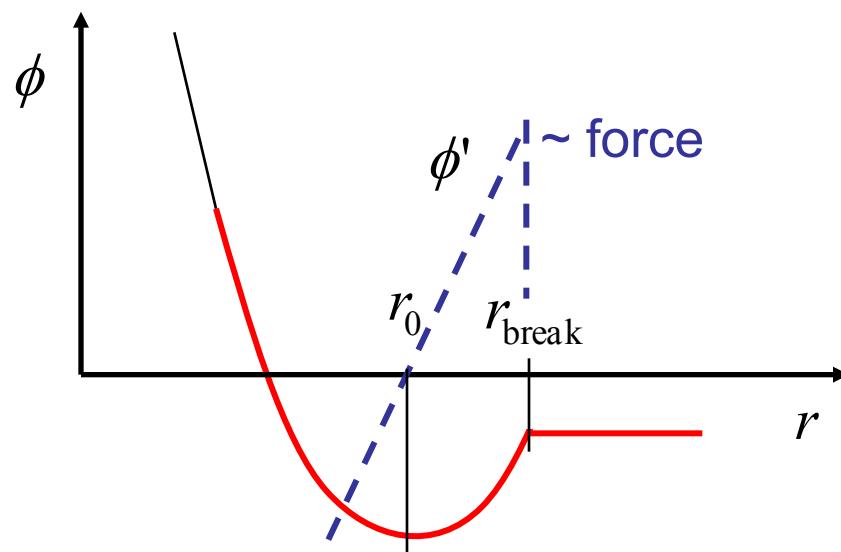
*whose bonds never break (bulk) and a potential  
 whose bonds break*

$$\phi = \begin{cases} \frac{1}{2} k_0 (r - r_0)^2 & r < r_{\text{break}} \\ \frac{1}{2} k_0 (r_{\text{break}} - r_0)^2 & r \geq r_{\text{break}} \end{cases}$$

# Harmonic and harmonic bond snapping potential



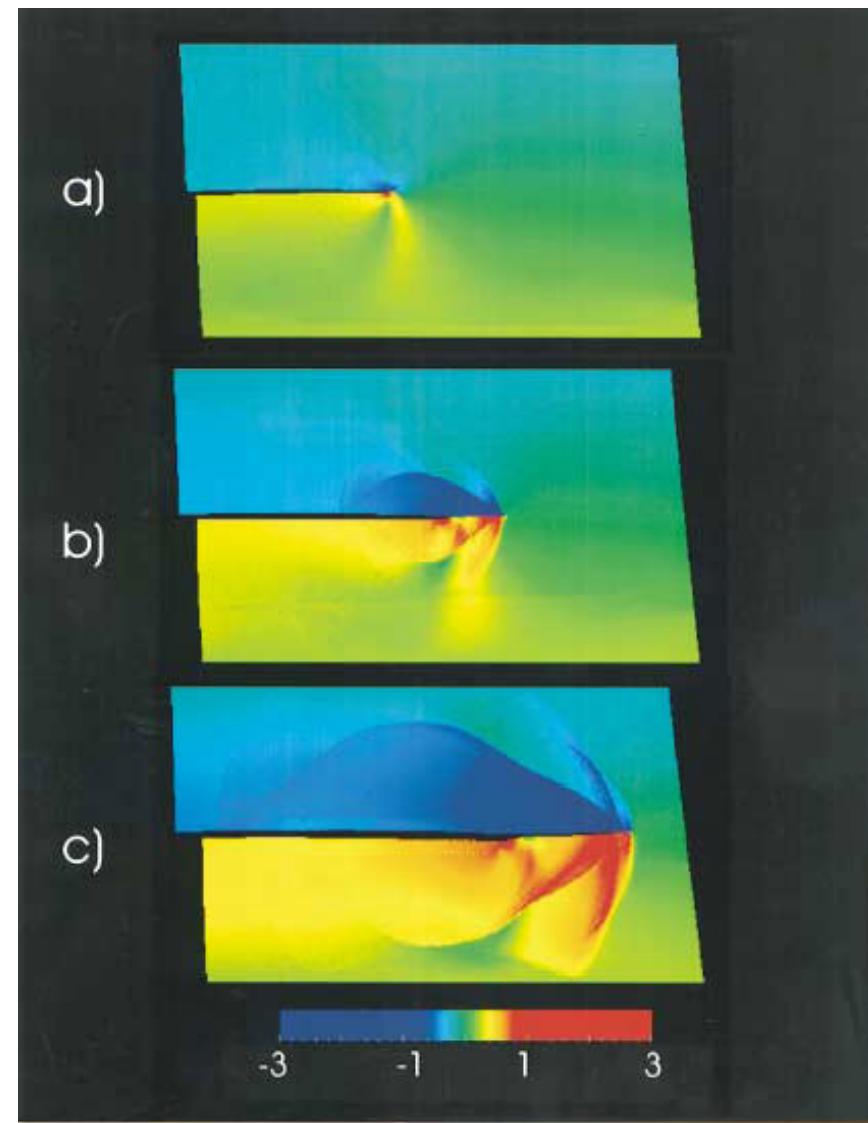
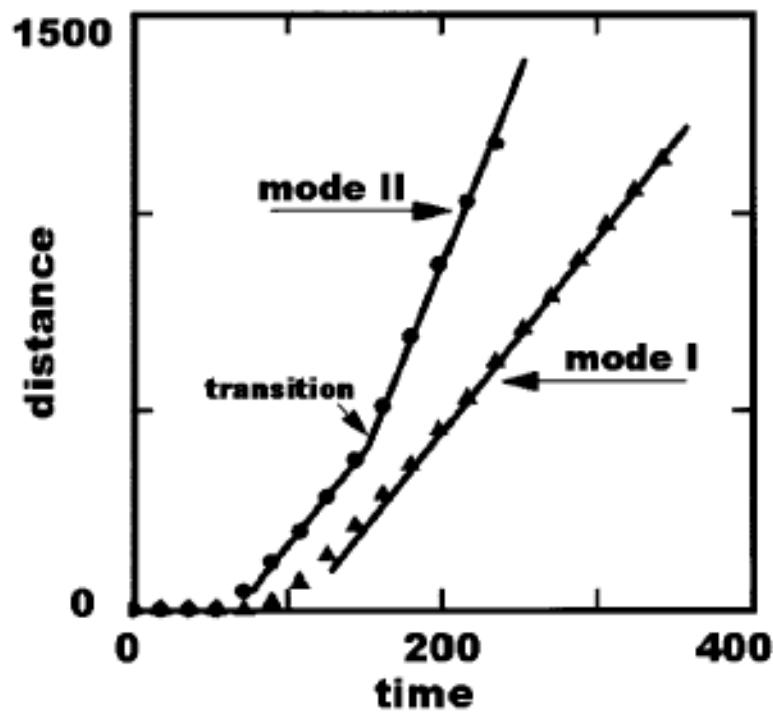
$$\phi = \frac{1}{2}k_0(r - r_0)^2$$



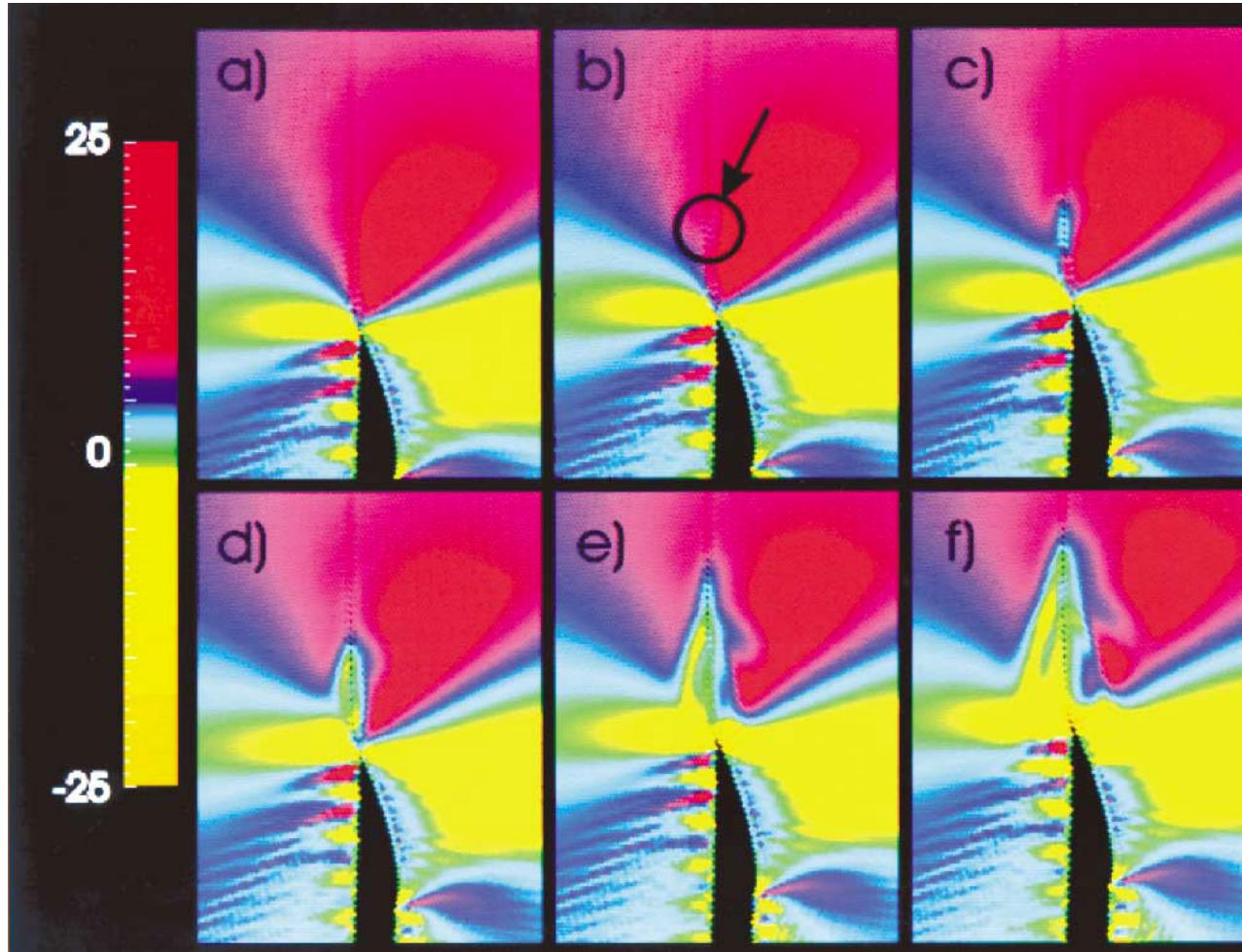
$$\phi = \begin{cases} \frac{1}{2}k_0(r - r_0)^2 & r < r_{\text{break}} \\ \frac{1}{2}k_0(r_{\text{break}} - r_0)^2 & r \geq r_{\text{break}} \end{cases}$$

*Application of atomistic model:  
Understand mechanism of intersonic  
fracture*

# MD simulations: intersonic fracture



# MD simulation: mechanism



*Daughter  
crack  
nucleation  
(ahead of  
mother  
crack)*

*Continuum theory: intersonic crack motion allowed, elucidates mechanism*

# Continuum analysis: reveals shear stress peak

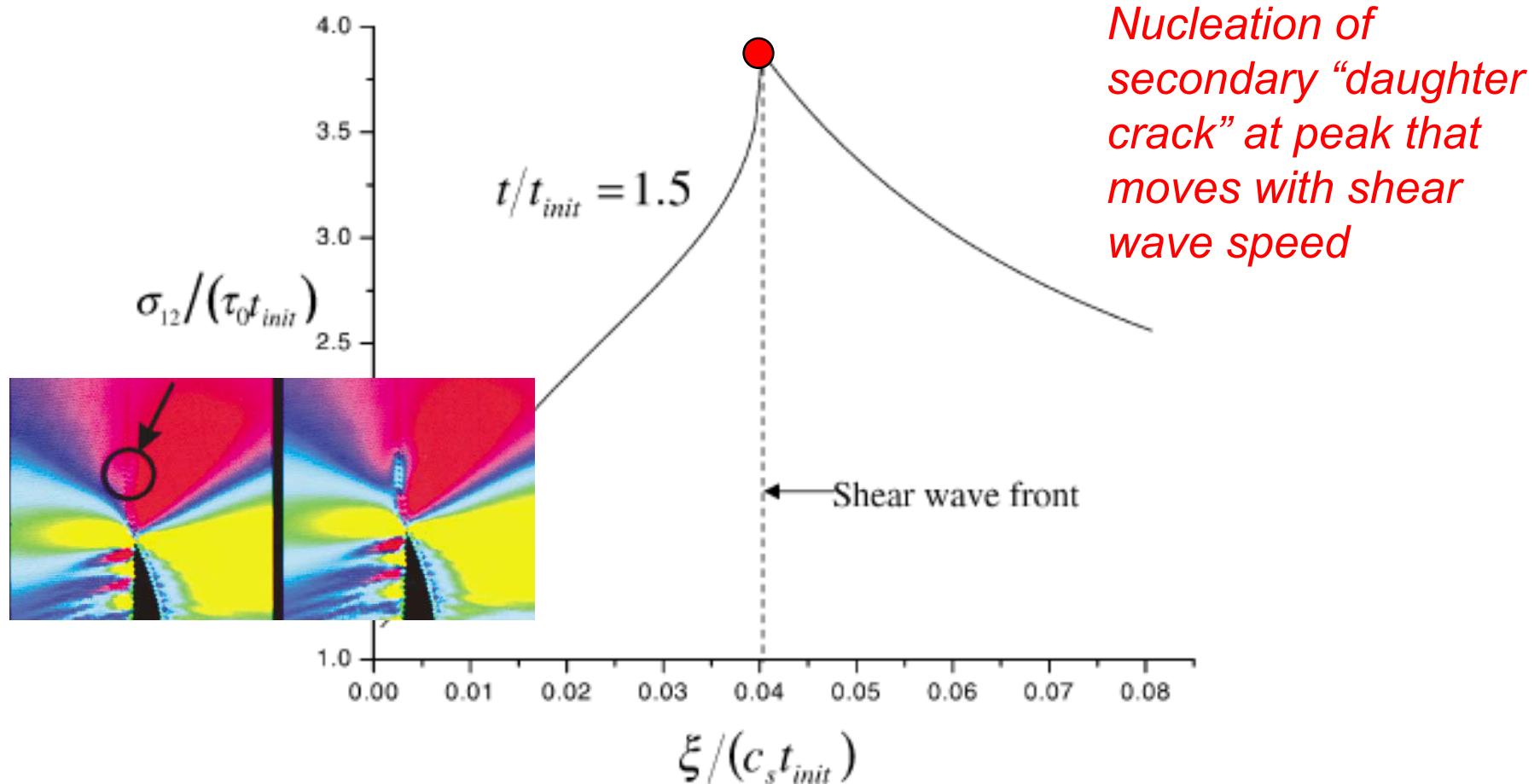
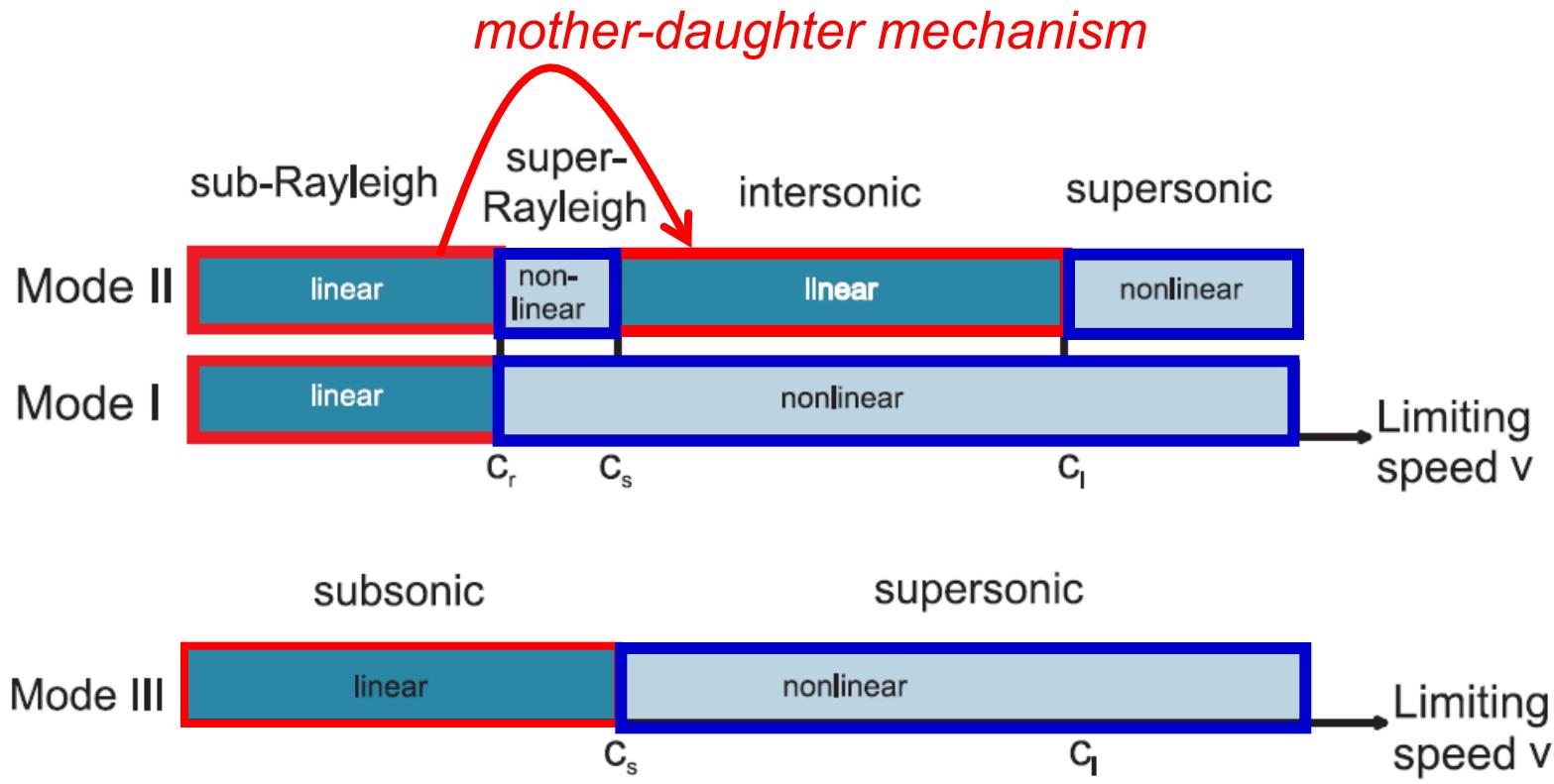


Fig. 5. The distribution of shear stress ahead of the mother crack moving at the Rayleigh wave speed. Note that there is a stress peak at the shear wavefront.

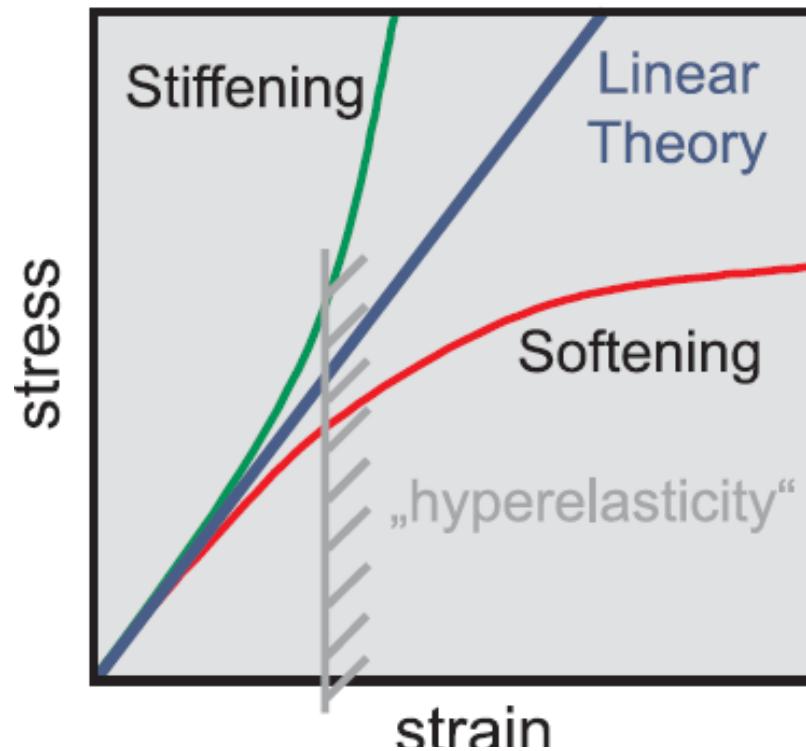
# Limiting speeds of cracks



- Under presence of hyperelastic effects, cracks can exceed the conventional barrier given by the wave speeds
- This is a “local” effect due to enhancement of energy flux
- Subsonic fracture due to local softening, that is, reduction of energy flux

## *Other fracture mechanisms*

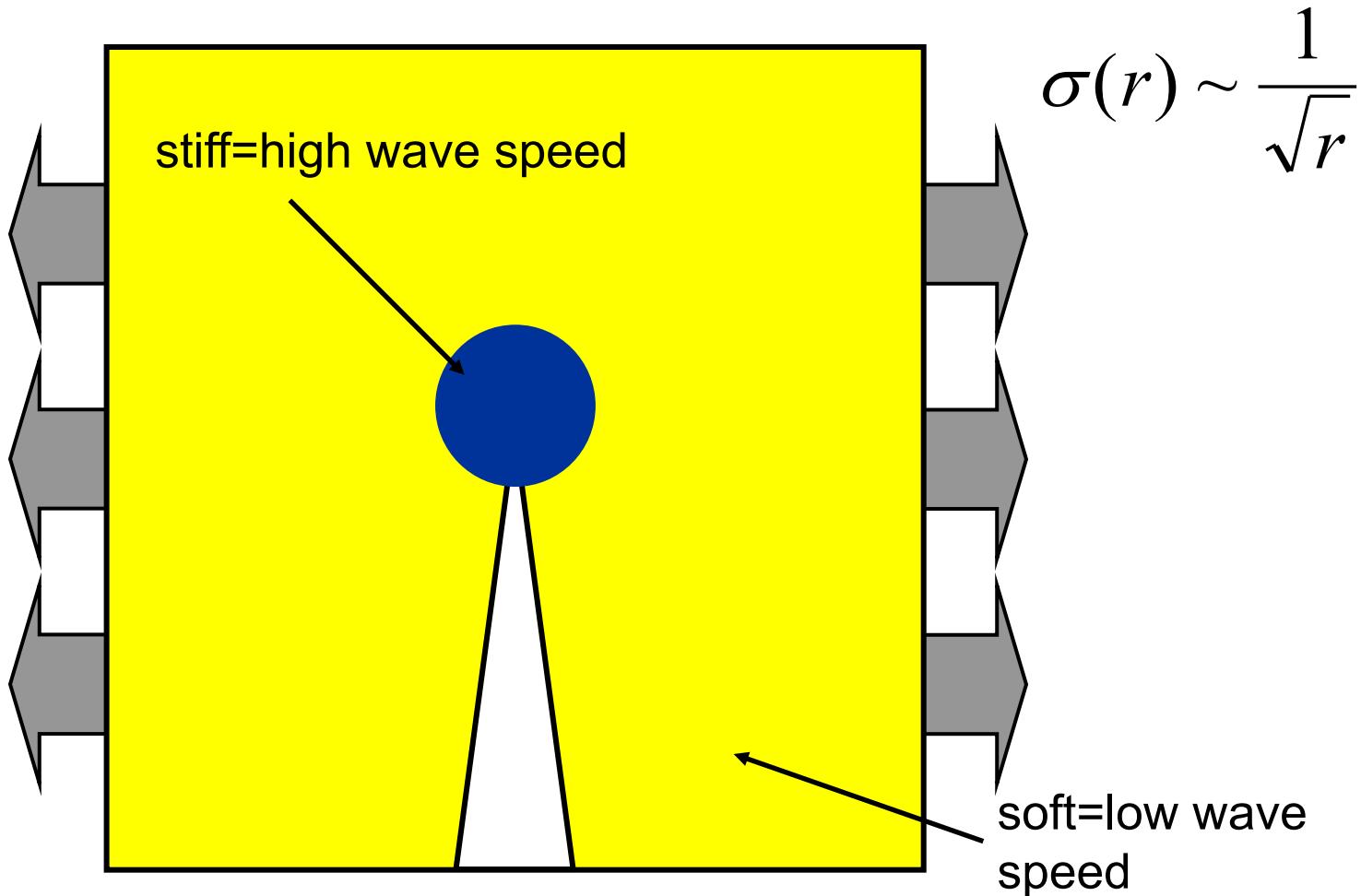
# Linear versus nonlinear elasticity=hyperelasticity



**Linear elasticity:** Young's modulus (stiffness) does not change with deformation

**Nonlinear elasticity = hyperelasticity:** Young's modulus (stiffness) changes with deformation

# Wave speeds close to crack



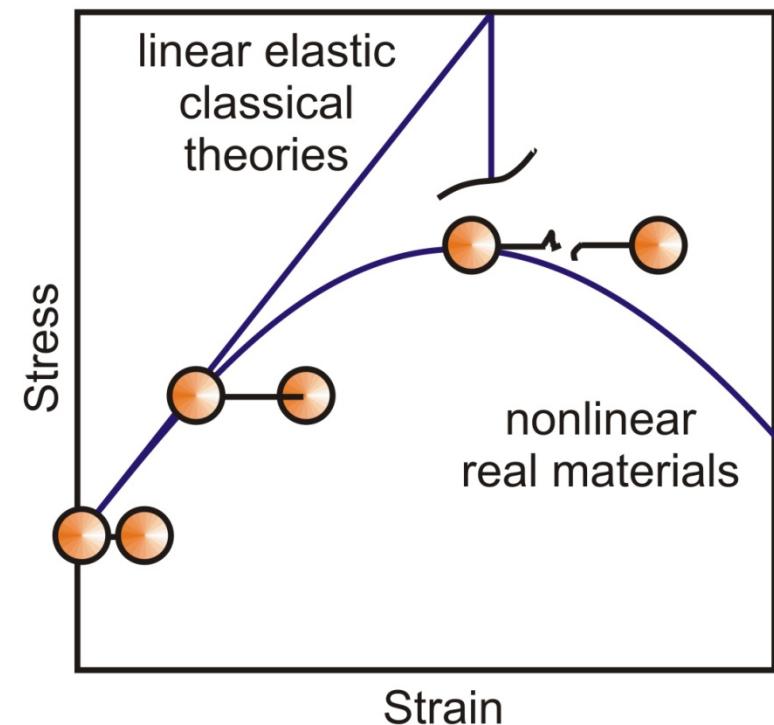
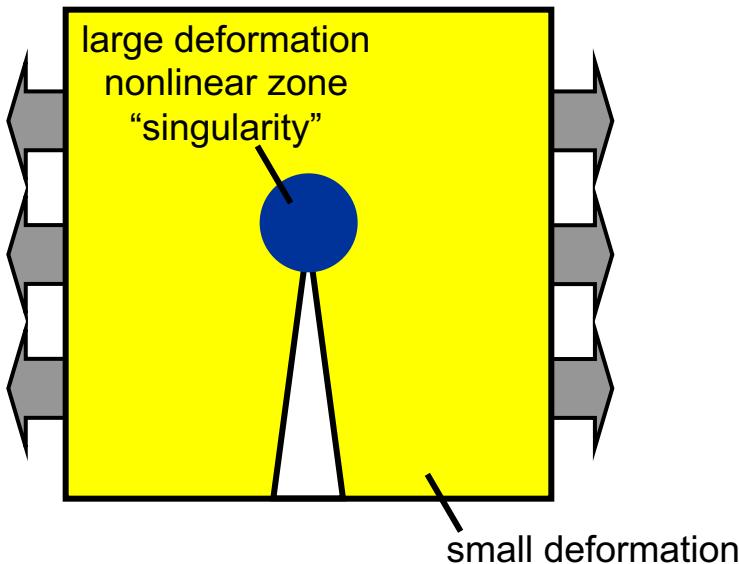
*Can this lead to crack speeds faster than limit predicted by linear elasticity?*

# Subsonic and supersonic fracture

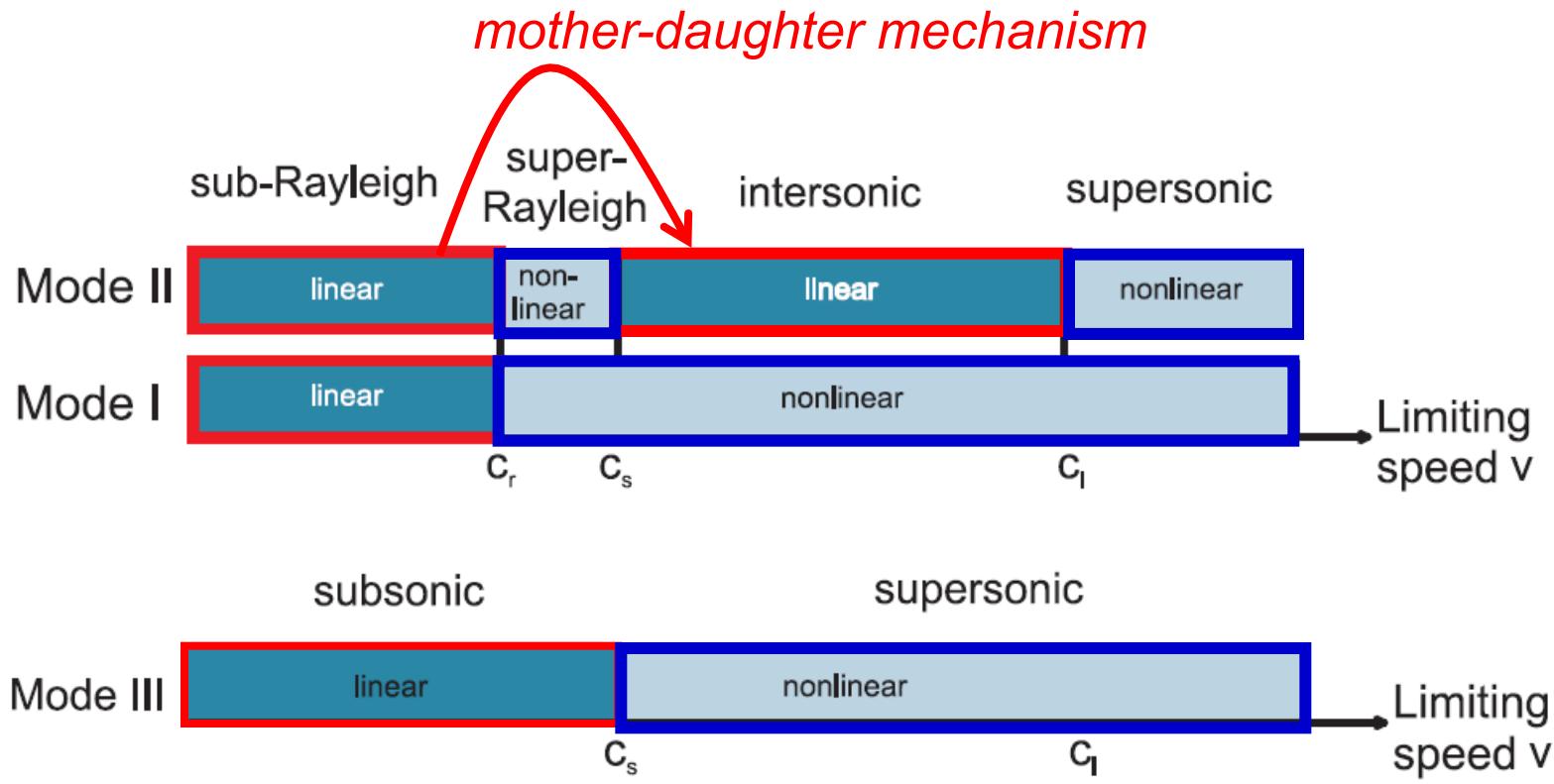
- Under certain conditions, material nonlinearities (that is, the behavior of materials under large deformation = hyperelasticity) becomes important
- This can lead to different limiting speeds than described by the model introduced above

$$\sigma(r) \sim \frac{1}{\sqrt{r}}$$

*Deformation field near a crack*



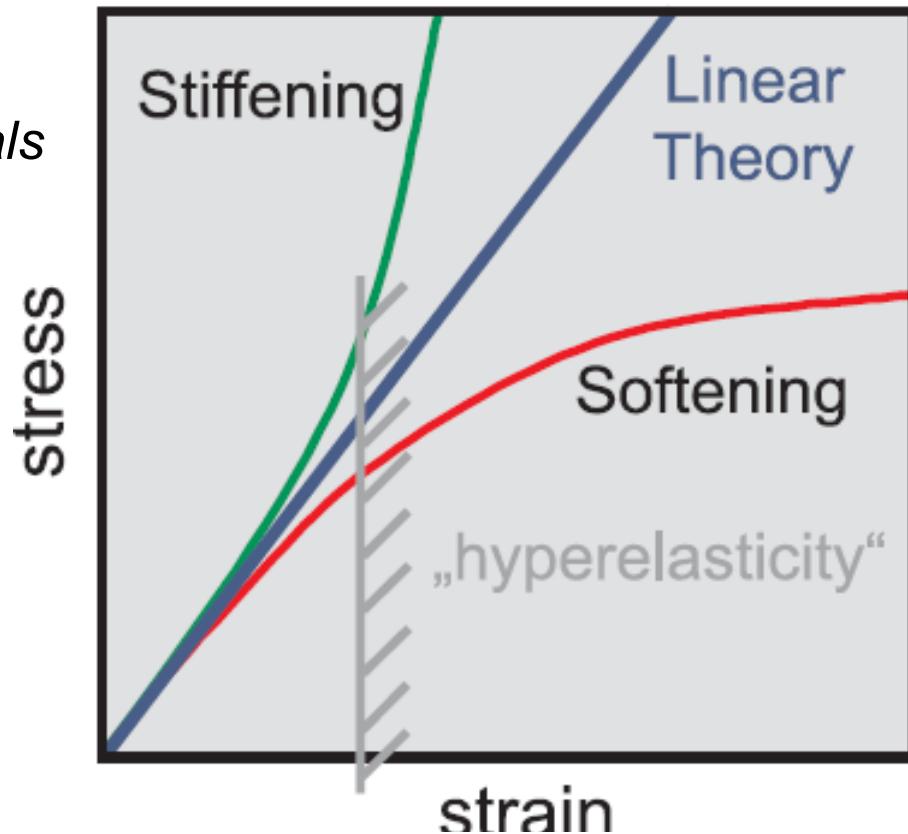
# Limiting speeds of cracks



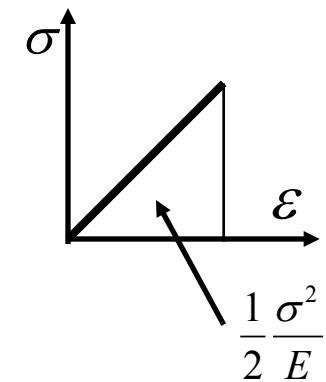
- Under presence of hyperelastic effects, cracks can exceed the conventional barrier given by the wave speeds
- This is a “local” effect due to enhancement of energy flux
- Subsonic fracture due to local softening, that is, reduction of energy flux

# Stiffening vs. softening behavior

*real  
materials*



*"linear elasticity"*



*Increased/decreased wave speed*

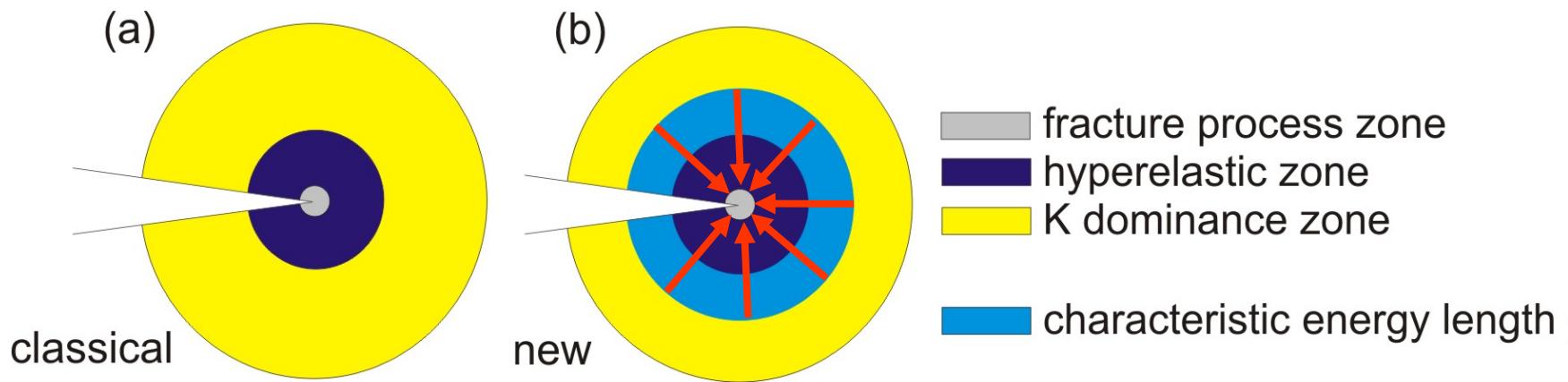
$$c_l = \sqrt{\frac{3\mu}{\rho}}$$

$$c_s = \sqrt{\frac{\mu}{\rho}}$$

$$c_R \approx \beta c_s$$

$$\beta \approx 0.923$$

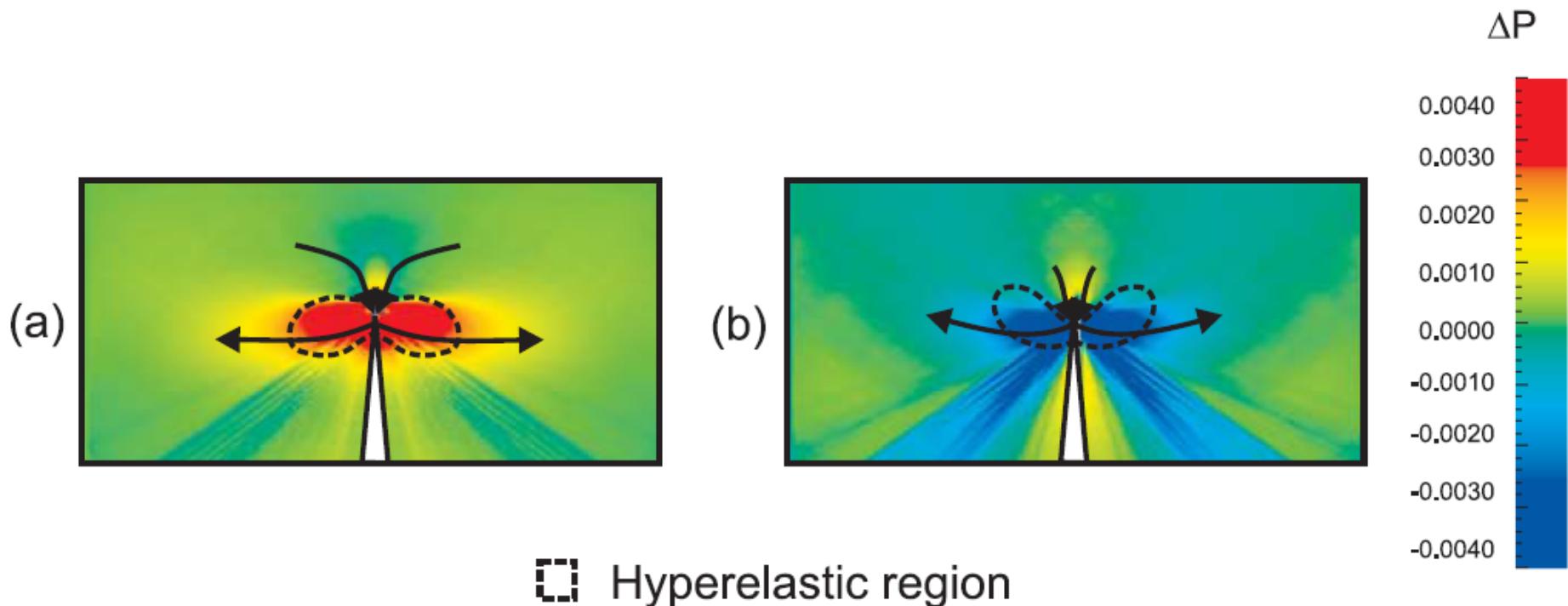
# Energy flux reduction/enhancement



**Energy flux related to wave speed:** high local wave speed, high energy flux, crack can move faster (and reverse for low local wave speed)

# Physical basis for subsonic/supersonic fracture

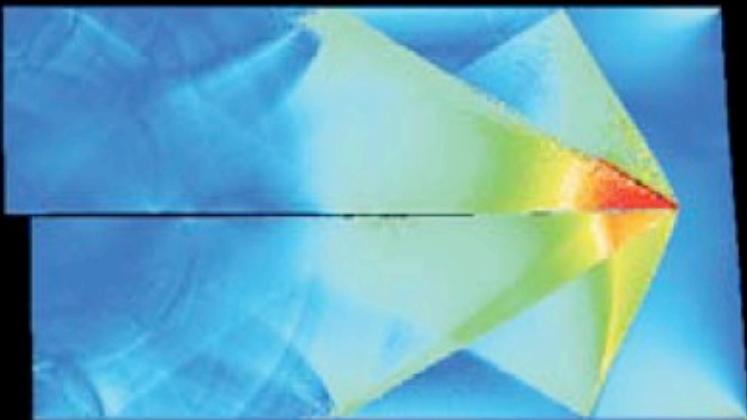
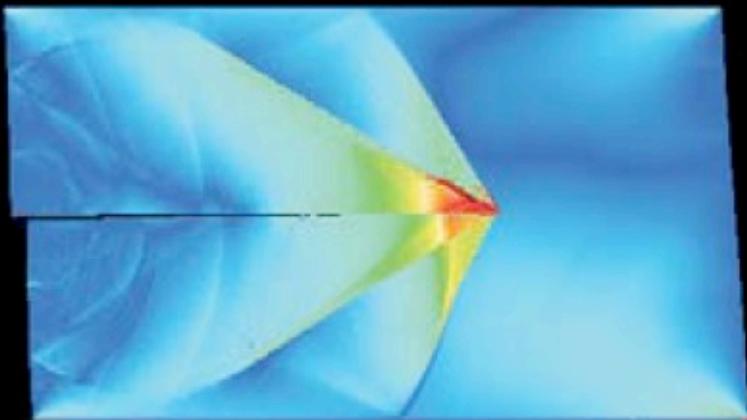
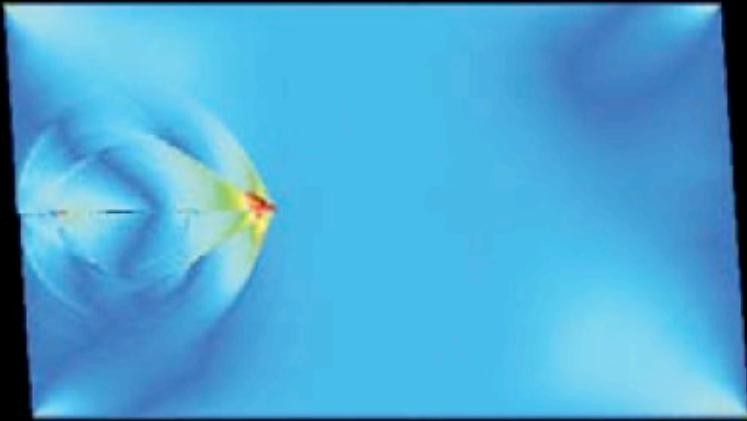
- Changes in energy flow at the crack tip due to changes in local wave speed (energy flux higher in materials with higher wave speed)
- Controlled by a characteristic length scale  $\chi$



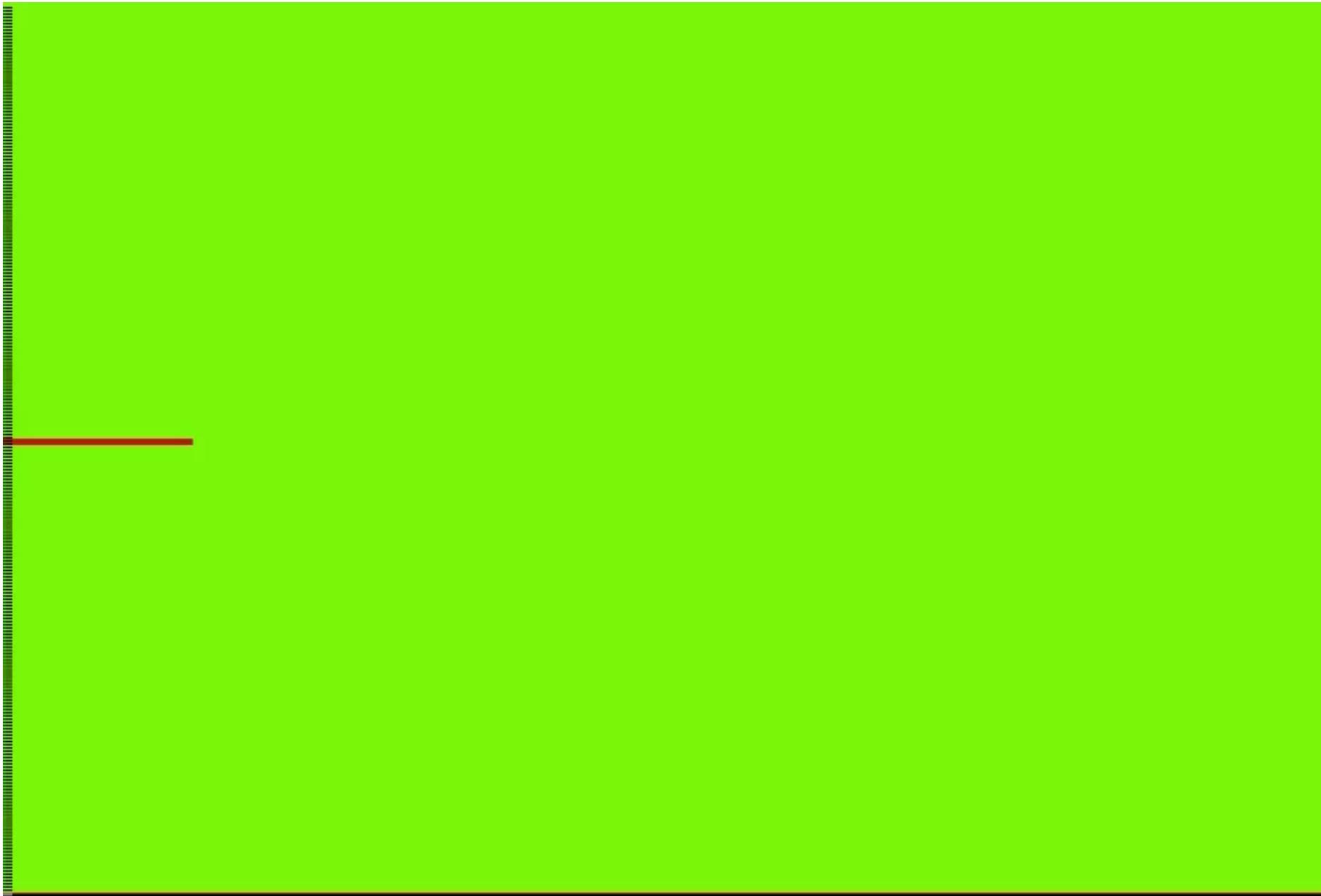
# Summary: atomistic mechanisms of brittle fracture

- Brittle fracture – **rapid spreading** of a small initial crack
- Cracks initiate based on **Griffith condition**  $G = 2\gamma_s$
- Cracks spread on the order of **sound speeds** (km/sec for many brittle materials)
- Cracks have a **maximum speed**, which is given by characteristic sound speeds for different loading conditions)
- Maximum speed can be altered if material is strongly nonlinear, leading to **supersonic or subsonic fracture**

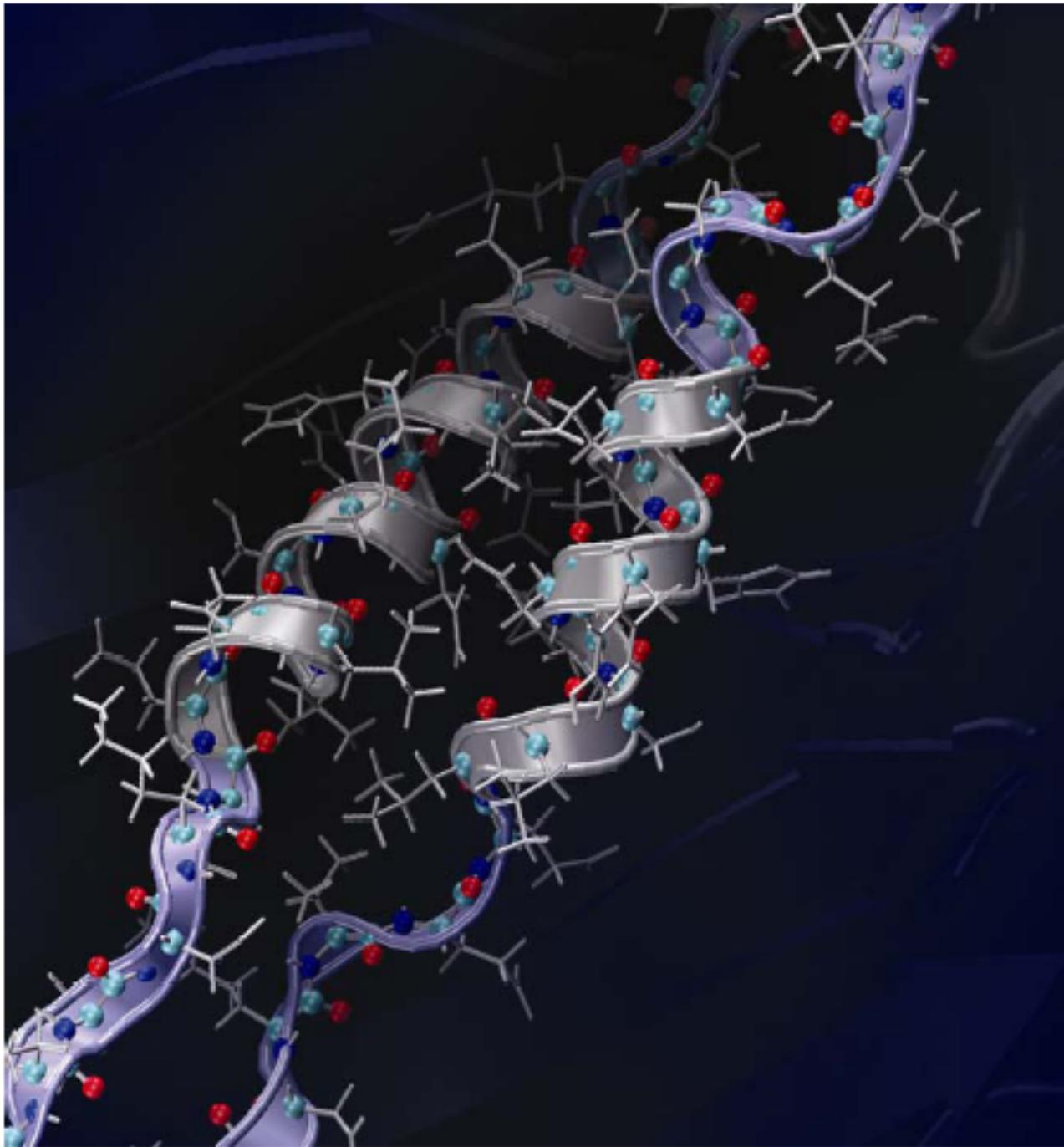




*Supersonic fracture*



## **2. Force fields for proteins (and polymers)**



# Significance of proteins

- Proteins are **basic building blocks of life**
- **Define tissues, organs, cells**
- Provide a **variety of functions and properties**, such as mechanical stability (strength), elasticity, catalytic activity (enzyme), electrochemical properties, optical properties, energy conversion
- Molecular simulation is an **important tool in the analysis of protein structures and protein materials**

***Goal here: To train you in the fundamentals of modeling techniques for proteins, to enable you to carry out protein simulations***

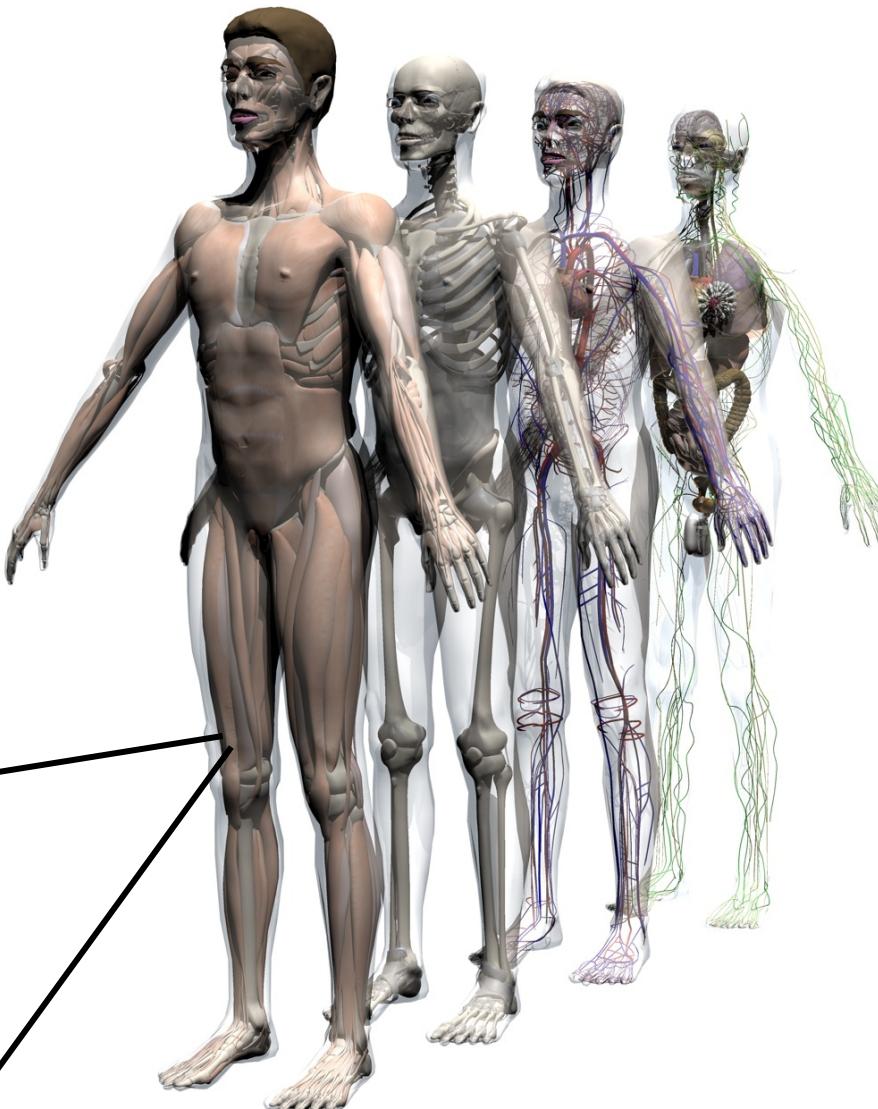
***Explain the significance of proteins (application)***

# Human body: composed of diverse array of protein materials

**Eye's cornea**  
(collagen material)

**Skin** (complex composite of collagen, elastin)

**Cells** (complex material/system based on proteins)



**Muscle tissue**  
(motor proteins)

**Nerve cells**

**Blood vessels**

**Tendon**  
(links bone, muscles)

**Cartilage** (reduce friction in joints)

**Bone** (structural stability)

# Cellular structure: Protein networks

**Cell nucleus**

**Actin network**

**Microtubulus**  
(e.g. cargo)

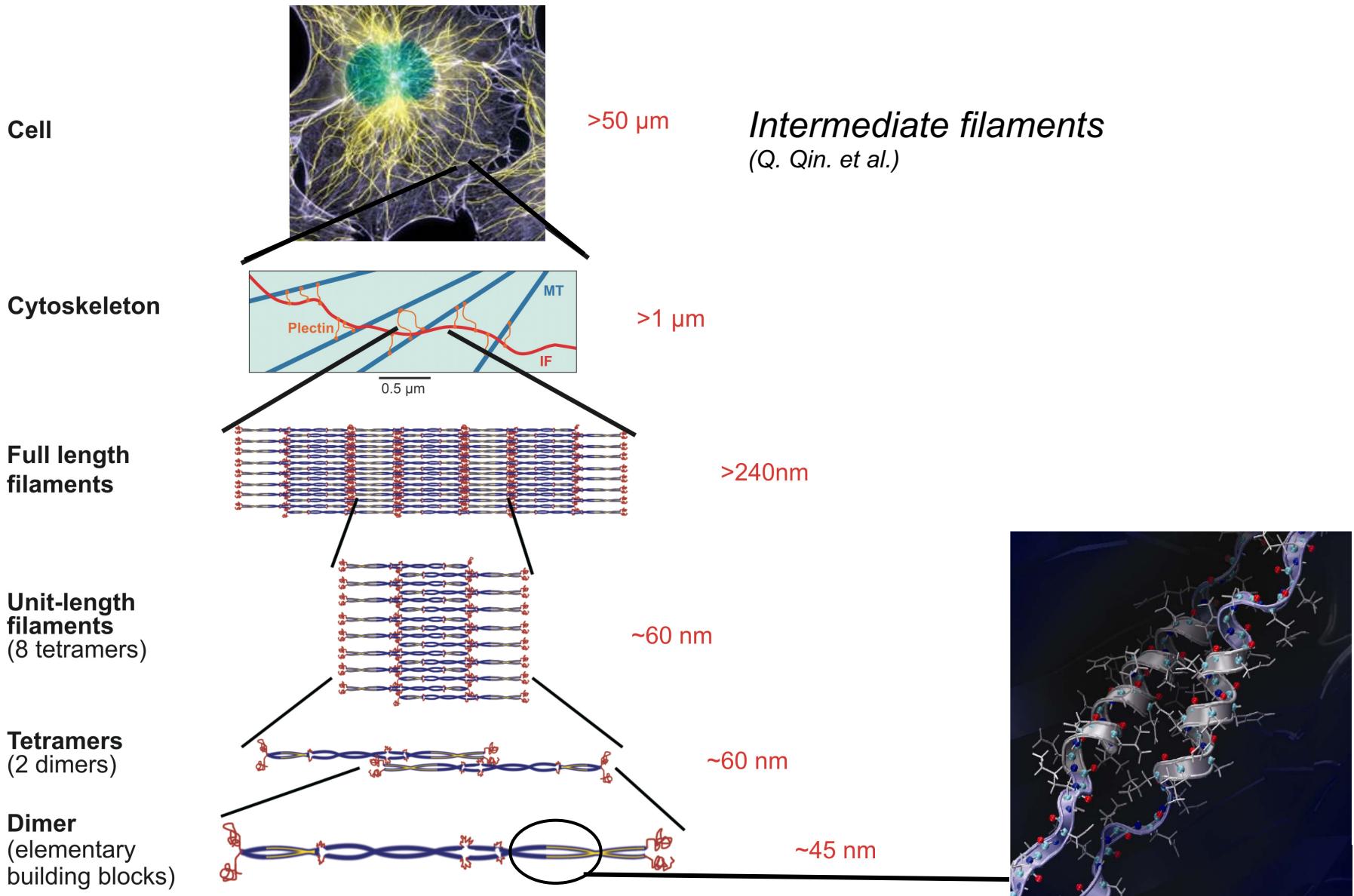
**Vimentin**  
(extensible,  
flexible, provide  
strength)

= cytoskeleton



Photo: Torsten Wittmann

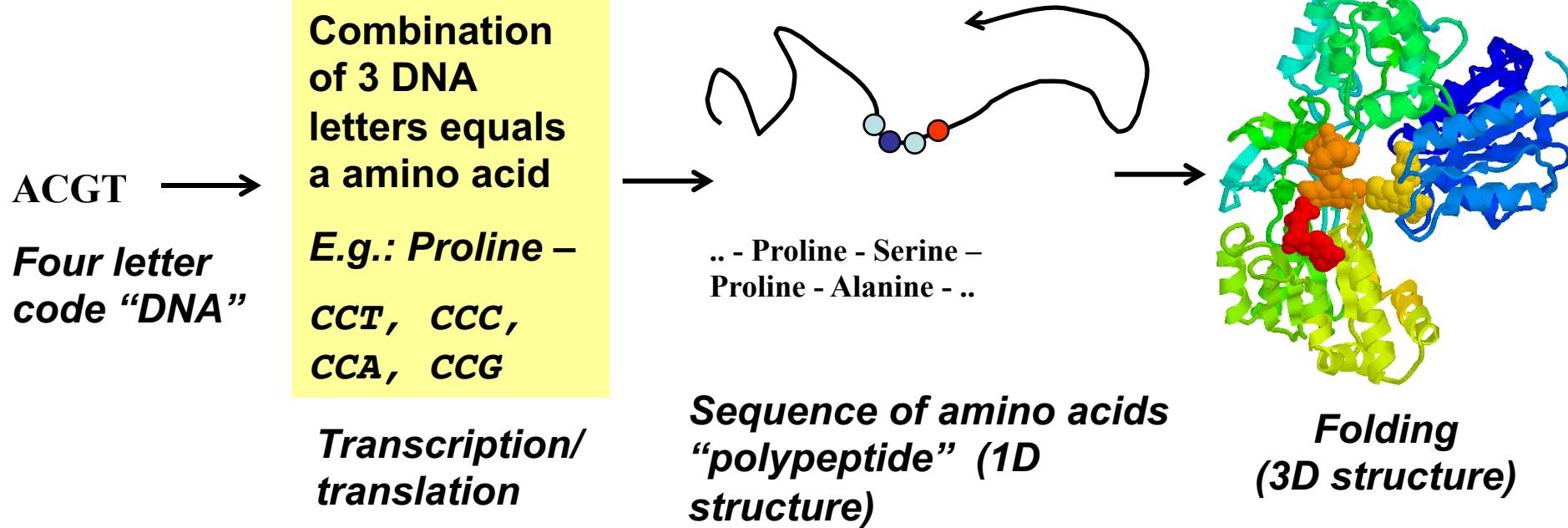
# Protein structures define the cellular architecture



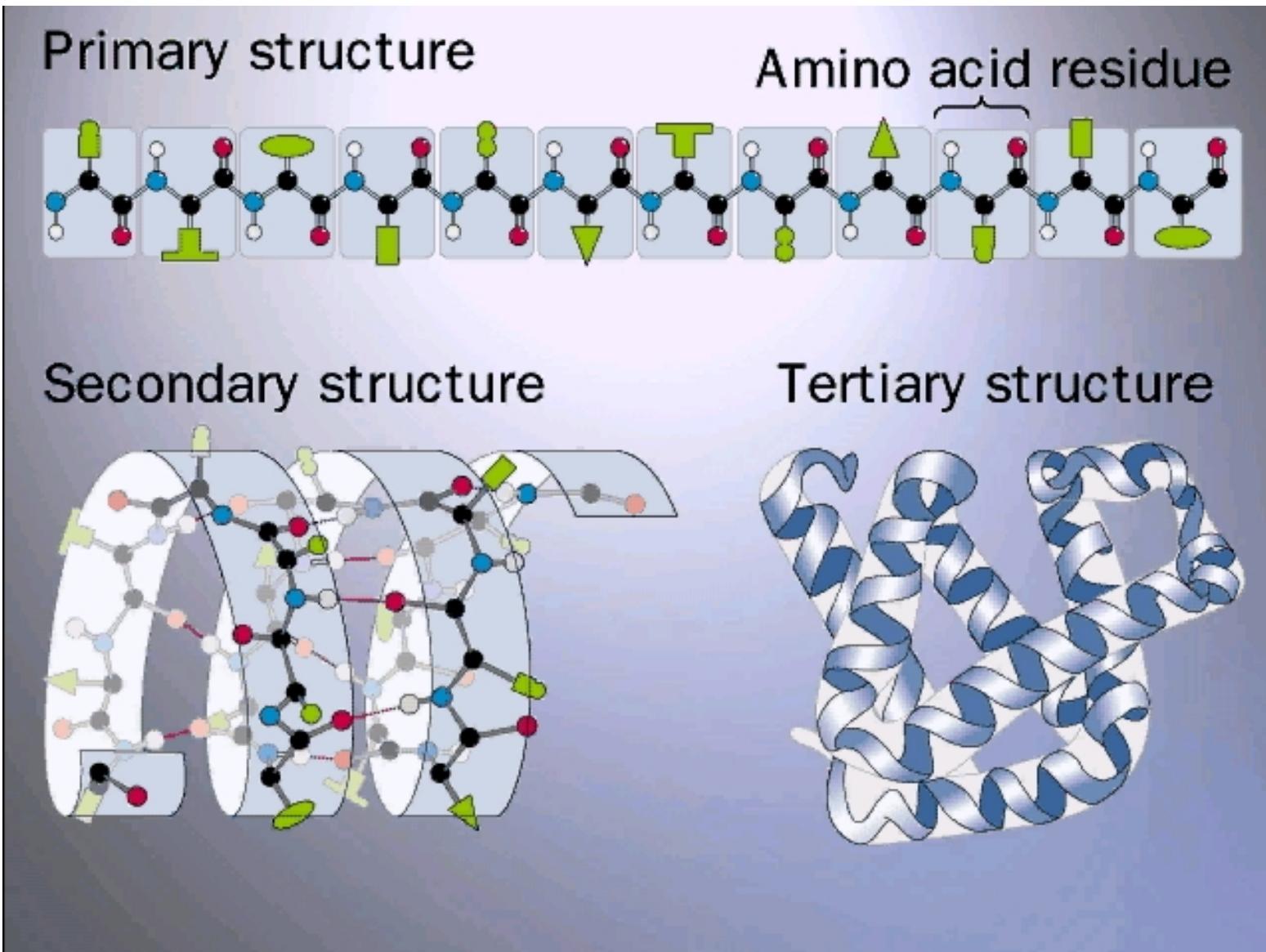
# How protein materials are made – the genetic code

- Proteins: Encoded by DNA (three “letters”), utilize 20 basic building blocks (amino acids) to form polypeptides
- Polypeptides arrange in complex folded 3D structures with specific properties

**1D structure transforms into complex 3D folded configuration**



# Primary, secondary, tertiary structure



# Alpha-helix (abbreviated as AH)

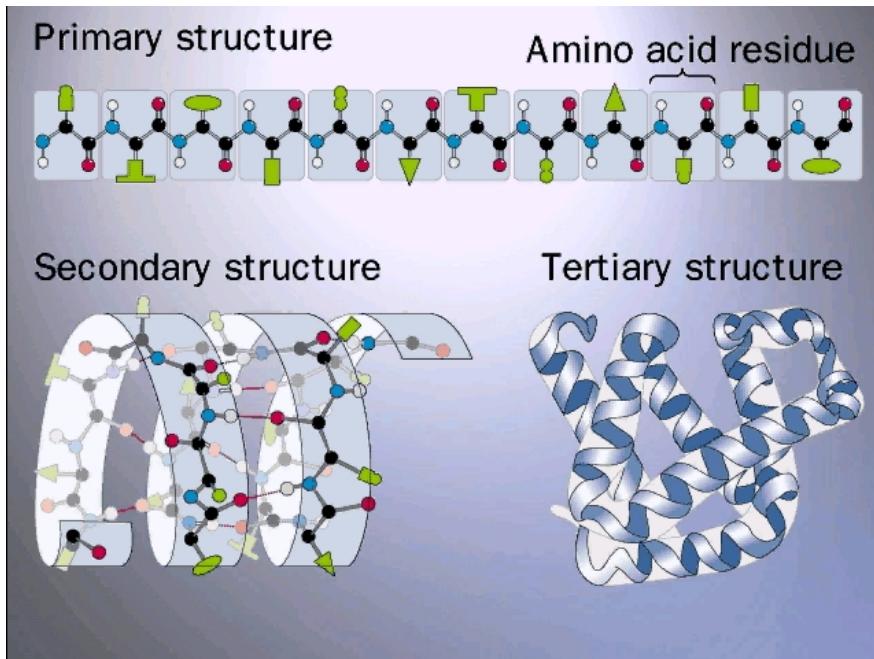
**Concept: hydrogen bonding (H-bonding)**

e.g. between O and H in  $\text{H}_2\text{O}$

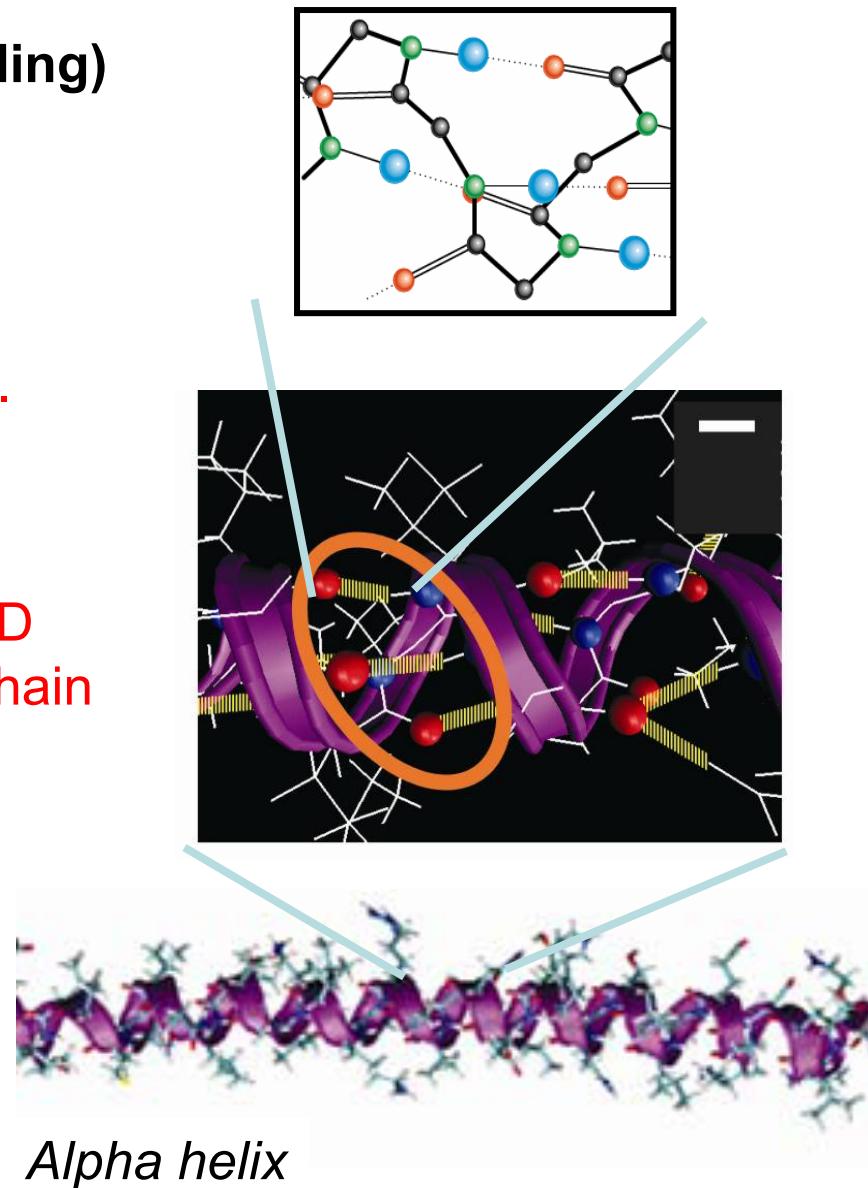
Between N and O in proteins

Drives formation of helical structures

AHs found in: hair, cells, wool, skin, etc.

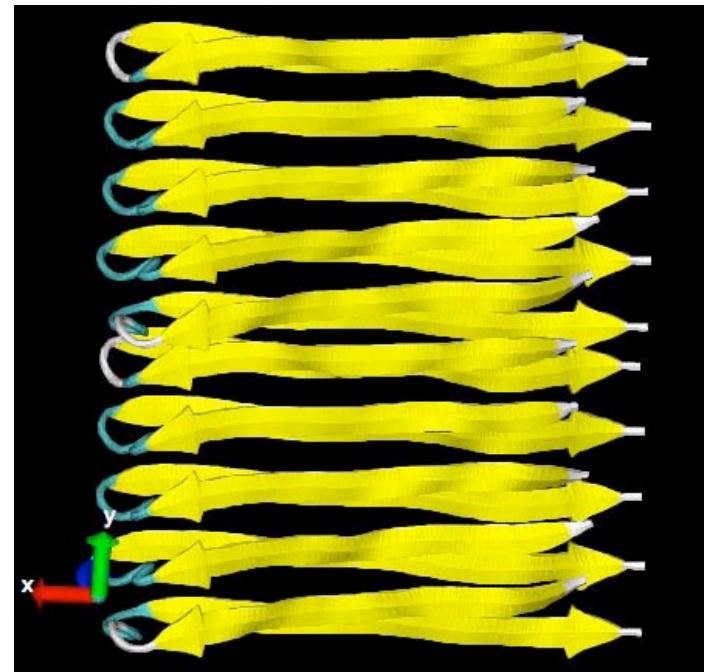
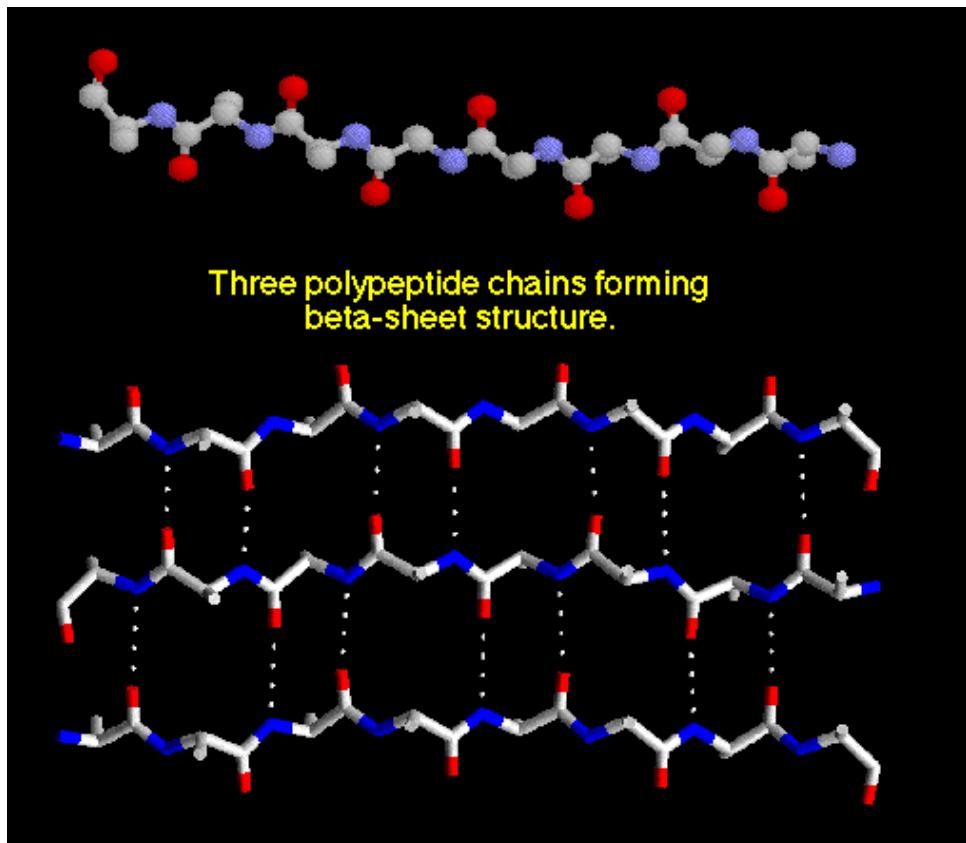


1D  
chain



# Beta-sheets (abbreviated as BS)

*Beta-sheet*



Found in many mechanically relevant proteins

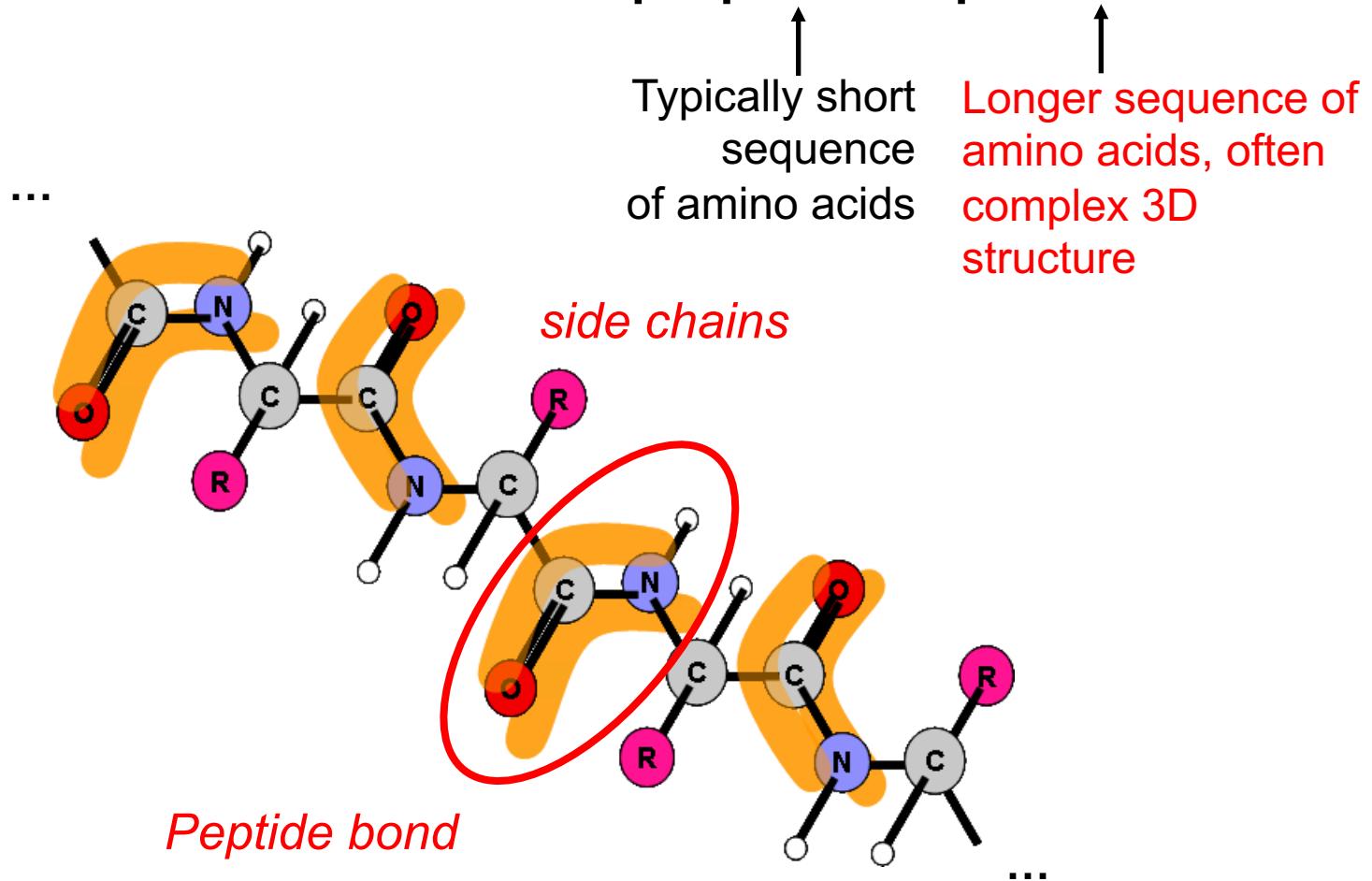
Spider silk

Fibronectin

Titin (muscle tissue)

Amyloids (Alzheimer's disease)

# Chemical structure of peptides/proteins

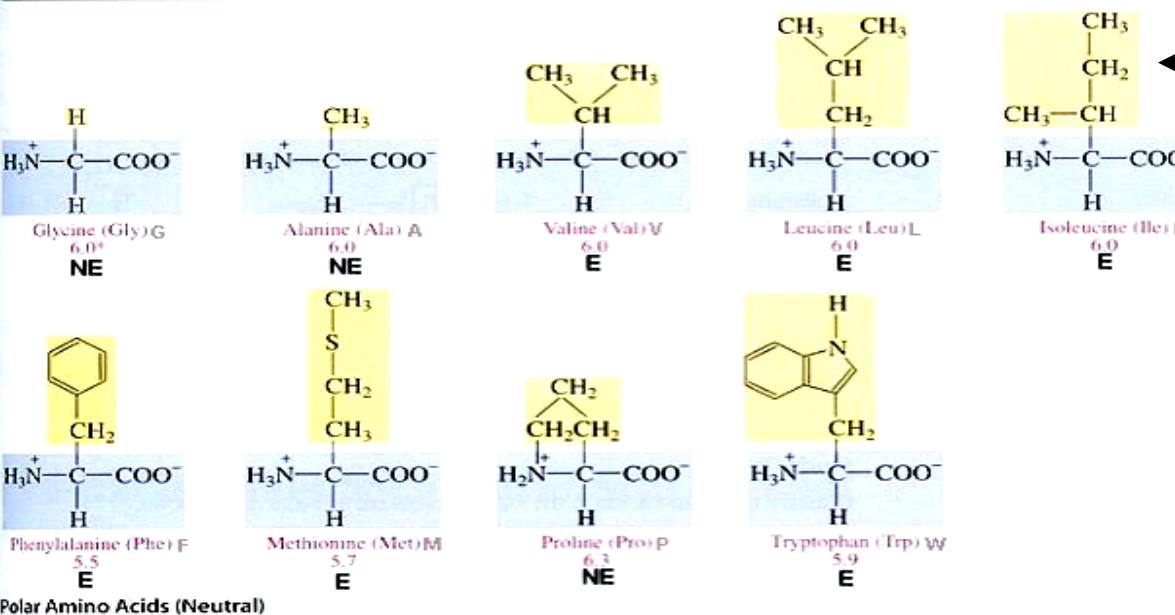


R = side chain, one of the 20 natural amino acids

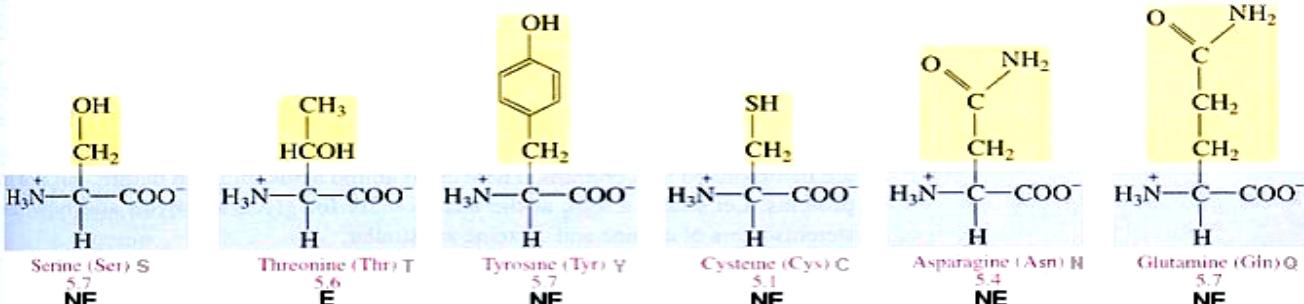
**20 natural amino acids differ in their side chain chemistry**

### Nonpolar Amino Acids

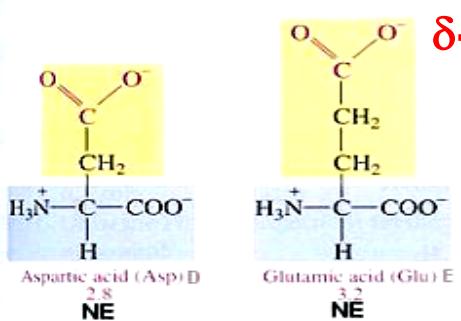
Forms peptide bond



### Polar Amino Acids (Neutral)



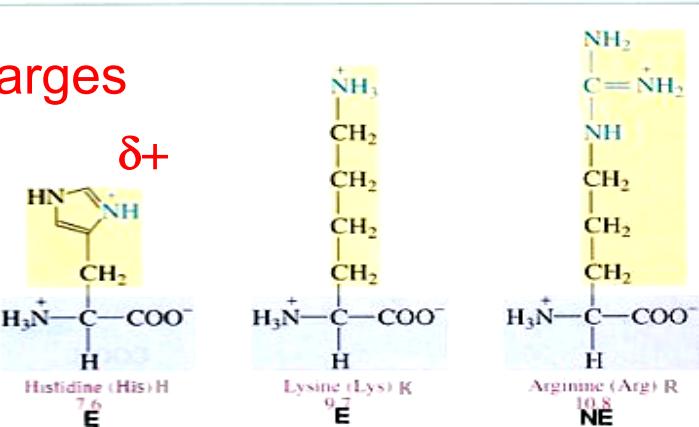
### Acidic Amino Acids



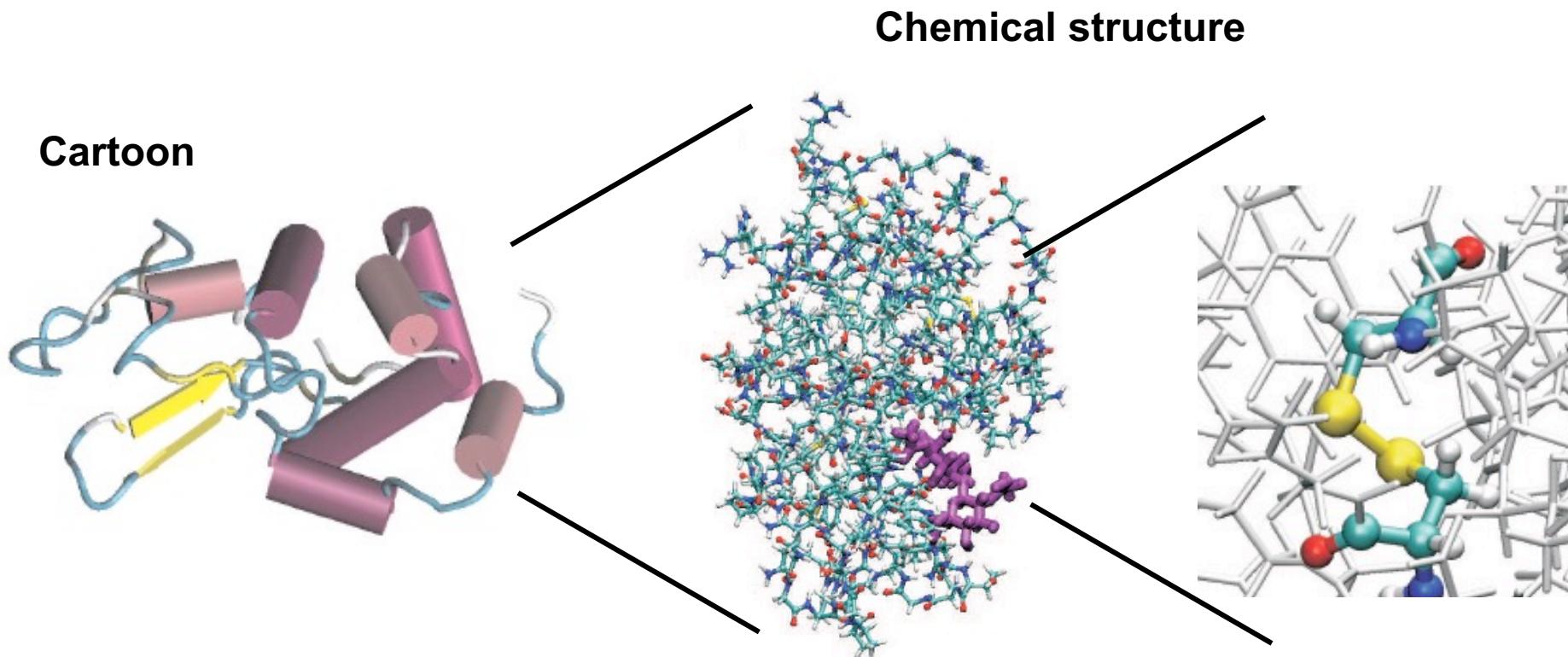
$\delta-$

charges

$\delta+$



# Chemistry, structure and properties are linked



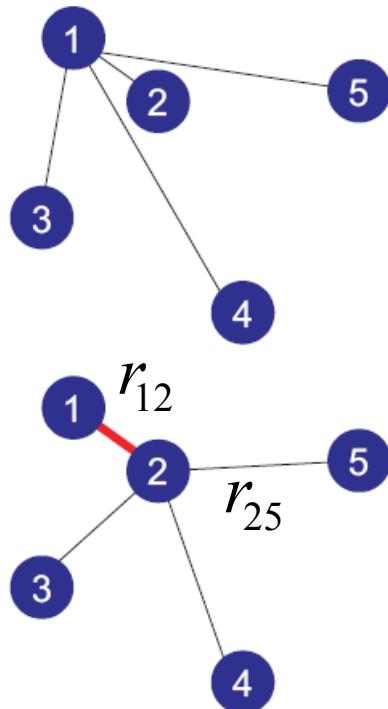
**Presence of various chemical bonds (chemical complexity):**

- Covalent bonds (C-C, C-O, C-H, C-N..)
- Electrostatic interactions (charged amino acid side chains)
- H-bonds (e.g. between H and O)
- vdW interactions (uncharged parts of molecules)

## **1.1 CHARMM force field**

# Pair potential: total energy

“simply” the sum of all energies of pairs of atoms



two “loops” over pairs of all particles

$$U_{total} = \frac{1}{2} \sum_{i=1, i \neq j}^N \sum_{j=1}^N \phi(r_{ij})$$

with  $\phi_{ij} = \phi(r_{ij})$

$$U_{total} = \frac{1}{2} (\phi_{12} + \phi_{13} + \phi_{14} + \phi_{1N} \dots + \phi_{21} + \phi_{23} + \dots + \phi_{2N} + \dots + \phi_{N-1,N})$$

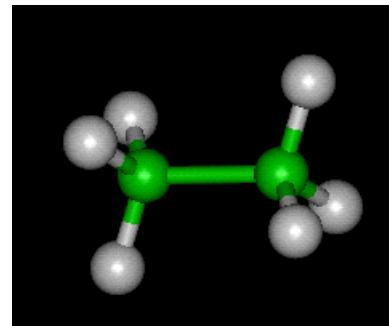
# Review: atomic interactions – different types of chemical bonds

- **Primary bonds (“strong”)**
  - Ionic (ceramics, quartz, feldspar - **rocks**)
  - Covalent (**silicon**)
  - Metallic (copper, nickel, **gold**, silver)  
(high melting point, 1000-5,000K)
- **Secondary bonds (“weak”)**
  - Van der Waals (**wax**, low melting point)
  - Hydrogen bonds (proteins, **spider silk**)  
(melting point 100-500K)
- Ionic: Non-directional (point charges interacting)
- Covalent: Directional (bond angles, torsions matter)
- Metallic: Non-directional (electron gas concept)

***Difference of material properties originates from different atomic Interactions: Concept: add different contributions (linear addition...)***

# Generalization: split energy contributions due to different chemical bonds

$$U_{total} = U_{Elec} + U_{Covalent} + U_{Metallic} + U_{vdW} + U_{H-bond}$$



Ethane  
 $C_2H_6$

Covalent bond described as

1. Bond stretching part (energy penalty for bond stretching)
2. Bending part (energy penalty for bending three atoms)
3. Rotation part (energy penalty for bond rotation,  $N \geq 4$ )

Consider ethane molecule as “**elastic structure**”

$$U_{Covalent} = U_{stretch} + U_{bend} + U_{rotate}$$

# Force fields for organics: Basic approach

$$U_{total} = U_{Elec} + U_{Covalent} + U_{Metallic} + U_{vdW} + U_{H\text{-bond}}$$

=0 for proteins

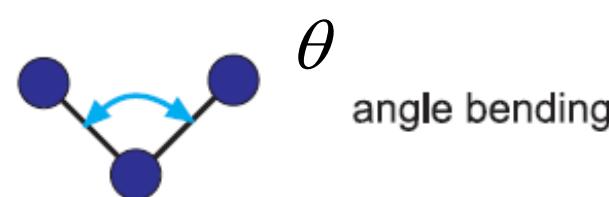
$$U_{Covalent} = U_{stretch} + U_{bend} + U_{rot}$$

$$\begin{cases} \phi_{stretch} = \frac{1}{2} k_{stretch} (r - r_0)^2 \\ U_{stretch} = \sum_{pairs} \phi_{stretch} \end{cases}$$



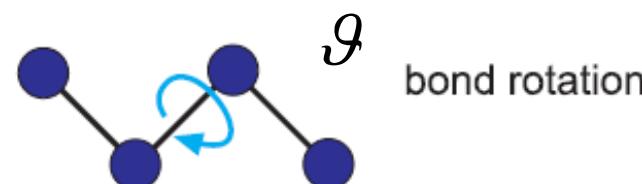
bond stretching

$$\begin{cases} \phi_{bend} = \frac{1}{2} k_{bend} (\theta - \theta_0)^2 \\ U_{bend} = \sum_{triplets} \phi_{bend} \end{cases}$$



angle bending

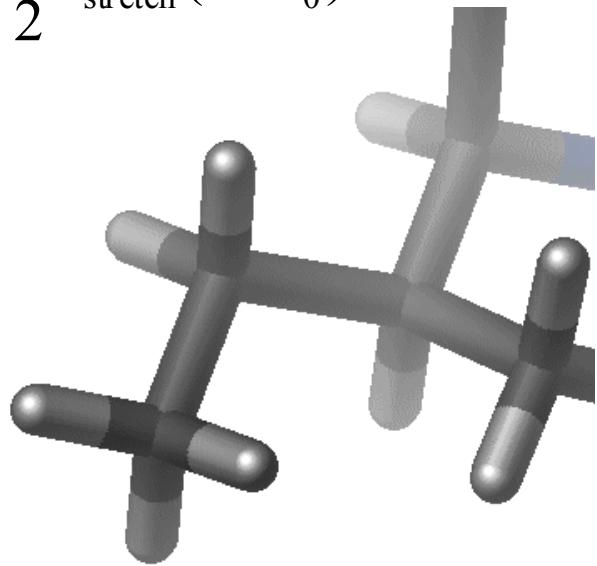
$$\begin{cases} \phi_{rot} = \frac{1}{2} k_{rot} (1 - \cos(\vartheta)) \\ U_{rot} = \sum_{quadruplets} \phi_{rot} \end{cases}$$



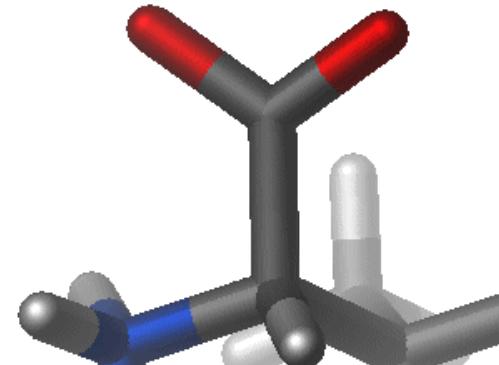
bond rotation

# Model for covalent bonds

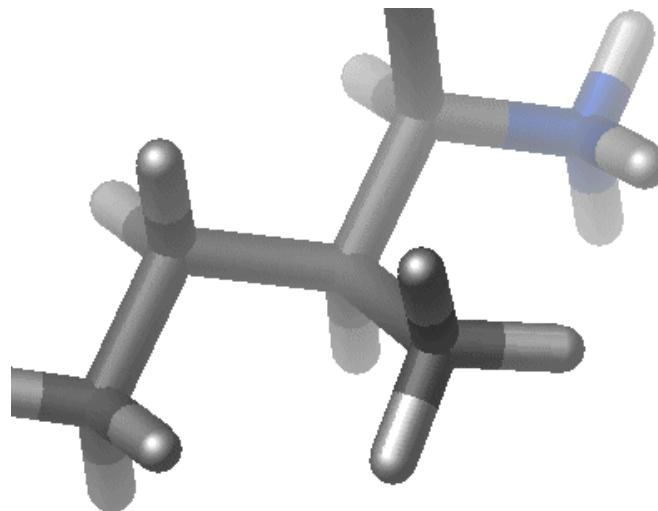
$$\phi_{\text{stretch}} = \frac{1}{2} k_{\text{stretch}} (r - r_0)^2$$



$$\phi_{\text{bend}} = \frac{1}{2} k_{\text{bend}} (\theta - \theta_0)^2$$



$$\phi_{\text{rot}} = \frac{1}{2} k_{\text{rot}} (1 - \cos(\vartheta))$$

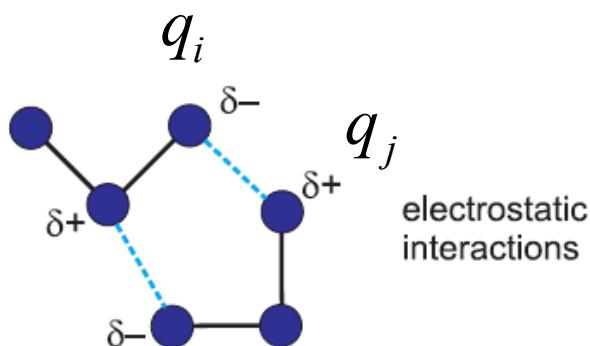


# Force fields for organics: Basic approach

$$U_{total} = U_{Elec} + U_{Covalent} + U_{Metallic} + U_{vdW} + U_{H\text{-bond}}$$

=0 for proteins

$U_{Elec}$



$U_{Elec}$  : Coulomb potential  $\phi(r_{ij}) = \frac{q_i q_j}{\epsilon_1 r_{ij}}$

partial charges

electrostatic constant

distance

$$\text{Coulomb forces } F(r_{ij}) = -\frac{q_i q_j}{\epsilon_1 r_{ij}^2}$$

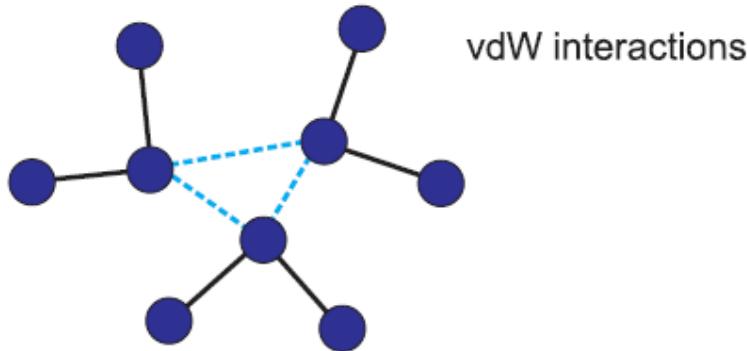
$$\epsilon_1 = 4\pi\epsilon_0 \quad \epsilon_0 = 1.602 \times 10^{-19} \text{ C}$$

# Force fields for organics: Basic approach

$$U_{total} = U_{Elec} + U_{Covalent} + U_{Metallic} + U_{vdW} + U_{H\text{-bond}}$$

=0 for proteins

$U_{vdW}$



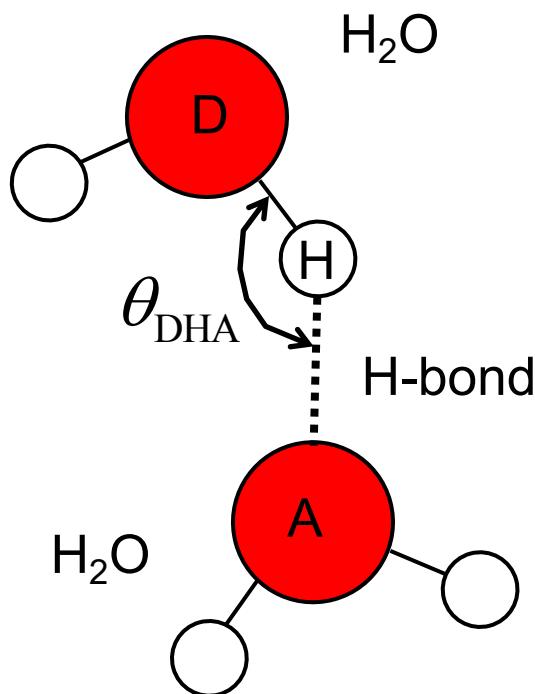
$$U_{vdW} : \text{ LJ potential } \phi(r_{ij}) = 4\epsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right]$$

LJ potential is particularly good model for vdW interactions (Argon) <sup>74</sup>

# H-bond model

$$U_{total} = U_{Elec} + U_{Covalent} + U_{Metallic} + U_{vdW} + U_{H-bond}$$

=0 for proteins



$$U_{H-bond}$$

Evaluated between acceptor (A) /donor(D) pairs

*Between electronegative atom and a H- atom  
that is bonded to another electronegative atom*

*Slightly modified LJ, different parameters*

$$U_{H-bond} : \phi(r_{ij}) = D_{H-bond} \left[ 5 \left( \frac{R_{H-bond}}{r_{ij}} \right)^{12} - 6 \left( \frac{R_{H-bond}}{r_{ij}} \right)^{10} \right] \cos^4(\theta_{DHA})$$

$r_{ij}$  = distance between D-A

# Summary

$$U_{total} = U_{Elec} + U_{Covalent} + U_{Metallic} + U_{vdW} + U_{H\text{-bond}}$$

=0 for proteins

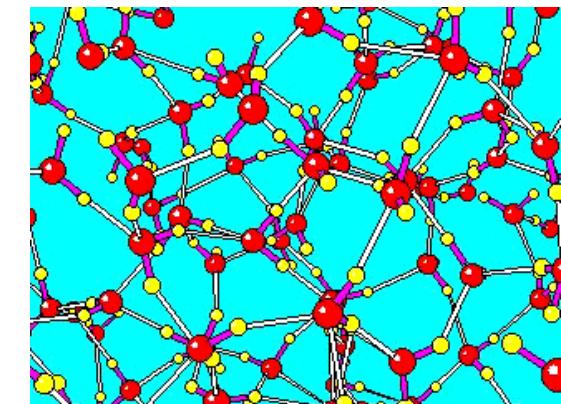
$$U_{Elec} : \text{ Coulomb potential } \phi(r_{ij}) = \frac{q_i q_j}{\epsilon_1 r_{ij}}$$

$$U_{Covalent} = U_{stretch} + U_{bend} + U_{rot}$$

$$\left\{ \begin{array}{l} \phi_{stretch} = \frac{1}{2} k_{stretch} (r - r_0)^2 \\ \phi_{bend} = \frac{1}{2} k_{bend} (\theta - \theta_0)^2 \\ \phi_{rot} = \frac{1}{2} k_{rot} (1 - \cos(\vartheta)) \end{array} \right.$$

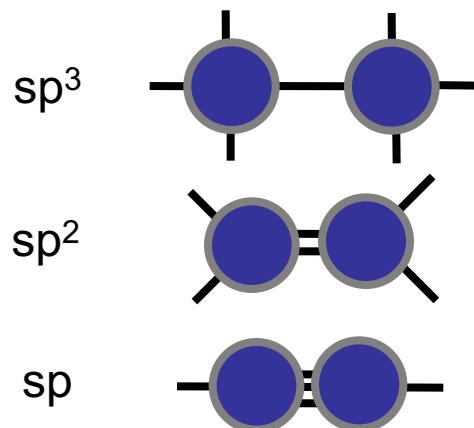
$$U_{vdW} : \text{ LJ potential } \phi(r_{ij}) = 4\epsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right]$$

$$U_{H\text{-bond}} : \phi(r_{ij}) = D_{H\text{-bond}} \left[ 5 \left( \frac{R_{H\text{-bond}}}{r_{ij}} \right)^{12} - 6 \left( \frac{R_{H\text{-bond}}}{r_{ij}} \right)^{10} \right] \cos^4(\theta_{DHA})$$



# The need for atom typing

- **Limited transferability** of potential expressions: Must use different potential for different chemistry
- Different chemistry is captured in **different “tags”** for atoms: **Element type** is expanded by **additional information** on particular chemical state
- Tags specify if a C-atom is in **sp<sup>3</sup>**, **sp<sup>2</sup>**, **sp** or in aromatic state (that is, to capture resonance effects)
- **Example atom tags:** CA, C\_1, C\_2, C\_3, C..., HN, HO, HC, ...

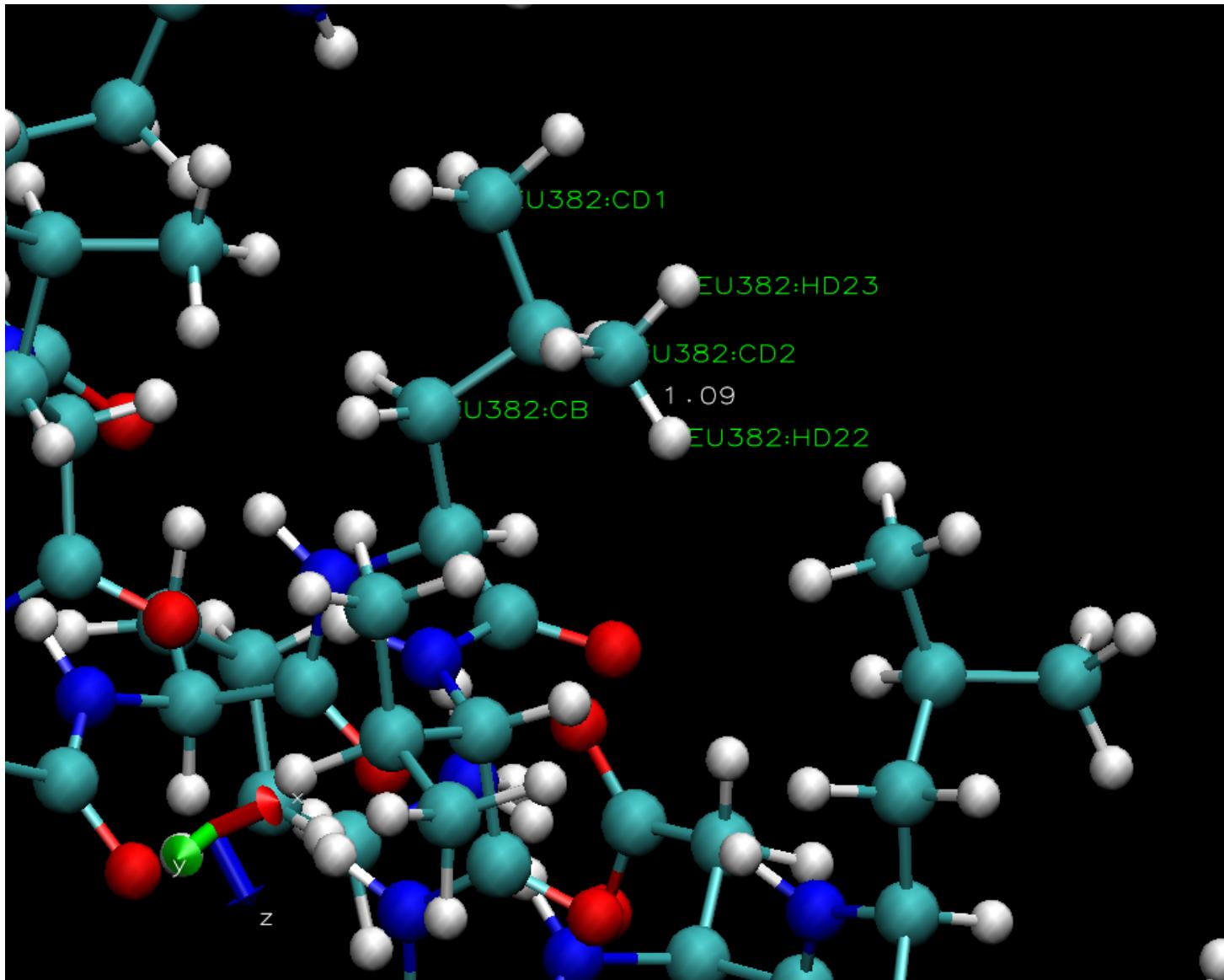


# Atom typing in CHARMM

Example of the RTF for the Alanine residue:

```
RESI ALA0.00
GROUP
ATOM N NH1 -0.47 ! | |
ATOM H N HN 0.31 : HN-N
ATOM C A CT1 0.07 ! | | HB1
ATOM H A HB 0.09 ! | | /
GROUP ! HA-CA--CB-HB2
ATOM C B CT3 -0.27 ! | | \
ATOM H B1 HA 0.09 ! | | HB3
ATOM H B2 HA 0.09 O=C
ATOM H B3 HA 0.09 ! | |
GROUP !
ATOM C C 0.51
ATOM O O -0.51
BOND CB CA N HN N CA
BOND C CA C +N CA HA CB HB1 CB HB2 CB HB3
DOUBLE O C
IMPR N -C CA HN C CA +N O
DONOR HN N
ACCEPTOR O C
IC -C CA *N HN 1.3551 126.4900 180.0000 115.4200 0.9996
IC -C N CA C 1.3551 126.4900 180.0000 114.4400 1.5390
IC N CA C +N 1.4592 114.4400 180.0000 116.8400 1.3558
IC +N CA *C O 1.3558 116.8400 180.0000 122.5200 1.2297
IC CA C +N +CA 1.5390 116.8400 180.0000 126.7700 1.4613
IC N C *CA CB 1.4592 114.4400 123.2300 111.0900 1.5461
IC N C *CA HA 1.4592 114.4400 -120.4500 106.3900 1.0840
IC C CA CB HB1 1.5390 111.0900 177.2500 109.6000 1.1109
IC HB1 CA *CB HB2 1.1109 109.6000 119.1300 111.0500 1.1119
IC HB1 CA *CB HB3 1.1109 109.6000 -119.5800 111.6100 1.1114
```

# VMD analysis of protein structure



# Common empirical force fields for organics and proteins

## Class I (experiment derived, simple form)

- CHARMM **pset #3**
- 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

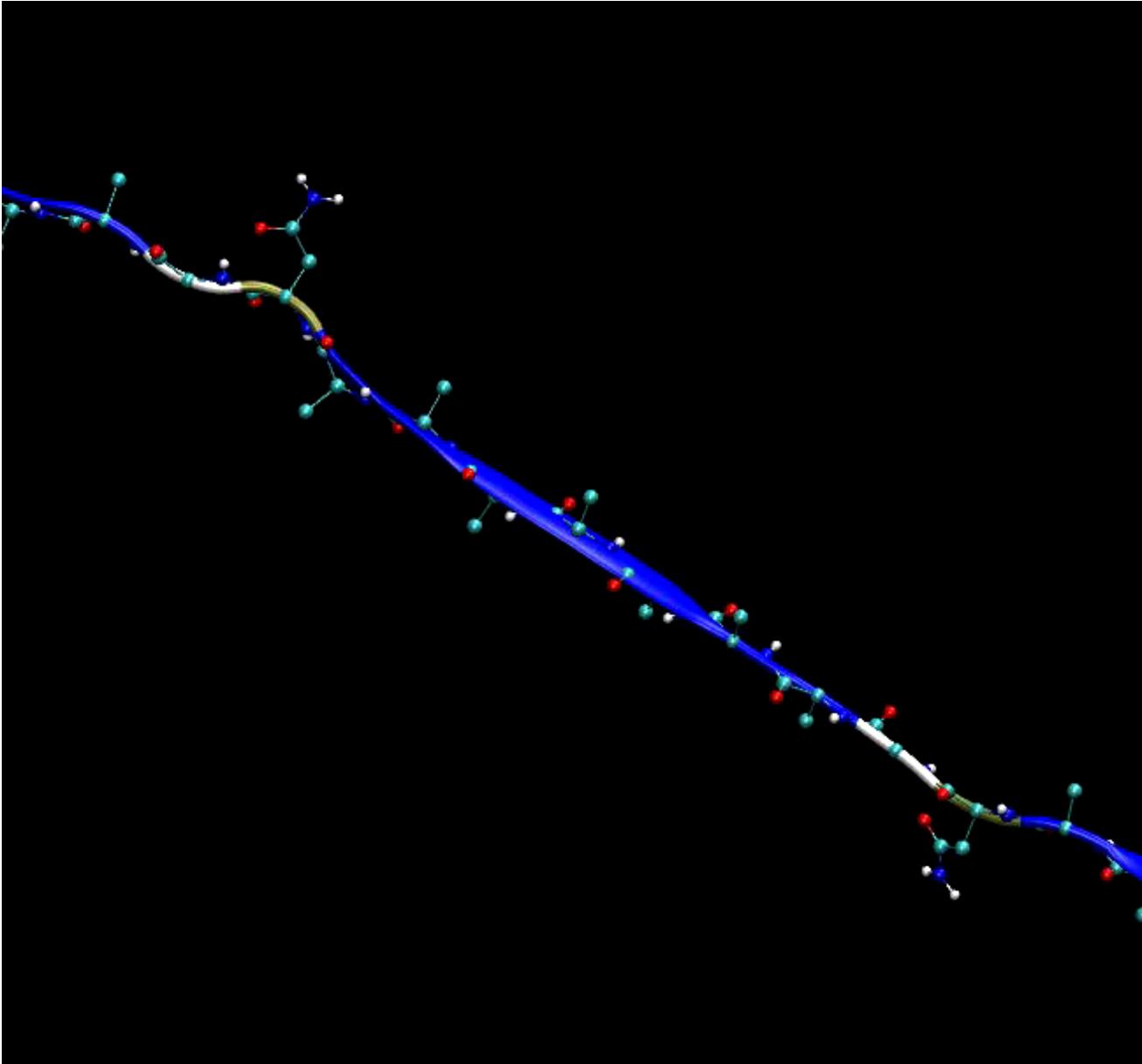
*Include anharmonic  
terms  
Derived from QM,  
more general*

# CHARMM force field

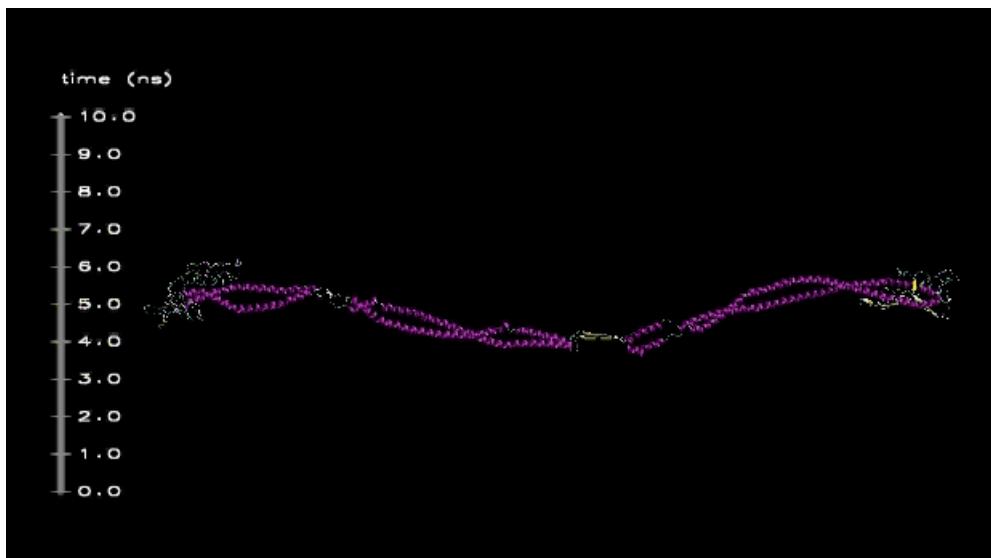
- Widely used and accepted model for protein structures
- Programs such as NAMD have implemented the CHARMM force field

**nanoHUB stretchmol module, study of a protein domain that is part of human vimentin intermediate filaments, collagen molecules, etc...**

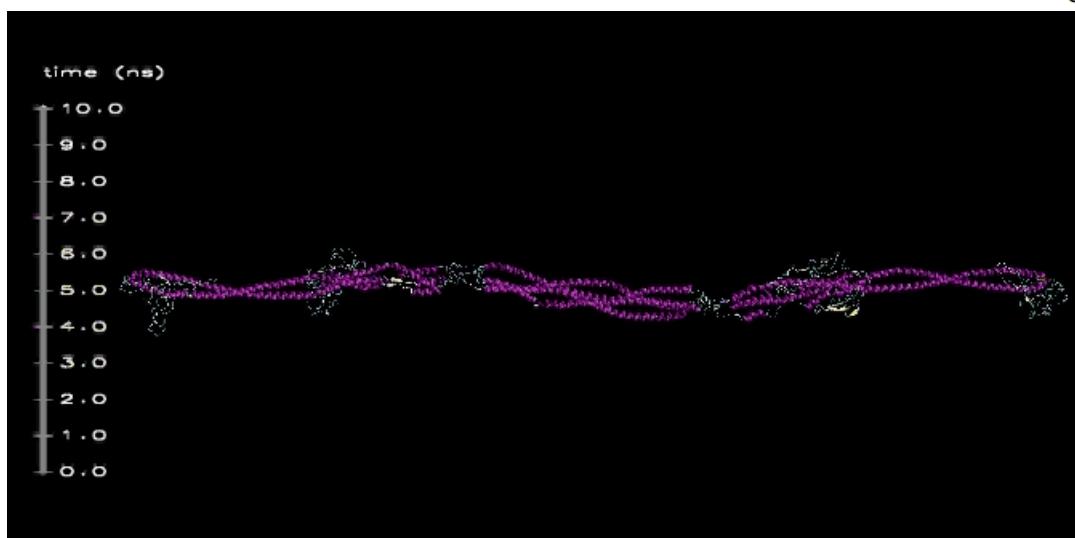
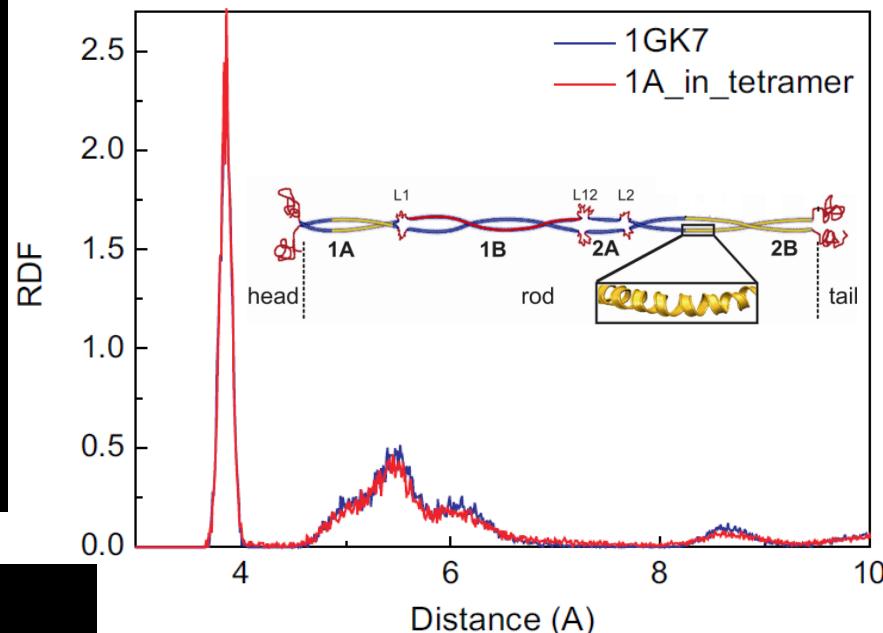
# Movie: protein folding with CHARMM



# Movies in equilibrium (temperature 300 K)



Dimer



Tetramer  
(increased effective  
bending stiffness,  
interaction via overlap  
& head/tail domain)