1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2011

Part I – Continuum and particle methods

Application to modeling brittle materials

Lecture 7

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Content overview

I. Particle and continuum methods

Lectures 2-13

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

II. Quantum mechanical methods

Lectures 14-26

1. It’s A Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. The Many-Body Problem: From Many-Body to Single-Particle
4. Quantum modeling of materials
5. From Atoms to Solids
6. Basic properties of materials
7. Advanced properties of materials
8. What else can we do?

Overview: Material covered so far…

- **Lecture 1: Broad introduction to IM/S**
- **Lecture 2**: **Introduction to atomistic and continuum modeling** (multi-scale modeling paradigm, difference between continuum and atomistic approach, case study: diffusion)
- **Lecture 3**: **Basic statistical mechanics – property calculation I** (property calculation: microscopic states vs. macroscopic properties, ensembles, probability density and partition function)
- **Lecture 4**: **Property calculation II** (Monte Carlo, advanced property calculation, introduction to chemical interactions)
- **Lecture 5: How to model chemical interactions I** (example: movie of copper deformation/dislocations, etc.)
- **Lecture 6: How to model chemical interactions II** (pair potentials, fracture – introduction)
- **Lecture 7: Application – MD simulation of materials failure**

Lecture 7: Application to modeling brittle materials

Outline:

1. Basic deformation mechanism in brittle materials - crack extension
2. Atomistic modeling of fracture
    - 2.1 Physical properties of atomic lattices
    - 2.2 Application
3. Bond order force fields - how to model chemical reactions

Goal of today's lecture:

- Apply our tools to model a particular material phenomena – brittle fracture (useful for pset #2)
- Learn basics in fracture of brittle materials
- Learn how to build a model to describe brittle fracture (from scratch)

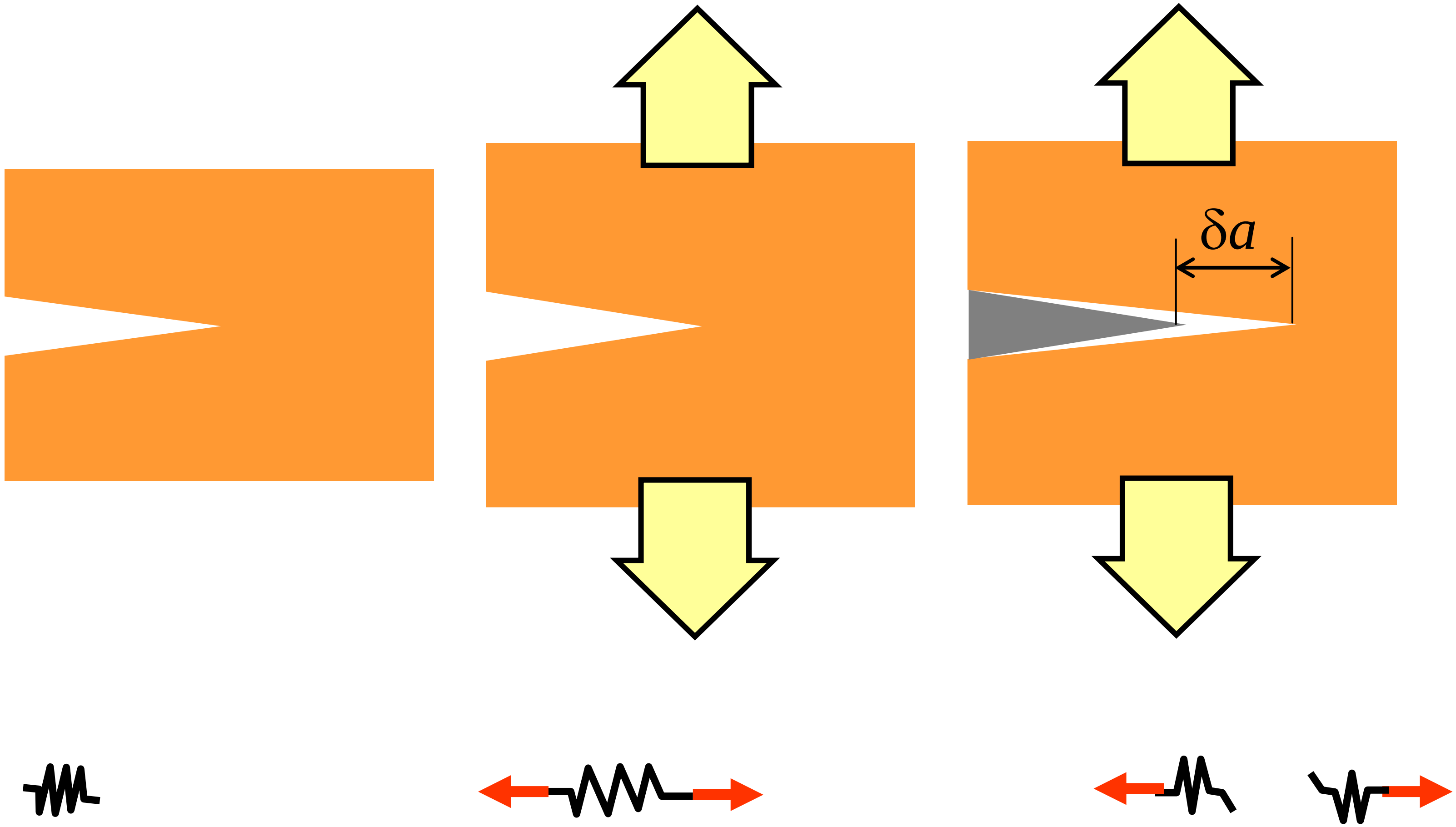
1. Basic deformation mechanism in brittle materials - crack extension

Brittle fracture

- Materials: **glass, silicon, many ceramics, rocks**

- At large loads, rather than accommodating a shape change, materials break

Basic fracture process: dissipation of elastic energy



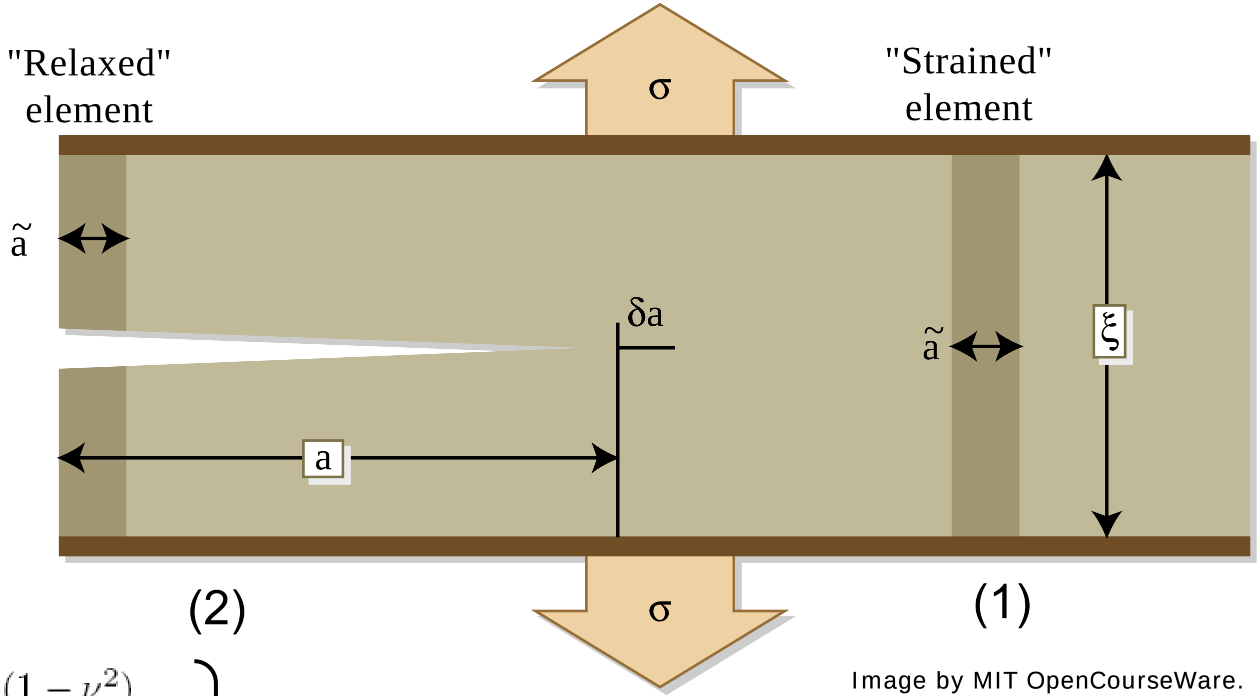
Undeformed

Stretching=store elastic energy

Release elastic energy dissipated into breaking chemical bonds

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 γ_s (energy necessary to create new surface, dimensions: energy/area, $\mathrm{Nm/m^2}$)



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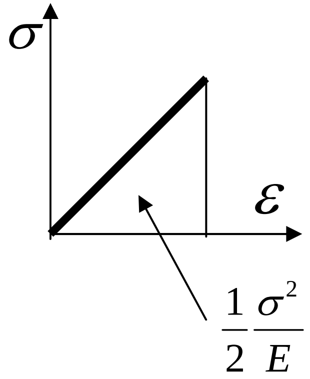


$$\left.\begin{array}{l} W_P^{(1)} = \dfrac{\sigma^2(1-\nu^2)}{2E}\xi\tilde{a}B \\[2em] W_P^{(2)} = 0 \end{array}\right\} W_P = W_P^{(1)} - W_P^{(2)} = \underbrace{\frac{1}{2}\frac{\sigma^2}{E}\xi\cancel{\tilde{a}B}}_{\text{change of elastic (potential) energy} = G} \overset{!}{=} \underbrace{2\gamma_s \cancel{B\tilde{a}}}_{\text{energy to create surfaces}}$$

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

Griffith condition for fracture initiation

- **Energy release rate** G, that is, the elastic energy released per unit crack advance must be equal or larger than the energy necessary to create new surfaces

$$G := \frac{1}{2}\frac{\sigma^2}{E}\xi = 2y_s$$

$$\boxed{G = 2\gamma_s}$$

- Provides **criterion to predict failure initiation**

- Calculation of G can be complex, but straightforward for thin strips as shown above

- Approach to calculate G based on "**stress intensity factor**" (see further literature, e.g. Broberg, Anderson, Freund, Tada)

Brittle fracture mechanisms

- Once nucleated, cracks in brittle materials spread rapidly, on the order of sound speeds

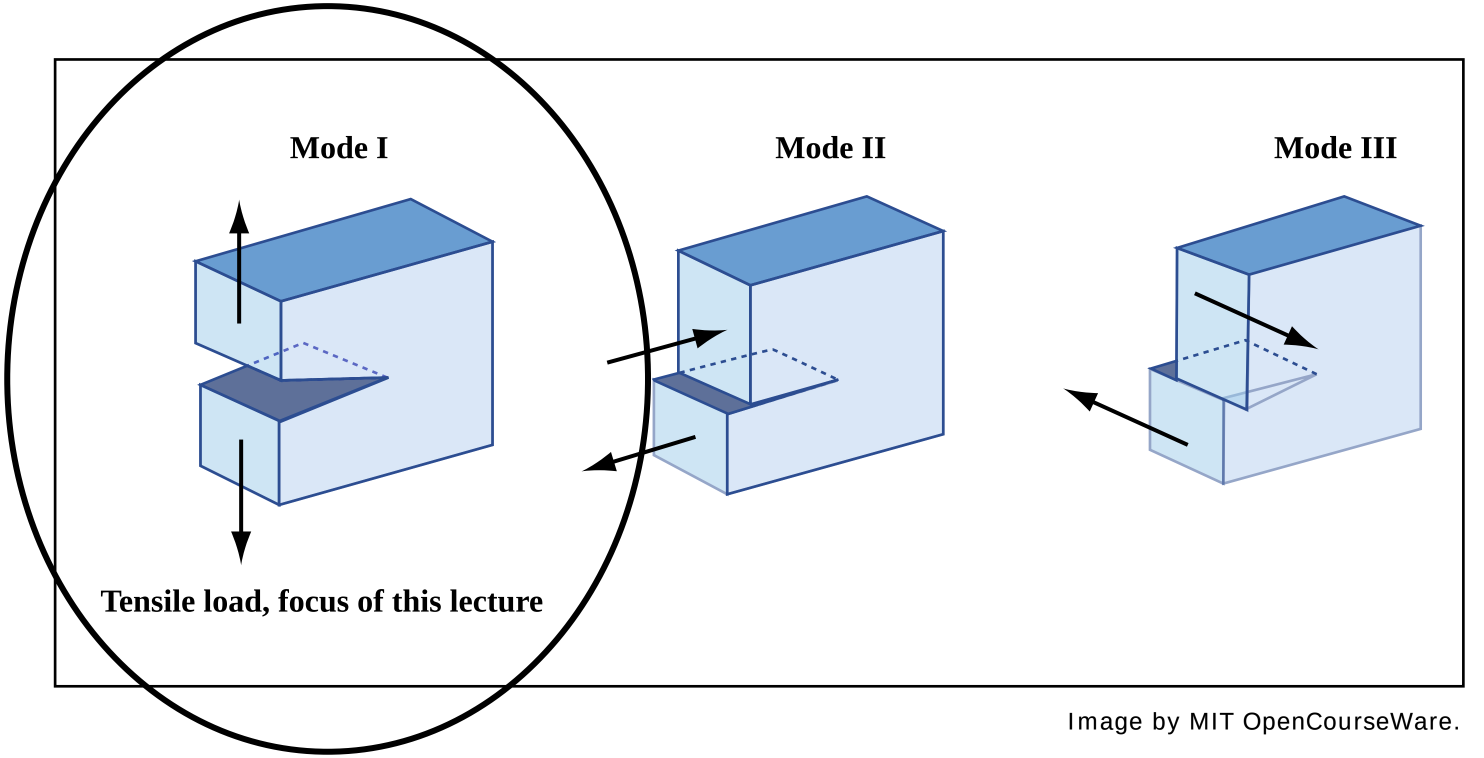
- Sound speeds in materials (=wave speeds):
  - Rayleigh-wave speed c_R (speed of surface waves)
  - shear wave speed c_s (speed of shear waves)
  - longitudinal wave speed c_l (speed of longitudinal waves)

- ***Maximum speeds of cracks is given by sound speeds, depending on mode of loading (mode I, II, III)***

Linear elastic continuum theory

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



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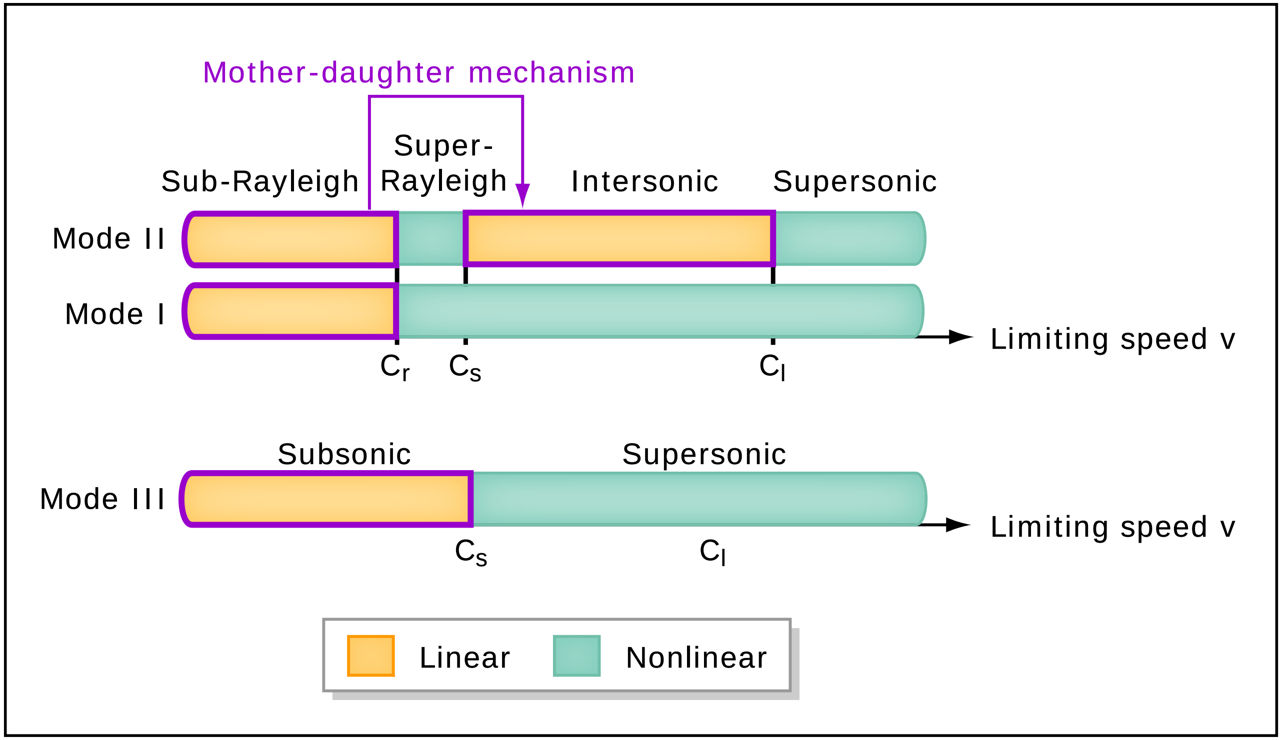
Limiting speeds of cracks: linear elastic continuum theory



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- 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

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

μ = shear modulus $\quad E = 8/3\mu \quad \mu = 3/8E$

Brittle fracture mechanisms: fracture is a multi-scale phenomenon, from nano to macro

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Physical reason for crack limiting speed

- Physical (mathematical) reason for the limiting speed is that it becomes increasingly difficult to increase the speed of the crack by adding a larger load
- When the crack approaches the limiting speed, the **resistance to fracture diverges to infinity (=dynamic fracture toughness)**

divergence

Driving force
(applied load)

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Please see: Fig. 6.15 in Buehler, Markus J. *Atomistic Modeling of Materials Failure*. Springer, 2008.

$$G = \frac{1}{2}\frac{\sigma^2}{E}\xi = f(y_s, v)$$

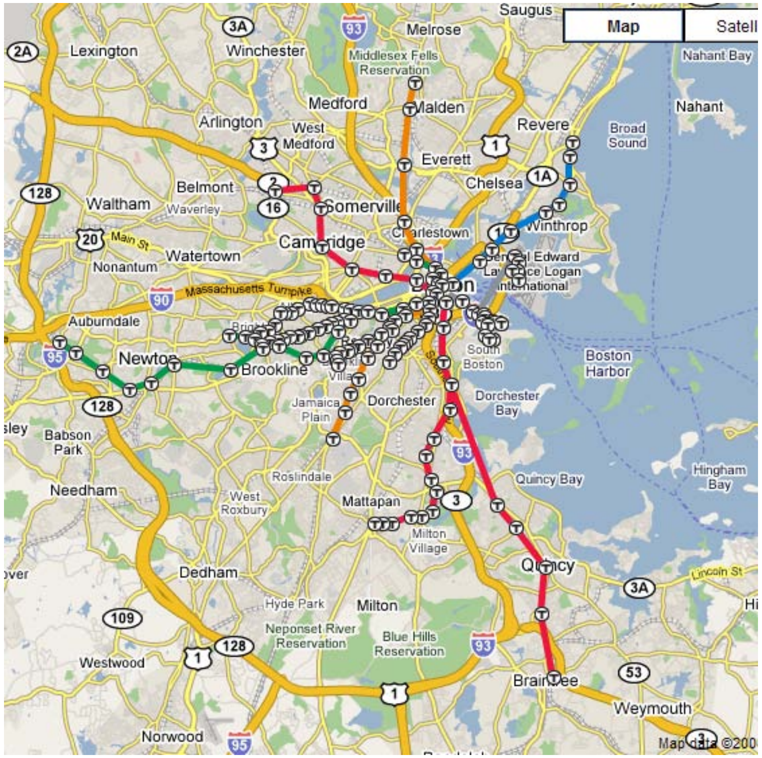
$$G \sim \frac{\sigma^2}{E}$$

2. Atomistic modeling of fracture

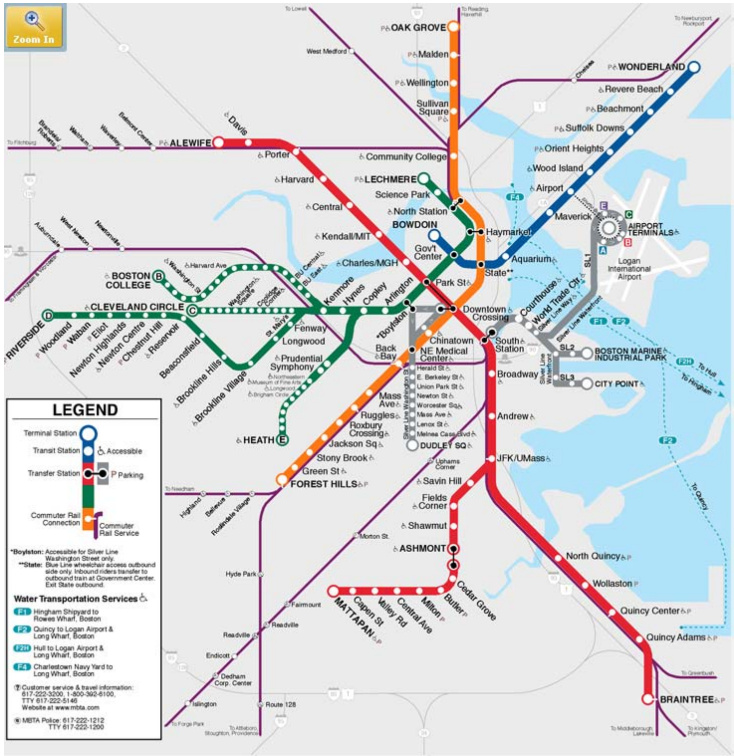
What is a model?

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

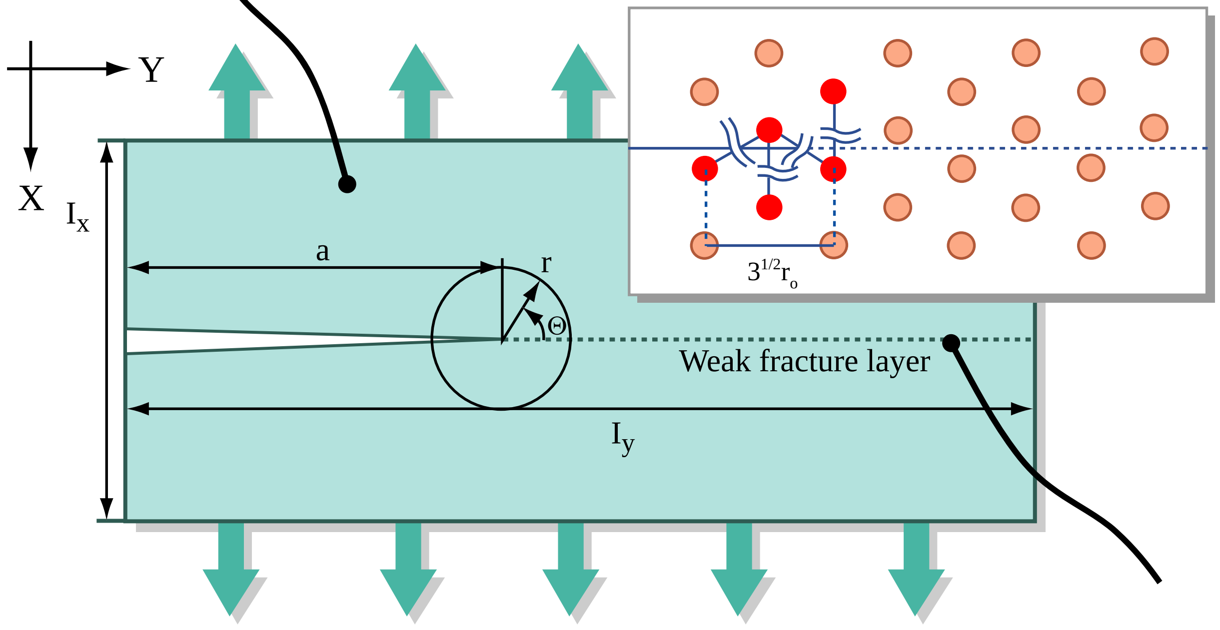
$$\phi = \frac{1}{2}k_0(r-r_0)^2$$

elasticity (store energy)

stable configuration of pair potential

↑

2D triangular (hexagonal) lattice



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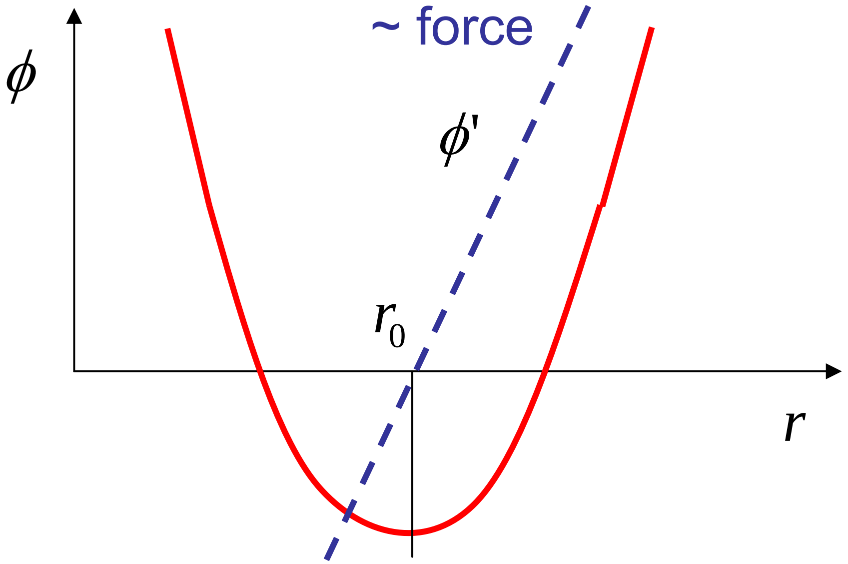
bond can break

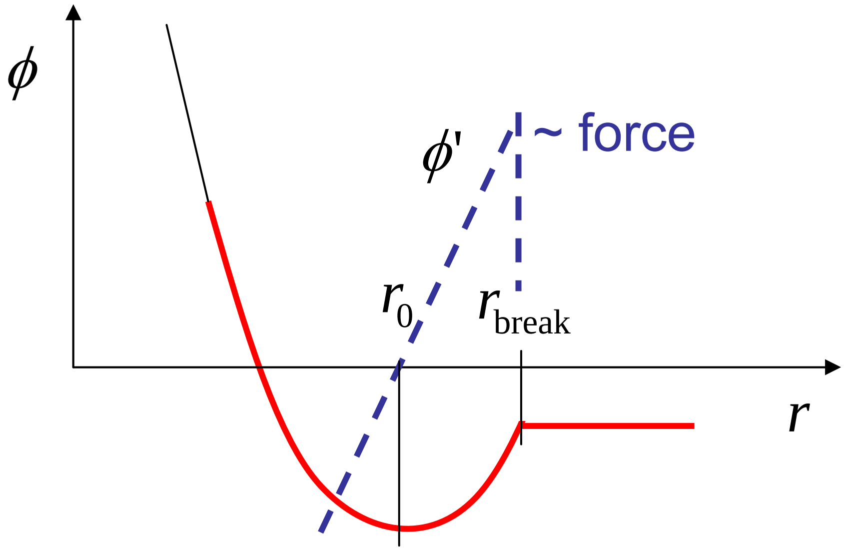
$$\phi = \begin{cases} \frac{1}{2}k_0(r-r_0)^2 & r < r_{\text{break}} \\ \frac{1}{2}k_0(r_{\text{break}}-r_0)^2 & r \geq r_{\text{break}} \end{cases}$$

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

Harmonic and harmonic bond snapping potential



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



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

2.1 Physical properties of atomic lattices

How to calculate elastic properties and fracture surface energy *– parameters to link with continuum theory of fracture*

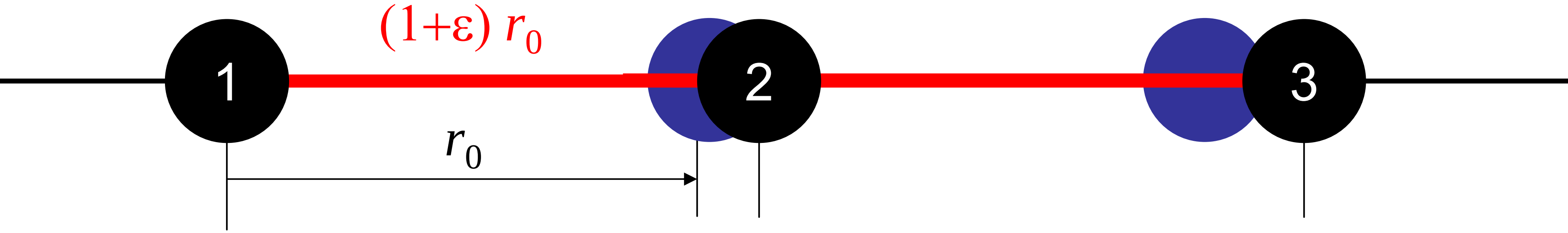
free energy density (energy per unit volume)

Stress $\sigma = \frac{\partial \psi(\varepsilon)}{\partial \varepsilon}$ Young's modulus $E = \frac{\partial^2 \psi(\varepsilon)}{\partial \varepsilon^2}$

$$\sigma = E\varepsilon$$

1D example – “Cauchy-Born rule”

- Impose homogeneous strain field on 1D string of atoms
- Then obtain $\sigma = E\varepsilon$ from that



$$r = (1+\varepsilon)\cdot r_0$$

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

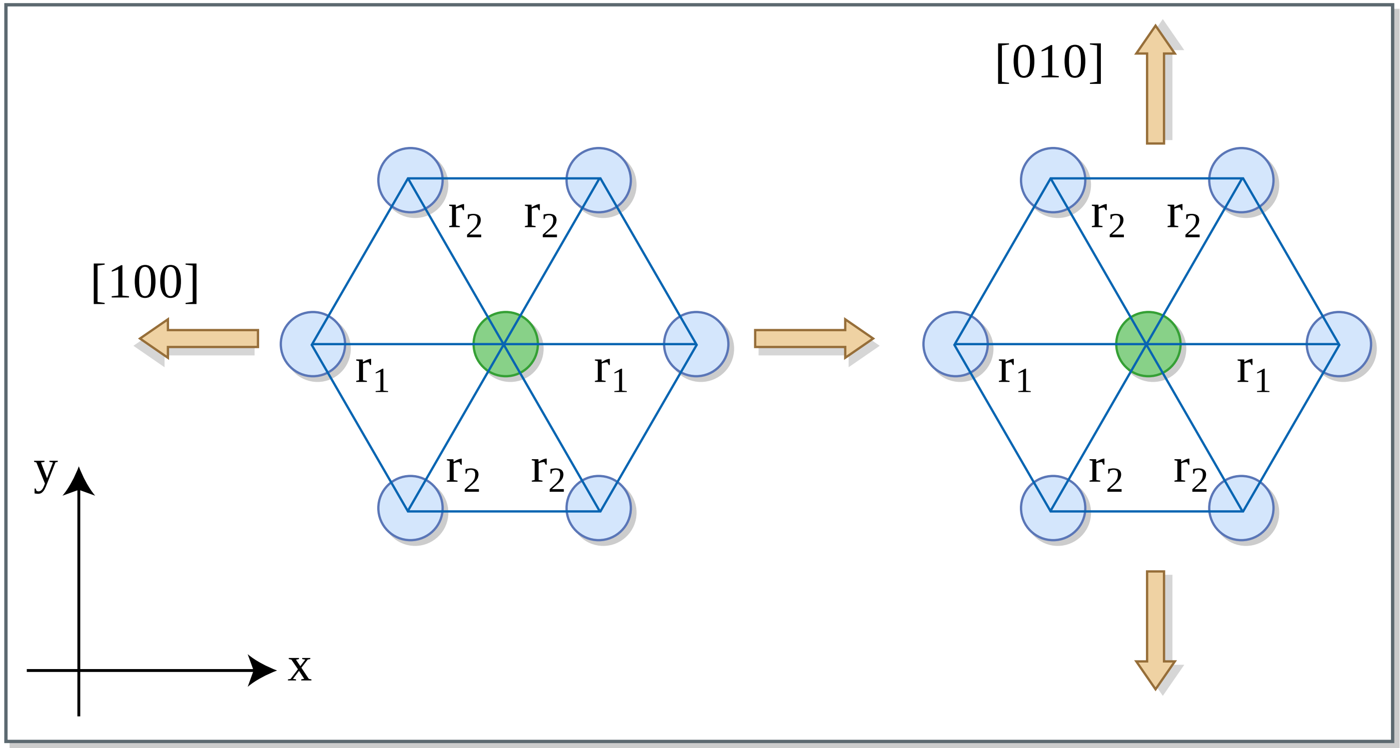
Strain energy density function

interatomic potential

$$\sigma = \frac{\partial \psi(\varepsilon)}{\partial \varepsilon} \qquad E = \frac{\partial^2 \psi(\varepsilon)}{\partial \varepsilon^2}$$

out-of-plane area ⟶ $r_0 \cdot D$ *atomic volume*

2D hexagonal lattice



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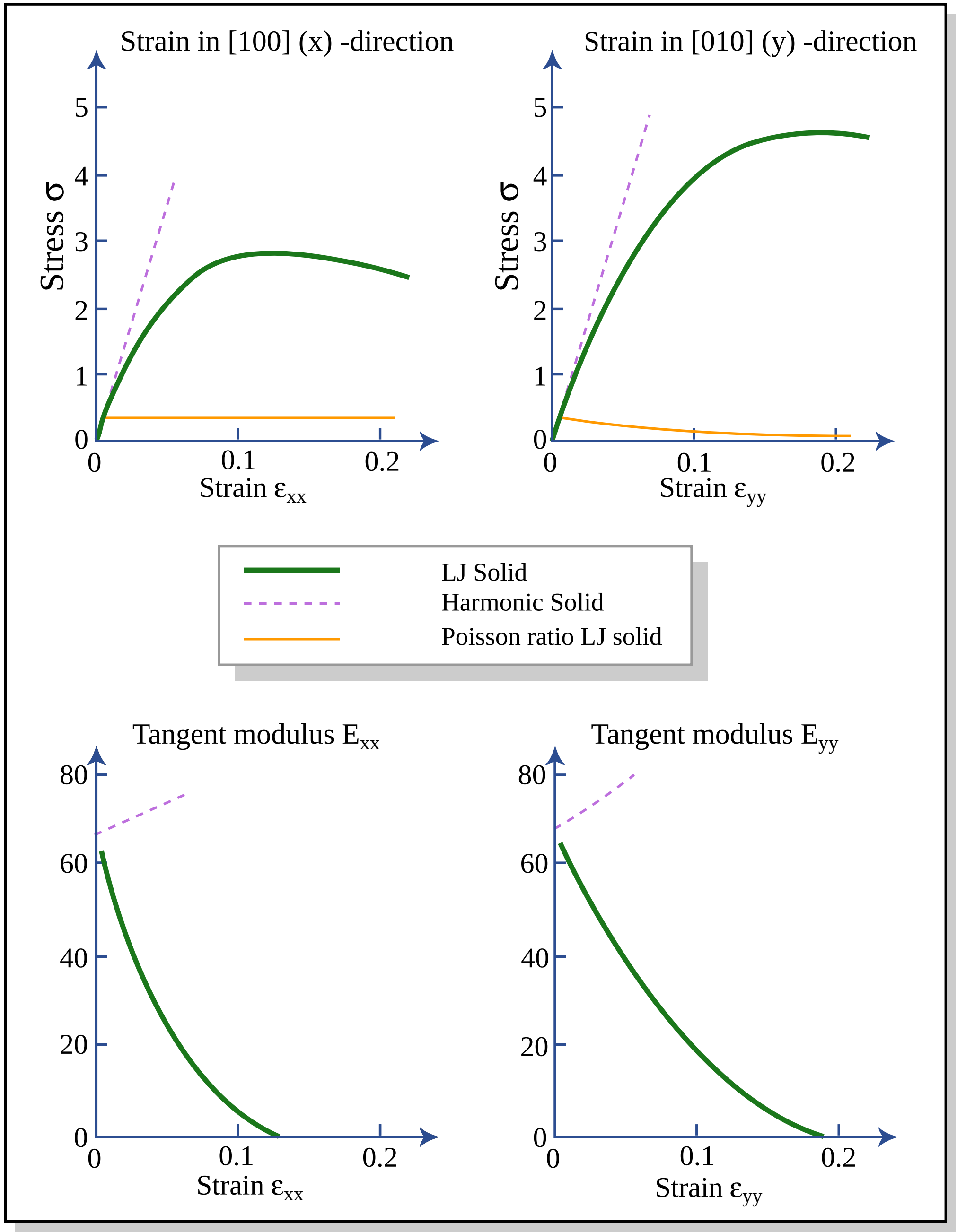
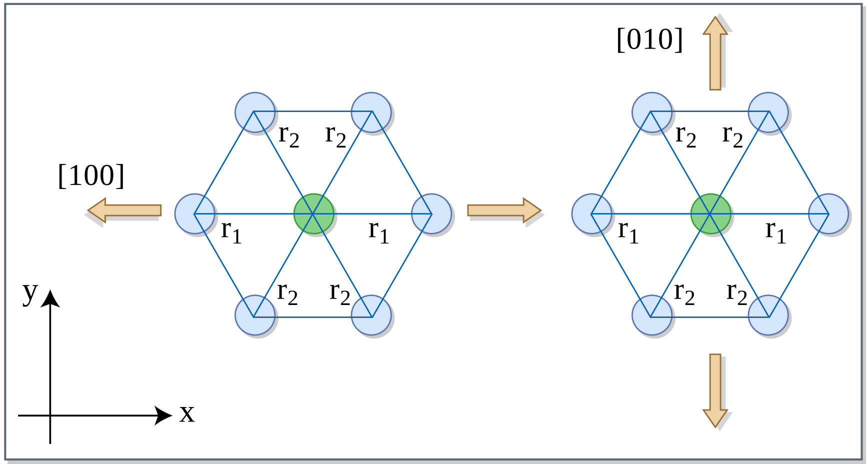
$$\phi'' = k$$

$$\psi(\varepsilon_{ij}) = \frac{\sqrt{3}}{8}\phi''\left(3\varepsilon_{11}^2 + 2\varepsilon_{11}\varepsilon_{22} + 3\varepsilon_{22}^2 + (\varepsilon_{21} + \varepsilon_{12})^2\right)$$

$$\sigma_{ij} = \frac{\partial\psi(\varepsilon_{ij})}{\partial\varepsilon_{ij}} \qquad c_{ijkl} = \frac{\partial^2\psi(\varepsilon_{ij})}{\partial\varepsilon_{ij}\partial\varepsilon_{kl}}$$

2D triangular lattice, LJ potential





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$$\varepsilon = 1$$

$$\sigma = 1$$

12:6 LJ potential

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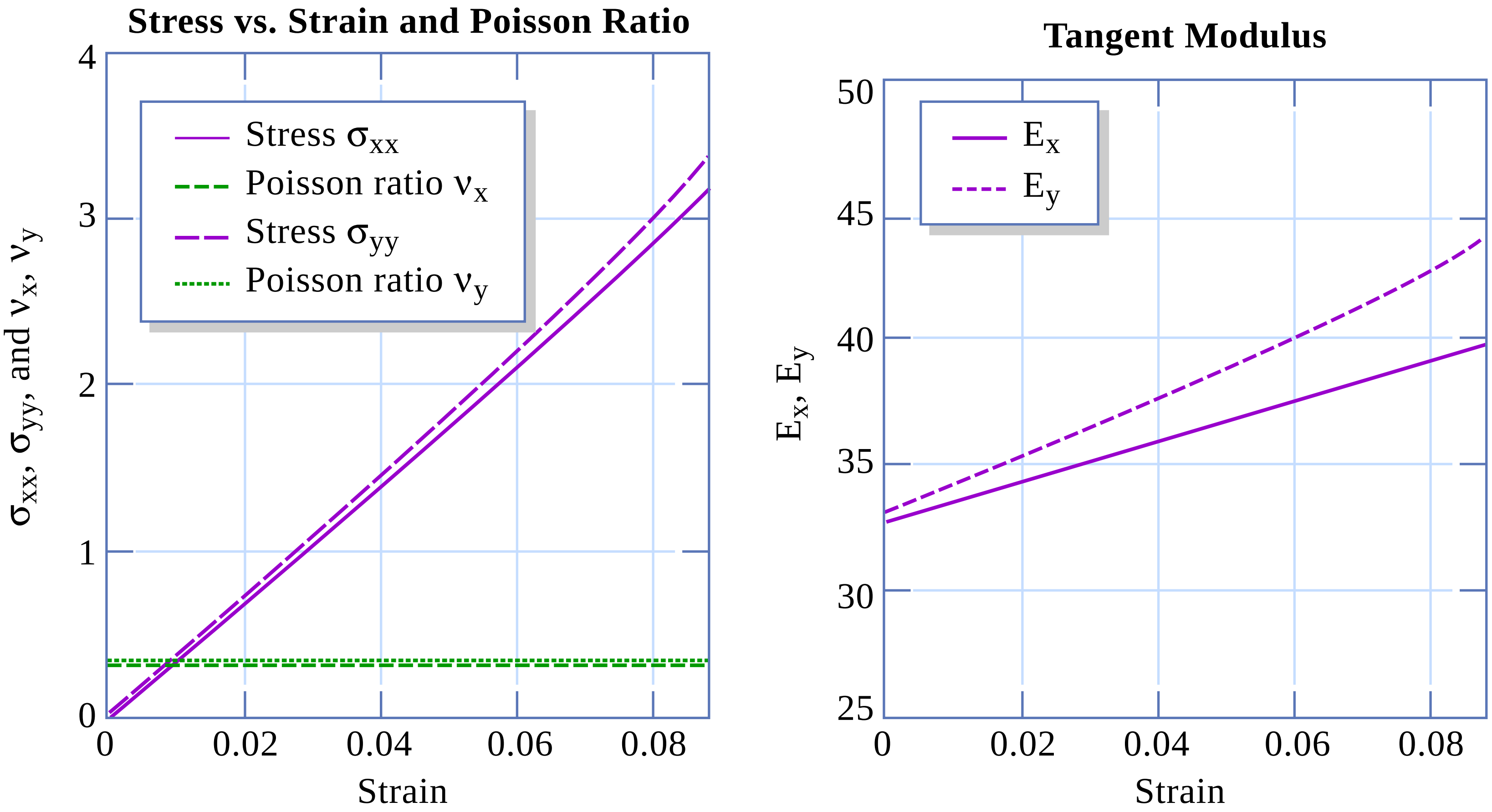
2D triangular lattice, harmonic potential



Elastic properties of the triangular lattice with harmonic interactions, stress versus strain (left) and tangent moduli E_x and E_y (right). The stress state is uniaxial tension, that is the stress in the direction orthogonal to the loading is relaxed and zero.

Image by MIT OpenCourseWare.

Elastic properties

$$E = \frac{2}{\sqrt{3}}k, \quad \mu = \frac{\sqrt{3}}{4}k$$

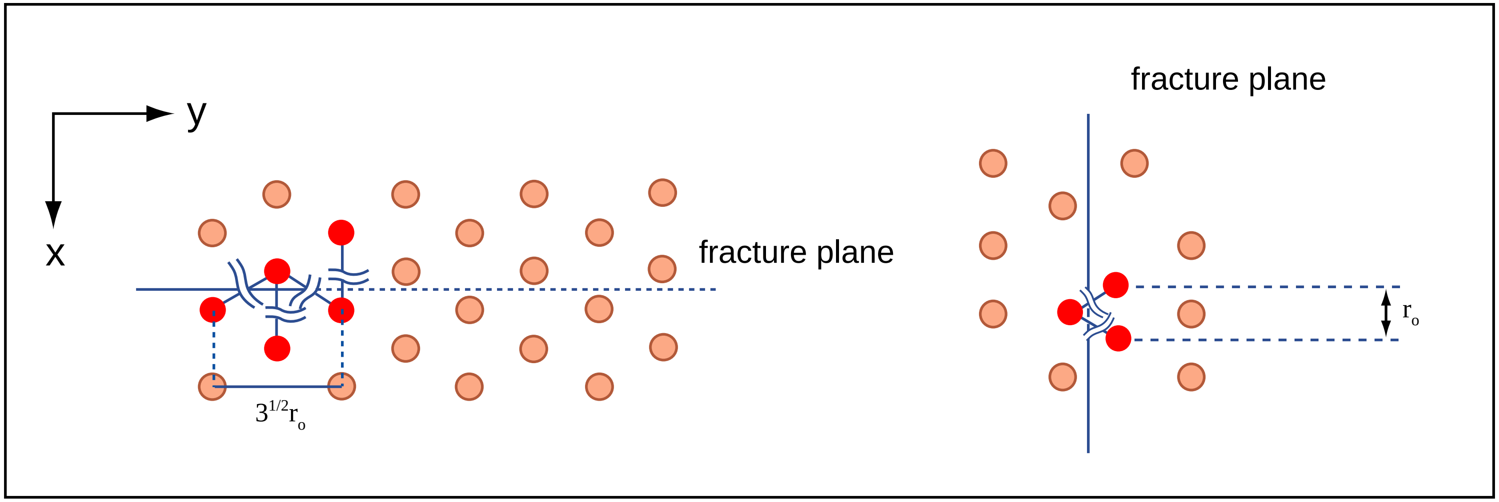
$$\phi'' = k$$

Enables to calculate wave speeds:

Spring constant k	Young's modulus E	Shear modulus μ	Poisson's ratio ν	c_l	c_s	c_R
$36\sqrt[3]{2} \approx 28.57$	33	12.4	0.33	6.36	3.67	3.39
$72\sqrt[3]{2} \approx 57.14$	66	24.8	0.33	9	5.2	4.8

Surface energy calculation

$$\gamma_s = -\frac{\Delta\phi}{d}$$



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Harmonic potential with bond snapping distance r_{break}

$$\gamma_s^{\text{bs,h}} = \frac{k(r_{\text{break}} - r_0)^2}{\sqrt{3}r_0}$$

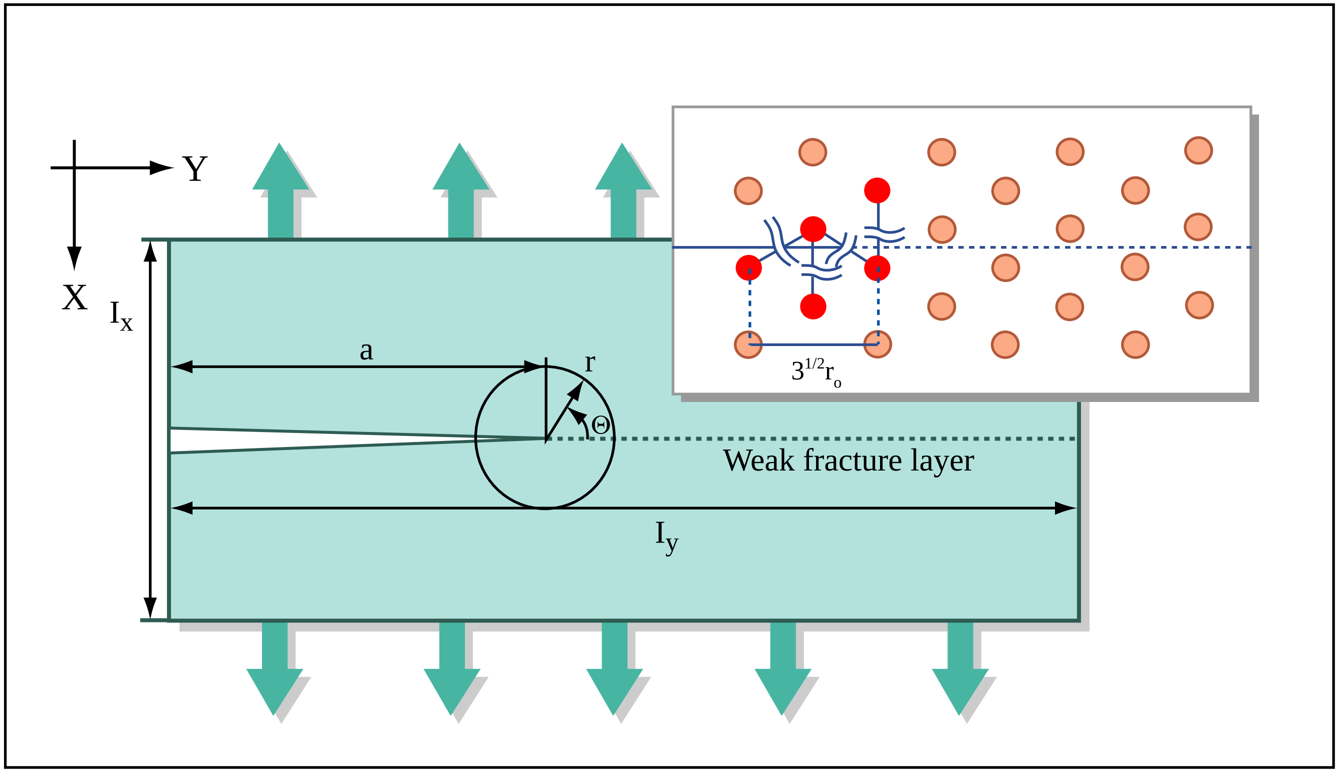
$$\gamma_s^{\text{bs,l}} = \frac{k(r_{\text{break}} - r_0)^2}{2r_0}$$

Note: out-of-plane unity thickness

2.2 Application

Focus: *effects of material nonlinearities (reflected in choice of model)*

Coordinate system and atomistic model



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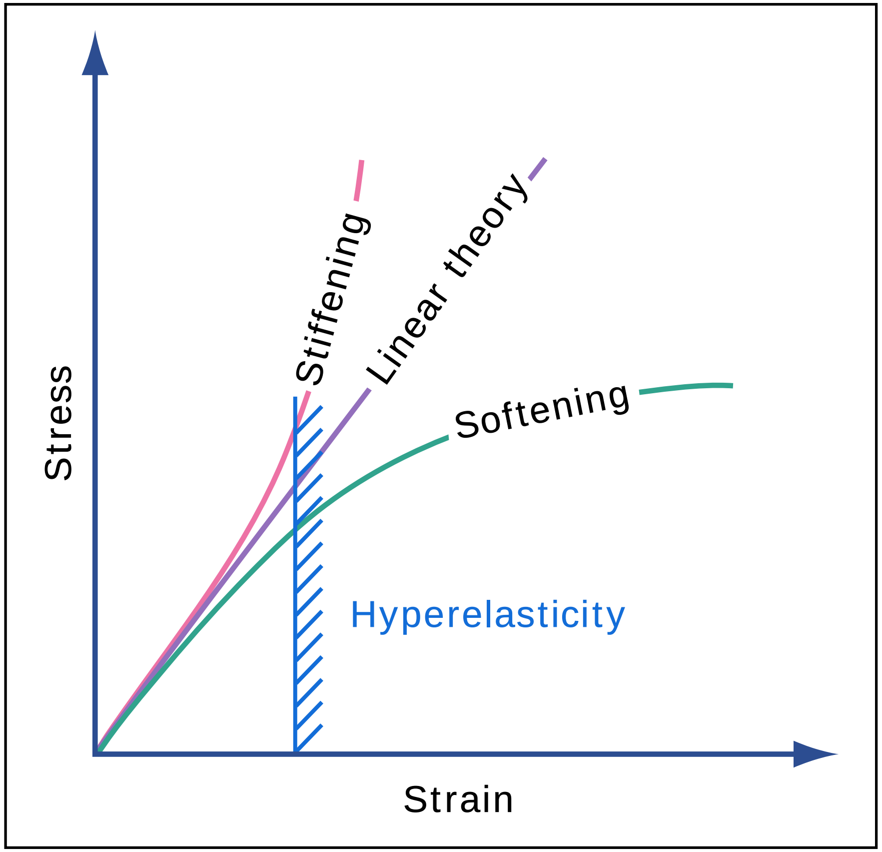
Pair potential to describe atomic interactions
Confine crack to a 1D path (weak fracture layer)

Linear versus nonlinear elasticity=hyperelasticity



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

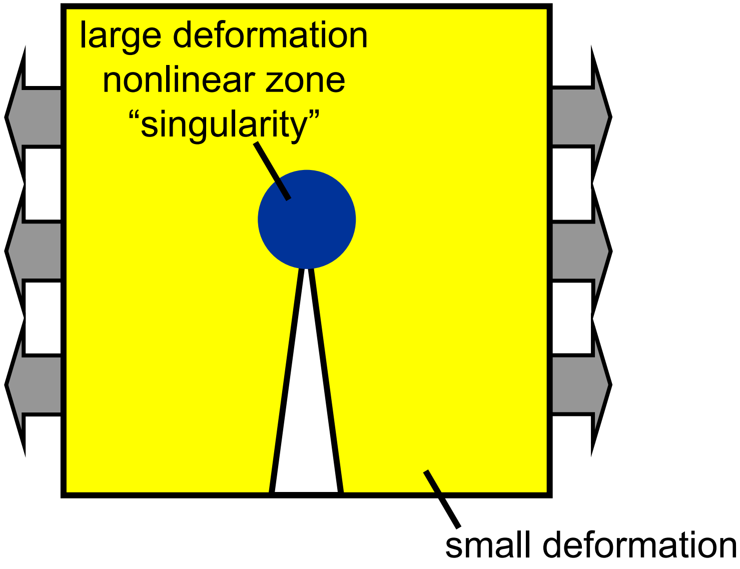
Nonlinear elasticity = hyperelasticity: Young’s modulus (stiffness) changes with deformation

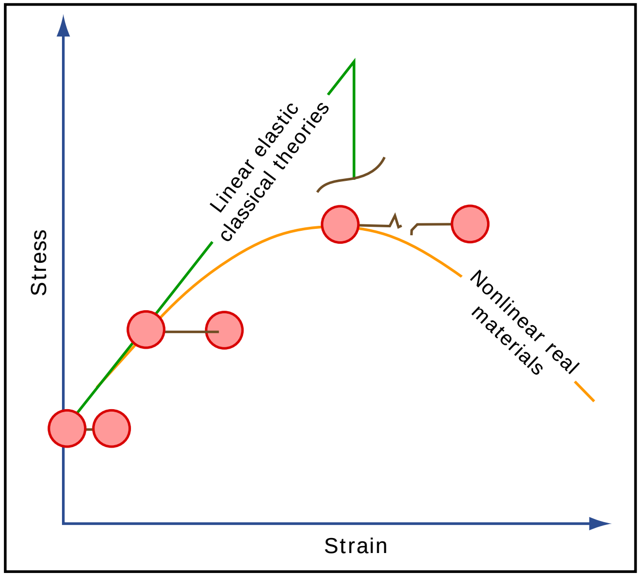
Subsonic and supersonic fracture

- 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





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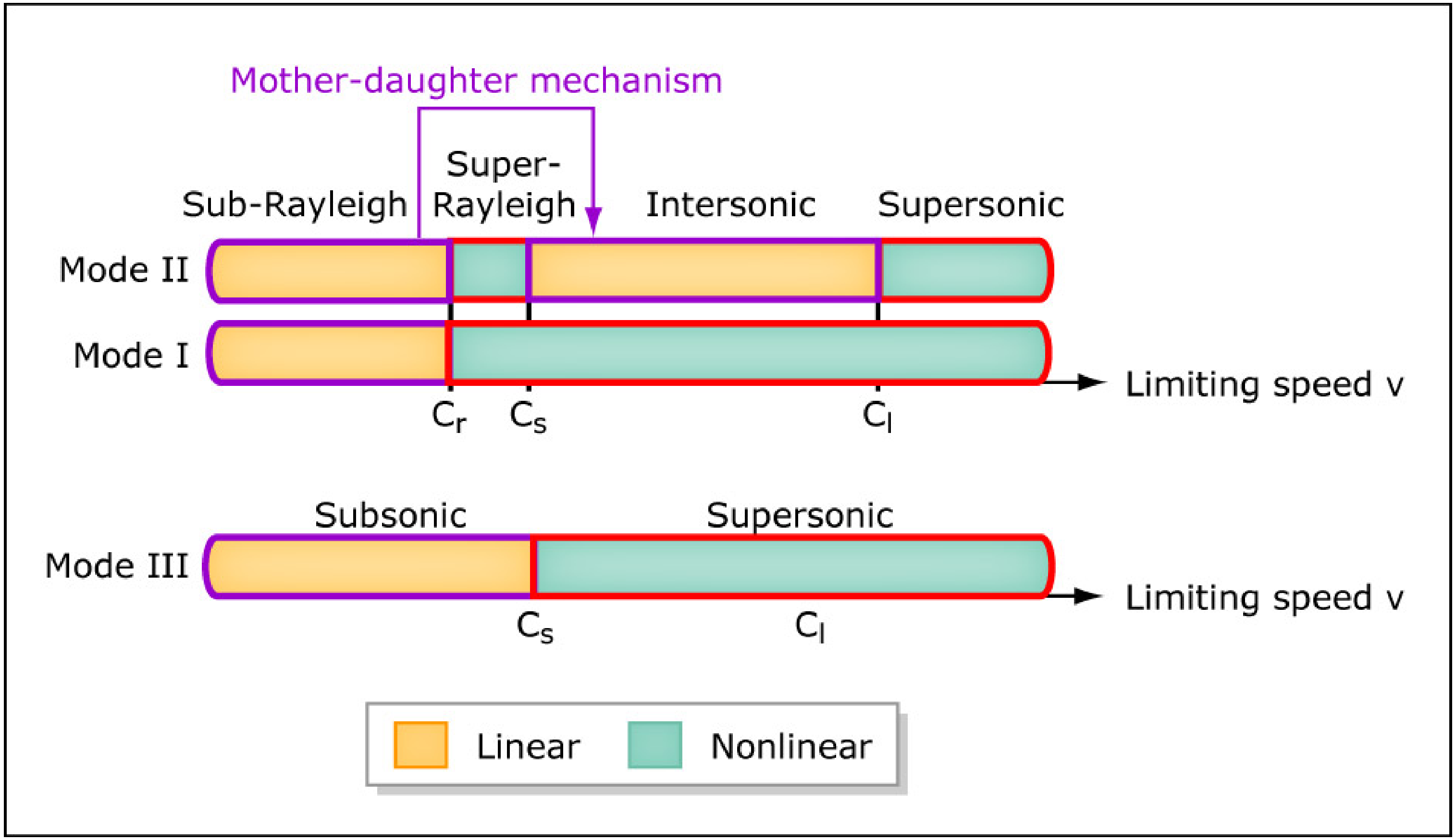
Limiting speeds of cracks



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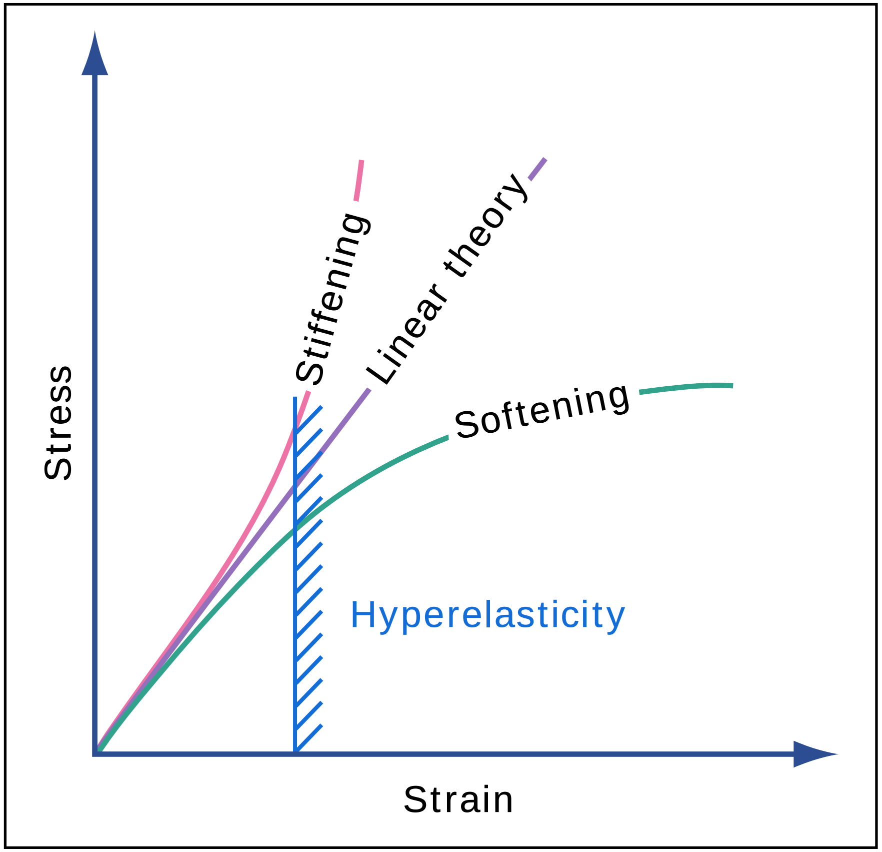
- Under presence of hyperelastic effects, cracks can exceed the conventional barrier given by the wave speeds
- This is a “local” effect due to enhancement of energy flux
- Subsonic fracture due to local softening, that is, reduction of energy flux

Stiffening vs. softening behavior

real materials



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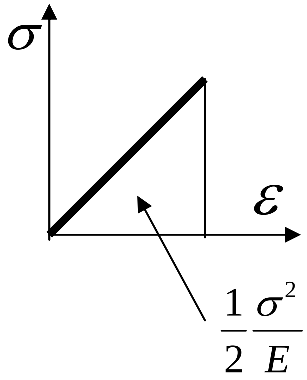
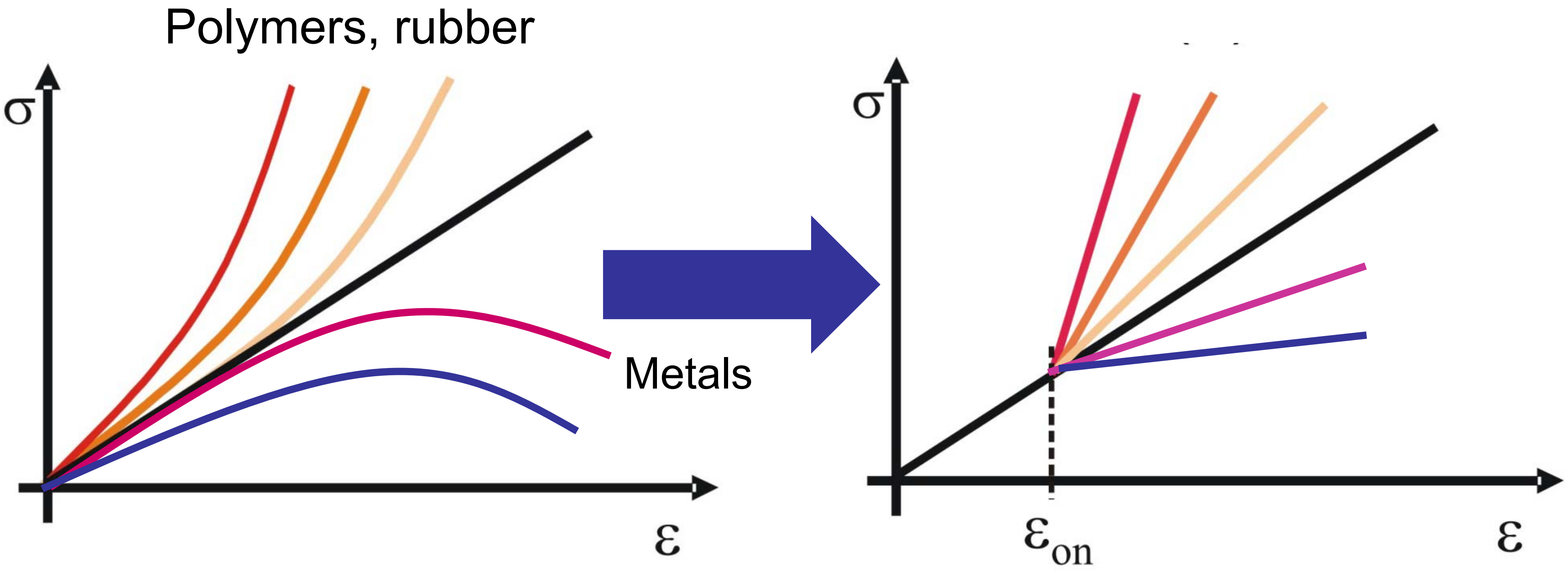
"linear elasticity"



Increased/decreased wave speed

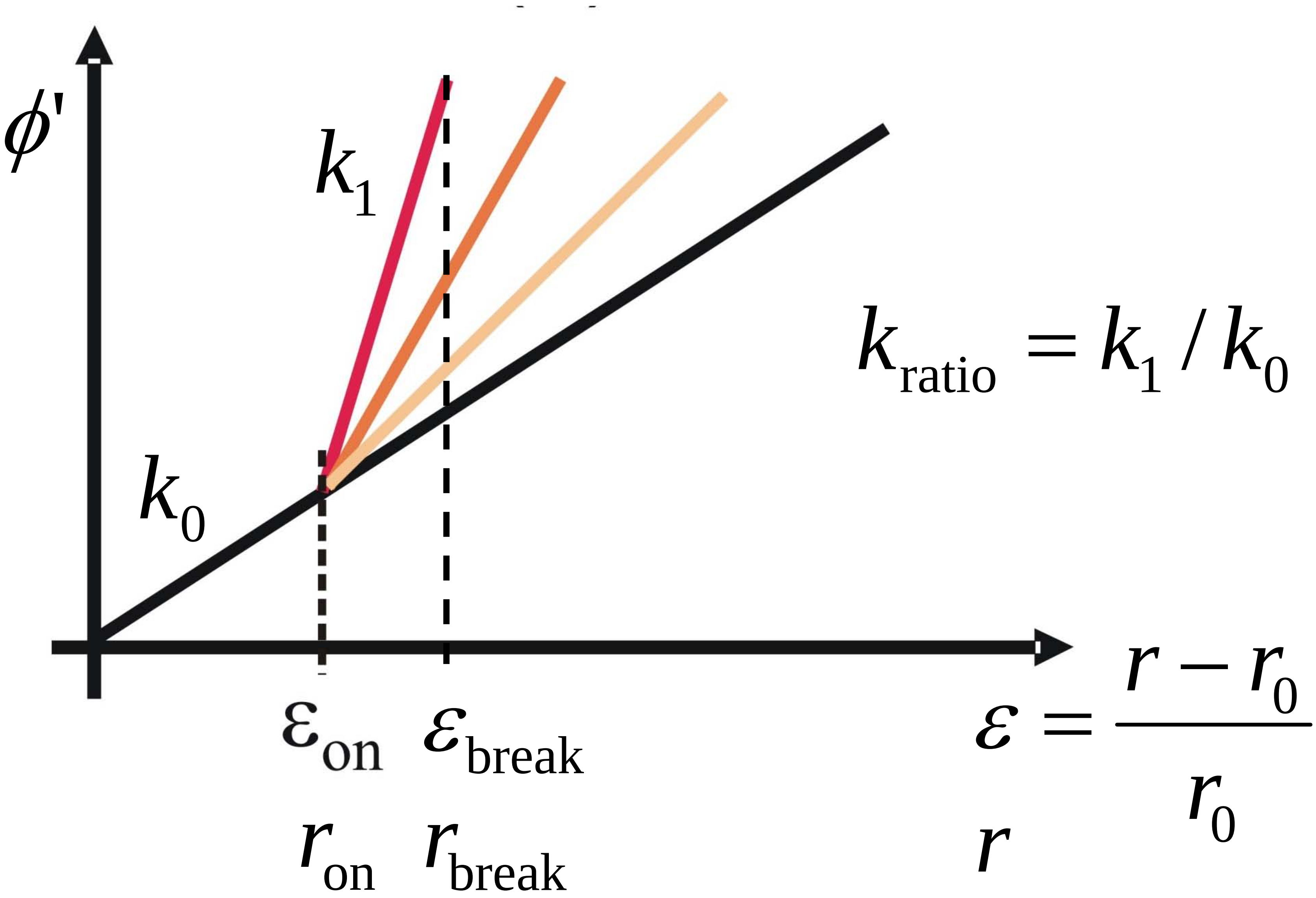
$$c_l = \sqrt{\frac{3\mu}{\rho}} \qquad c_s = \sqrt{\frac{\mu}{\rho}} \qquad c_R \approx \beta c_s \qquad \beta \approx 0.923$$

MD model development: biharmonic potential



- **Stiffness change under deformation**, with different strength
- Atomic bonds break at critical atomic separation
- **Want:** simple set of parameters that control these properties (as few as possible, to gain generic insight)

Biharmonic potential – control parameters



$$k_{\text{ratio}} = k_1 / k_0$$

$$\varepsilon = \frac{r - r_0}{r_0}$$

Biharmonic potential definition

The biharmonic potential is defined as:

$$\phi \quad (r_{ij}) = \begin{cases} a_0 + \frac{1}{2}k_0(r_{ij} - r_0)^2 & \text{if } r_{ij} < r_{\text{on}}, \\ a_1 + \frac{1}{2}k_1(r_{ij} - r_1)^2 & \text{if } r_{ij} \geq r_{\text{on}} \end{cases}$$

where r_{on} is the critical atomic separation for the onset of the hyperelastic effect, and

$$a_1 = a_0 + \frac{1}{2}k_0(r_{\text{on}} - r_0)^2 - \frac{1}{2}k_1(r_{\text{on}} - r_1)^2$$

and

$$r_1 = \frac{1}{2}(r_{\text{on}} + r_0)$$

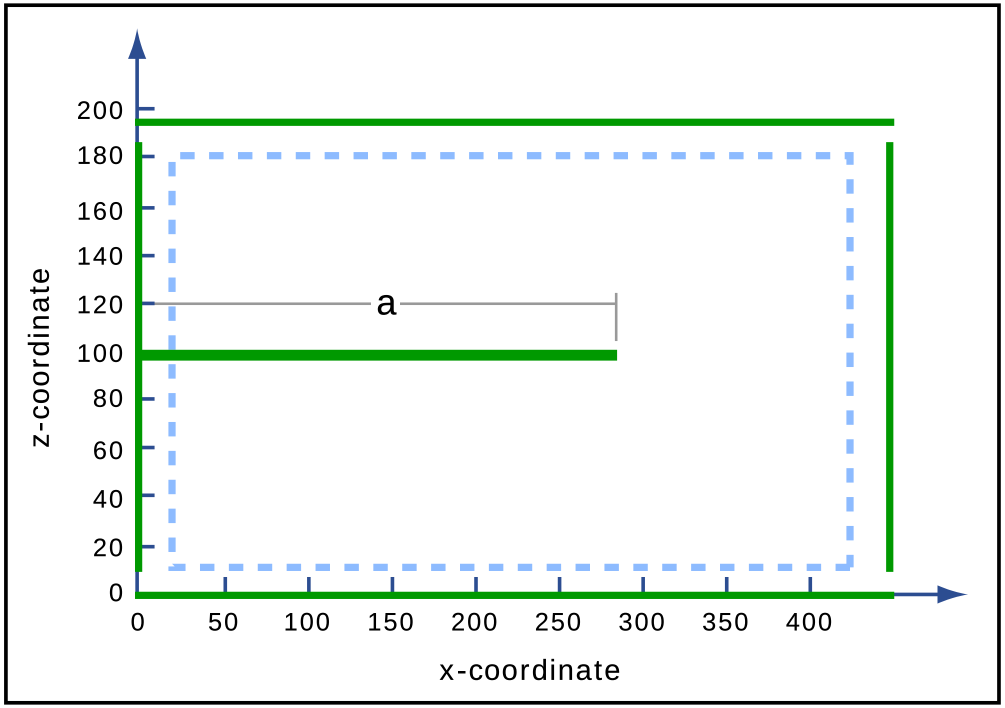
are found by continuity conditions of the potential at $r = r_{\text{on}}$.

The values k_0 and k_1 refer to the small- and large-strain spring constants.

Energy filtering: visualization approach

- Only plot atoms associated with higher energy
- Enables determination of crack tip (atoms at surface have higher energy, as they have fewer neighbors than atoms in the bulk)

Energy of atom i $$U_i = \sum_{j=1}^{N} \phi(r_{ij})$$



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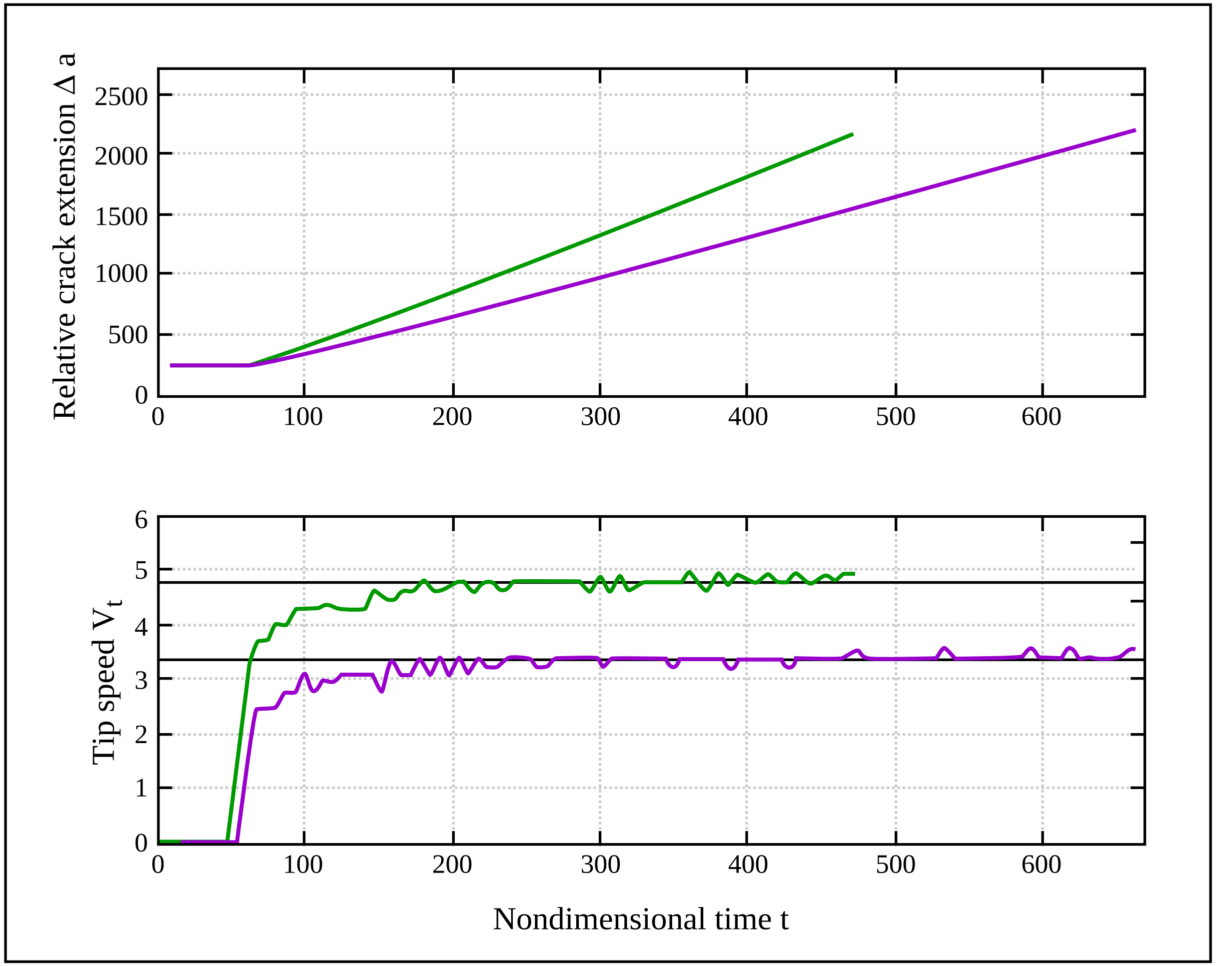
MD simulation results: confirms linear continuum theory



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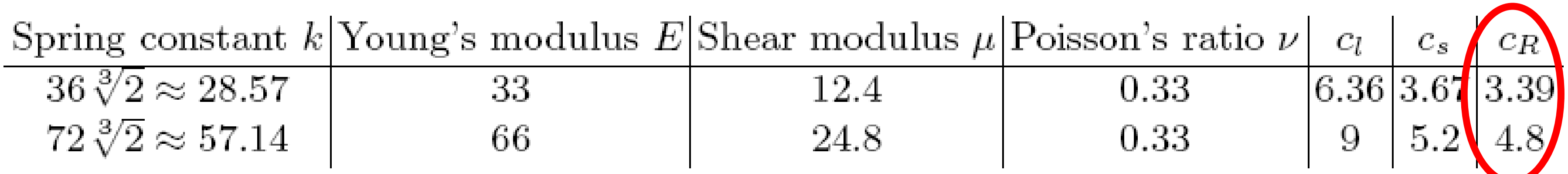
a (*t*)

crack speed
=time derivative of *a*

$v(t)=da/dt$



Spring constant k	Young's modulus E	Shear modulus μ	Poisson's ratio ν	c_l	c_s	c_R
$36\sqrt[3]{2} \approx 28.57$	33	12.4	0.33	6.36	3.67	3.39
$72\sqrt[3]{2} \approx 57.14$	66	24.8	0.33	9	5.2	4.8

Virial stress field around a crack

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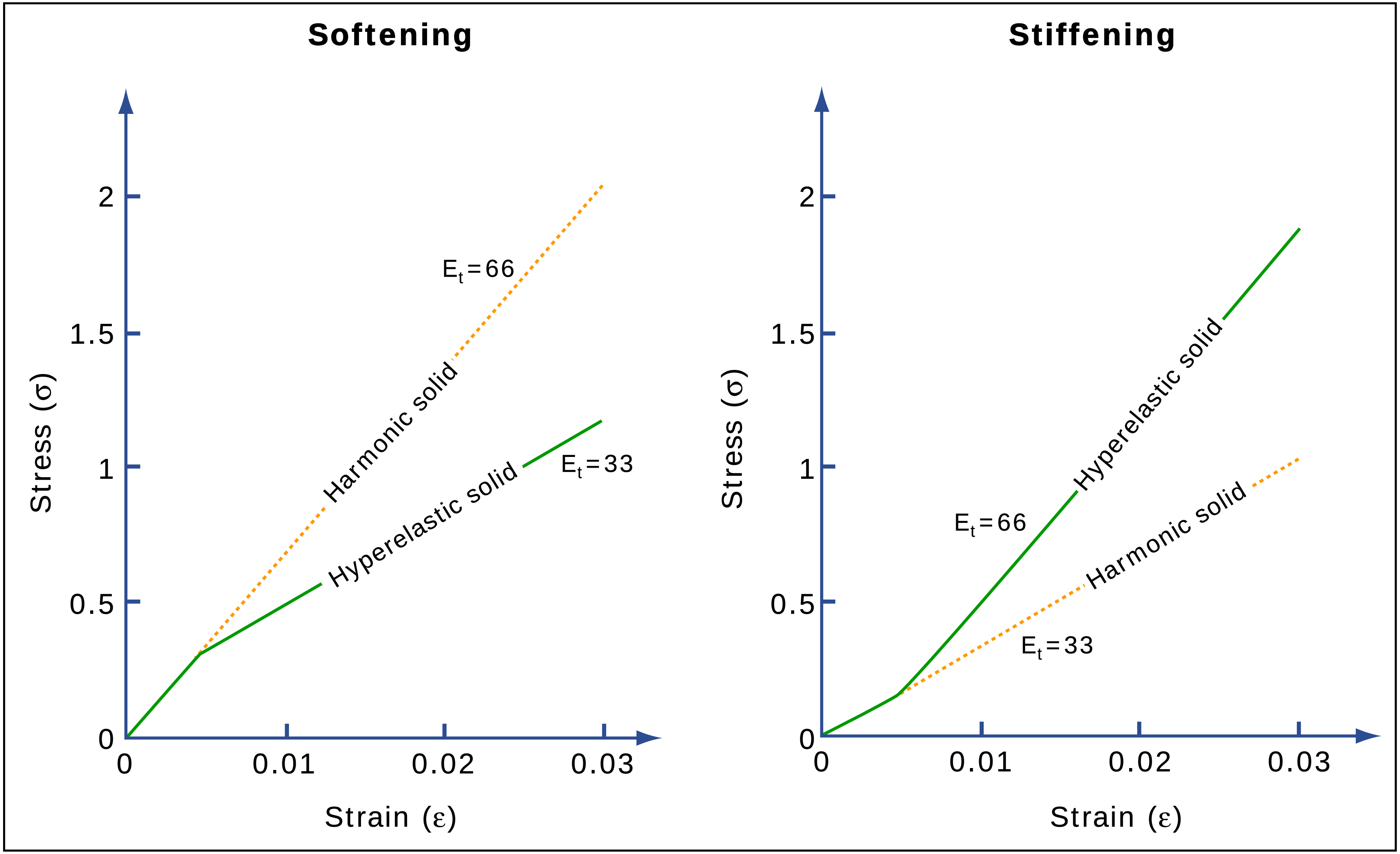
Please see: Fig. 6.30 in Buehler, Markus J. *Atomistic Modeling of Materials Failure*. Springer, 2008.

large stresses
at crack tip
- induce bond failure

Biharmonic potential – bilinear elasticity



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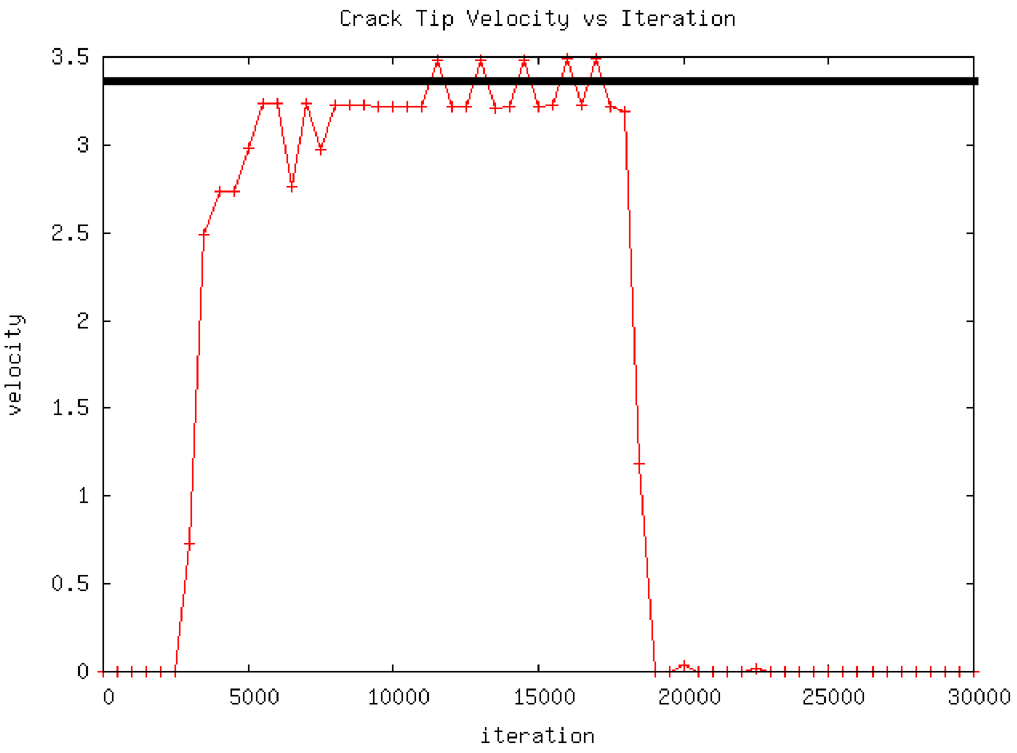
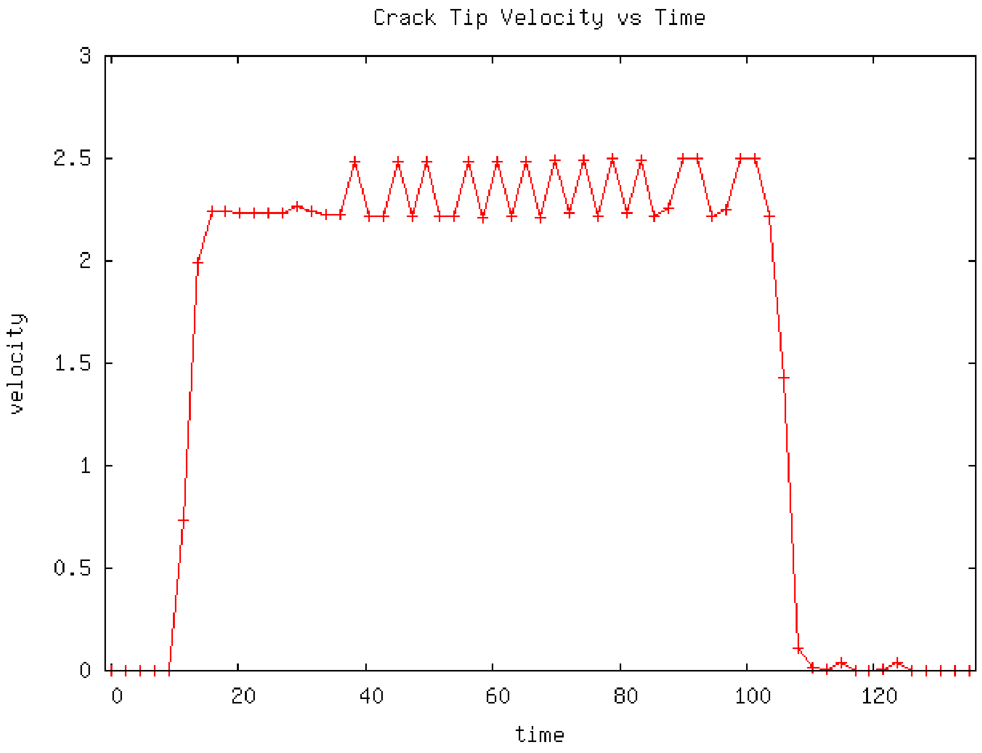
Harmonic system



Subsonic fracture

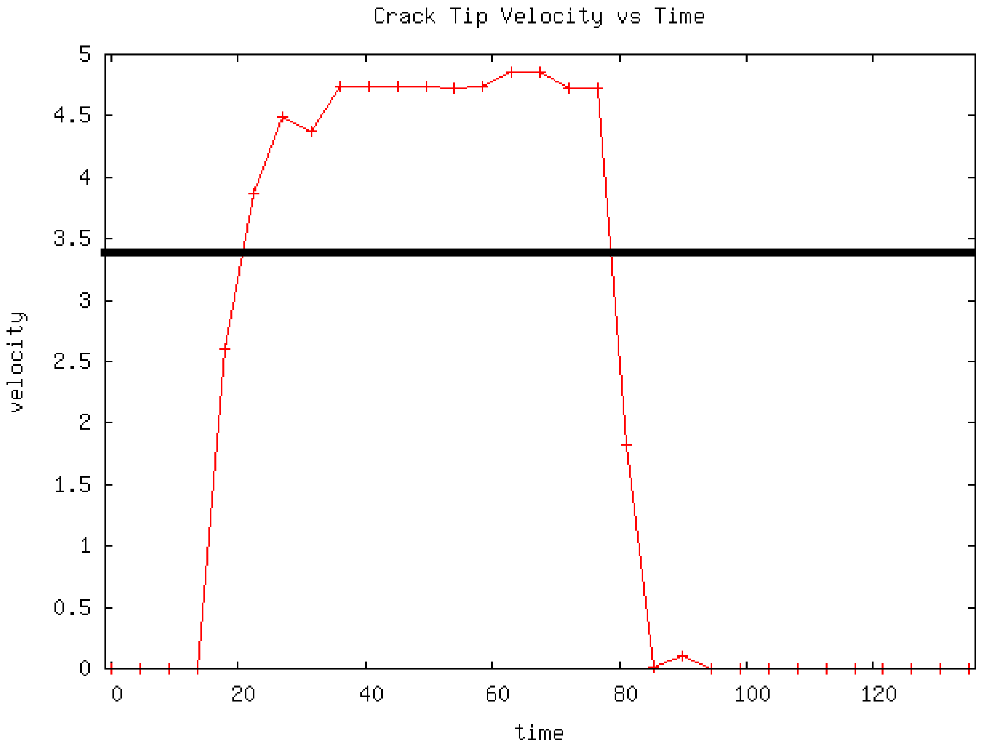
- Softening material behavior leads to subsonic fracture, that is, the crack can never attain its theoretical limiting speed
- Materials: metals, ceramics



$< 3.4 = c_R$

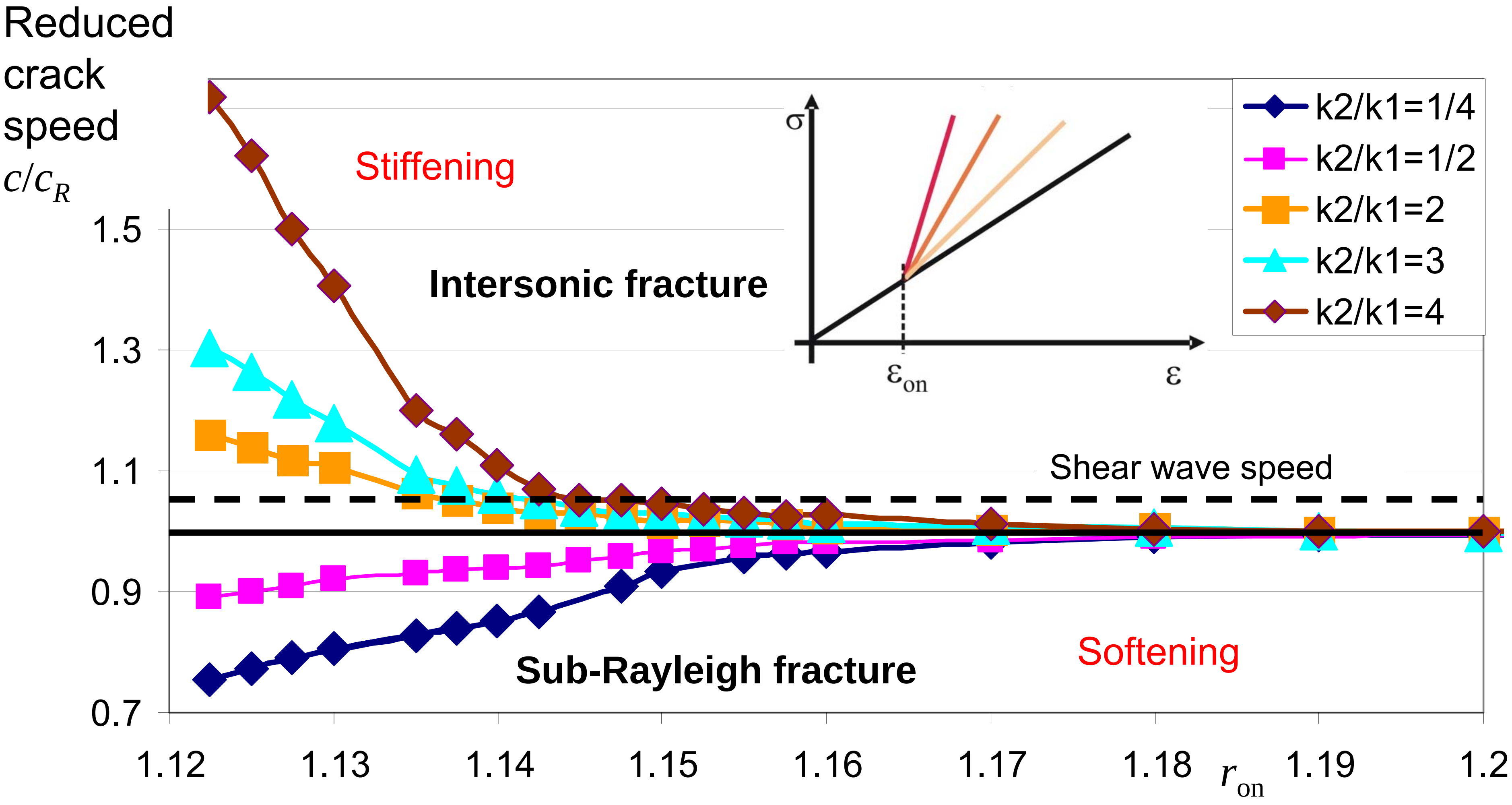
Supersonic fracture

- Stiffening material behavior leads to subsonic fracture, that is, the crack can exceed its theoretical limiting speed
- Materials: polymers



$> 3.4 = c_R$

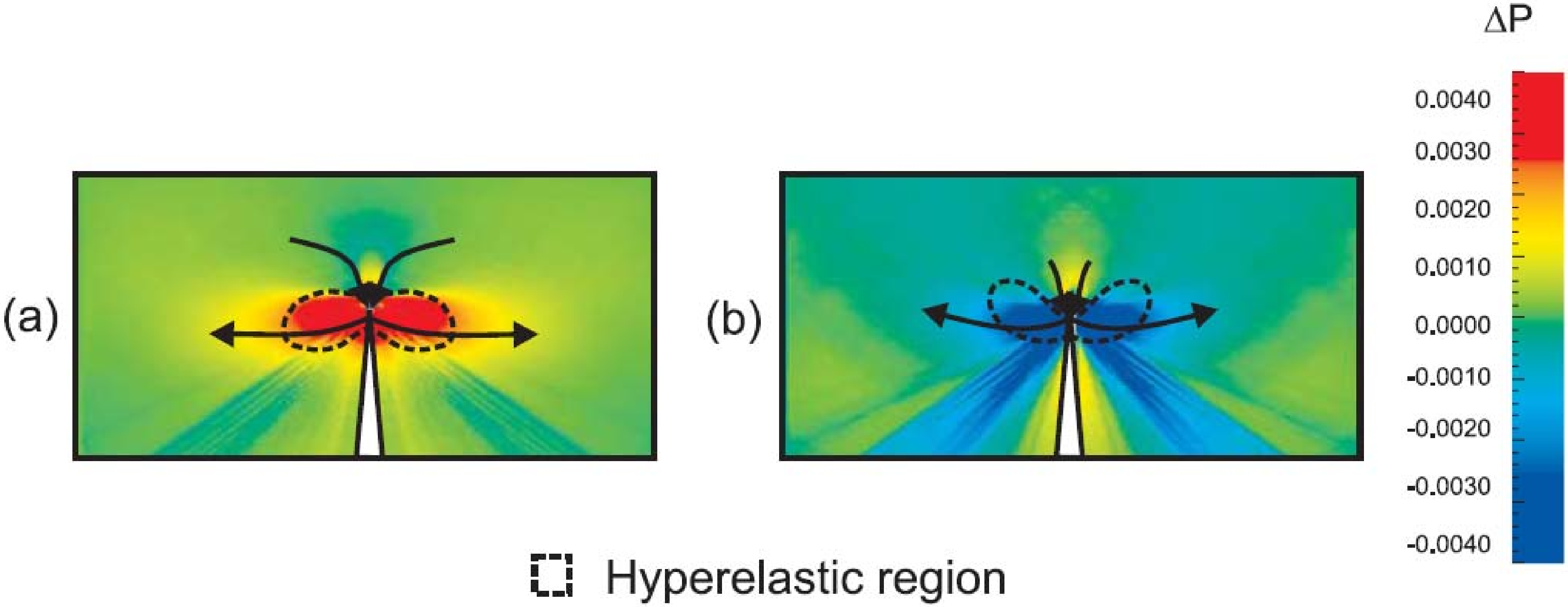
Different ratios of spring constants



Stiffening and softening effect: Increase or reduction of crack 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 χ



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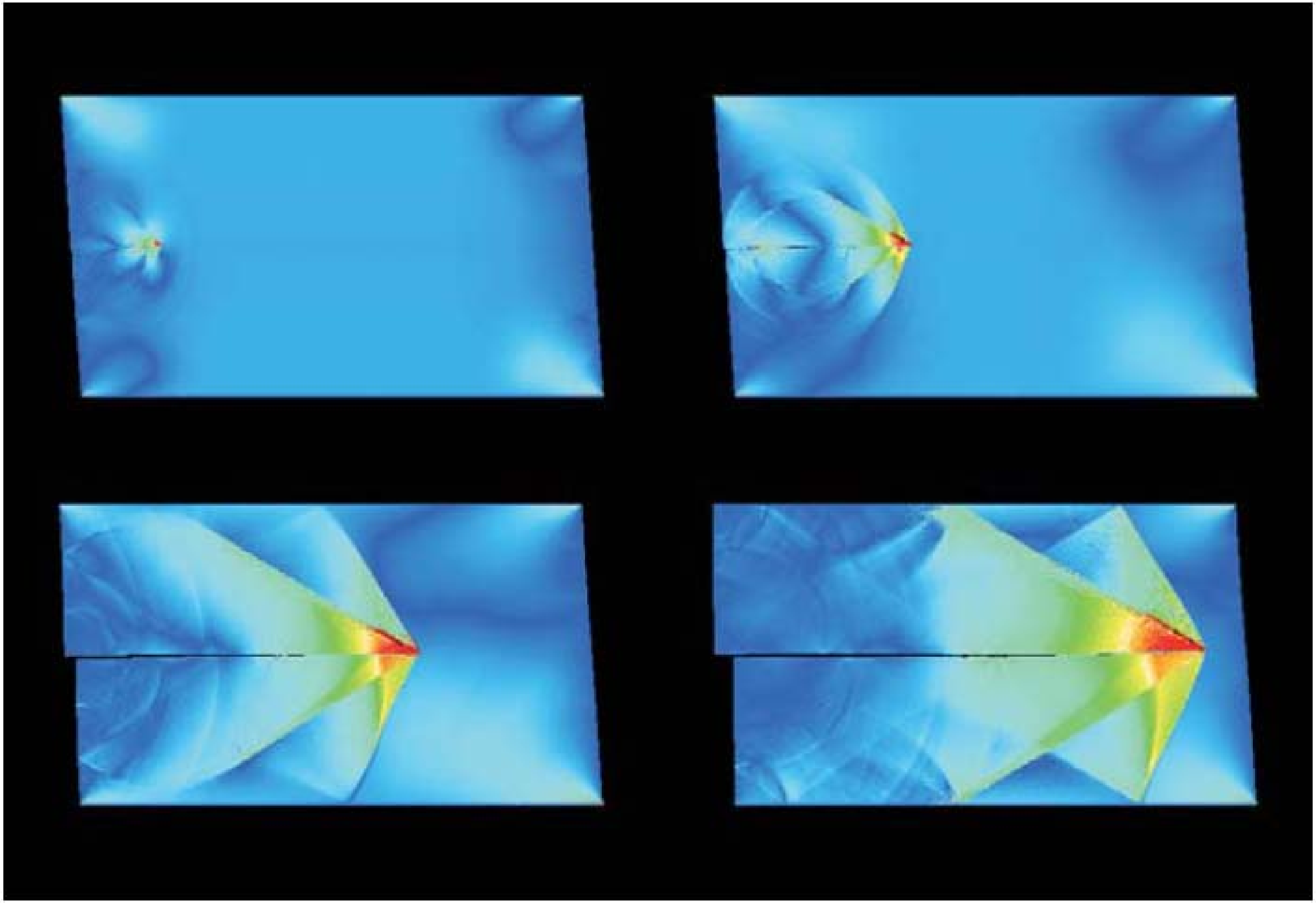
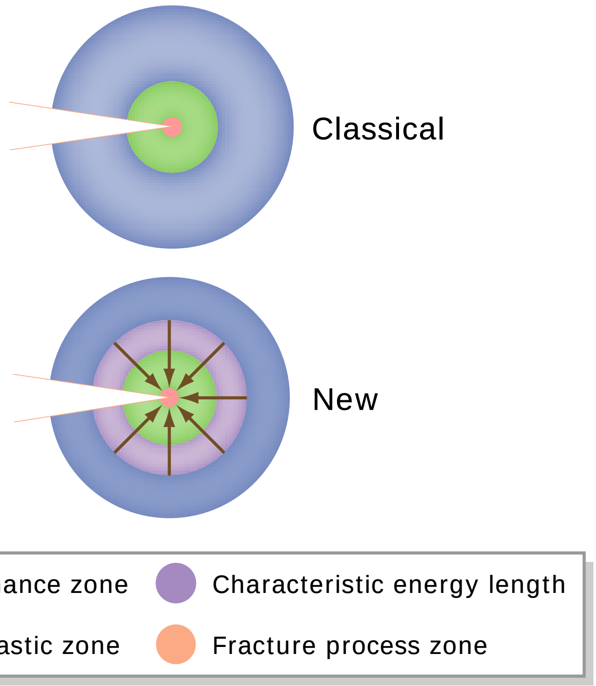
Source: Buehler, M., F. Abraham, and H. Gao. "Hyperelasticity Governs Dynamic Fracture at a Critical Length Scale." *Nature* 426 (2003): 141-6. © 2003.

Supersonic fracture: mode II (shear)



Please see: Buehler, Markus J., Farid F. Abraham, and Huajian Gao. "Hyperelasticity Governs Dynamic Fracture at a Critical Length Scale." *Nature* 426 (November 13, 2003): 141-6.

Theoretical concept: energy flux reduction/enhancement



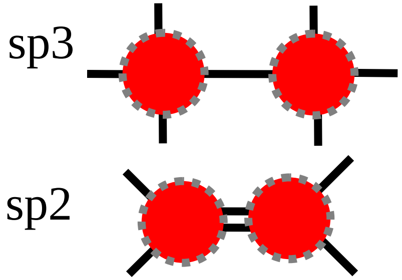
Energy Flux Related to Wave Speed: High local wave speed, high energy flux, crack can move faster (and reverse for low local wave speed).

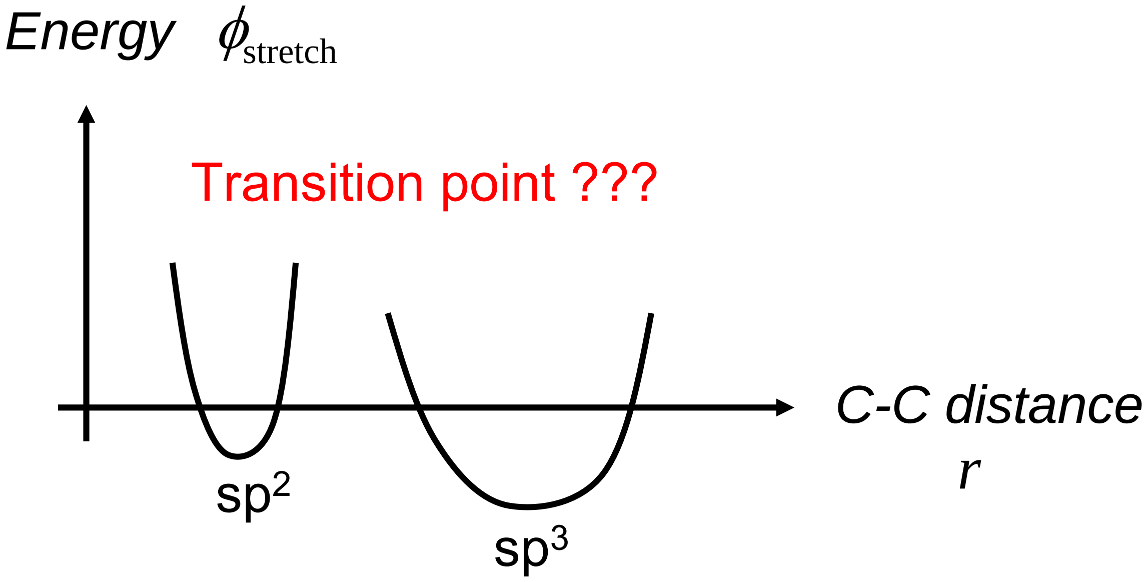
Image by MIT OpenCourseWare.

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

3. Bond order force fields - how to model chemical reactions

Challenge: chemical reactions





CHARMM-type potential can not describe chemical reactions

Why can not model chemical reactions with |spring-like potentials?

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

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

Set of parameters only valid for particular molecule type / type of chemical bond

$$k_{\text{stretch},sp^2} \neq k_{\text{stretch},sp^3}$$

Reactive potentials or reactive force fields *overcome these limitations*

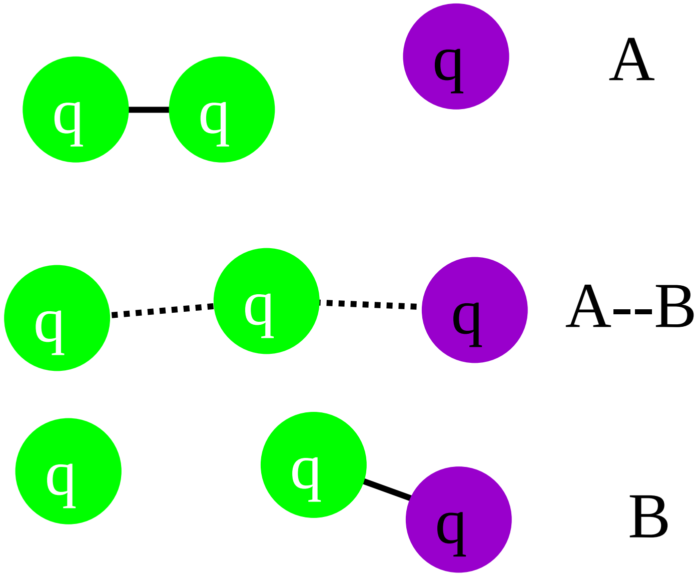
Key features of reactive potentials

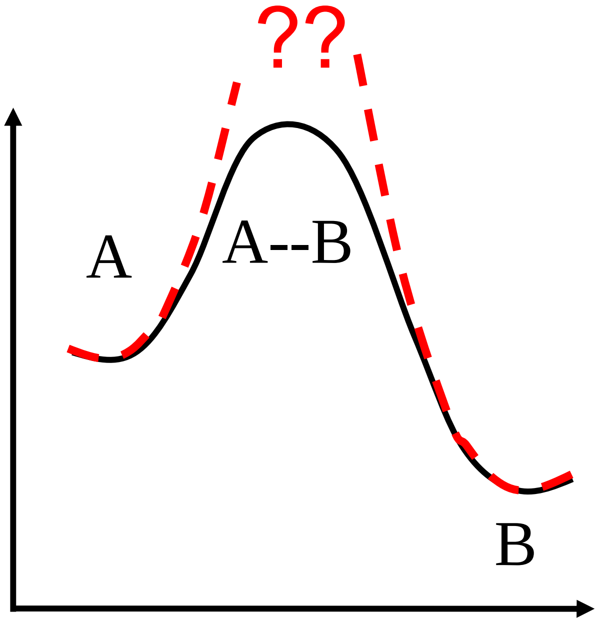
- How can one accurately describe the transition energies during chemical reactions?

- Use computationally more efficient descriptions than relying on purely quantum mechanical (QM) methods (see part II, **methods limited to 100 atoms**)

$$H-C\equiv C-H \xrightarrow{+H_2} H_2-C=C-H_2$$

involves processes with electrons





Key features of reactive potentials

- Molecular model that is capable of describing **chemical reactions**
- **Continuous energy landscape during reactions** (key to enable integration of equations)
- No typing necessary, that is, atoms can be sp, sp2, sp3… w/o further “tags” – **only element types**
- **Computationally efficient** (that is, should involve finite range interactions), so that large systems can be treated (> 10,000 atoms)
- **Parameters with physical meaning** (such as for the LJ potential)

Theoretical basis: bond order potential

Concept: Use pair potential that depends on atomic environment (similar to EAM, here applied to covalent bonds)

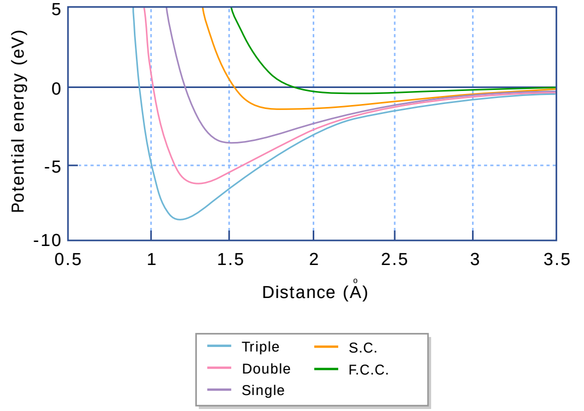
$$\phi(r_{ij}) = \phi_{\mathrm{R}}(r_{ij}) - M_{ij}\phi_A(r_{ij})$$

$$\downarrow$$

$$M_{ij} \sim Z^{-\delta}$$

Modulate strength of attractive part
(e.g. by coordination, or "bond order")

Abell, Tersoff



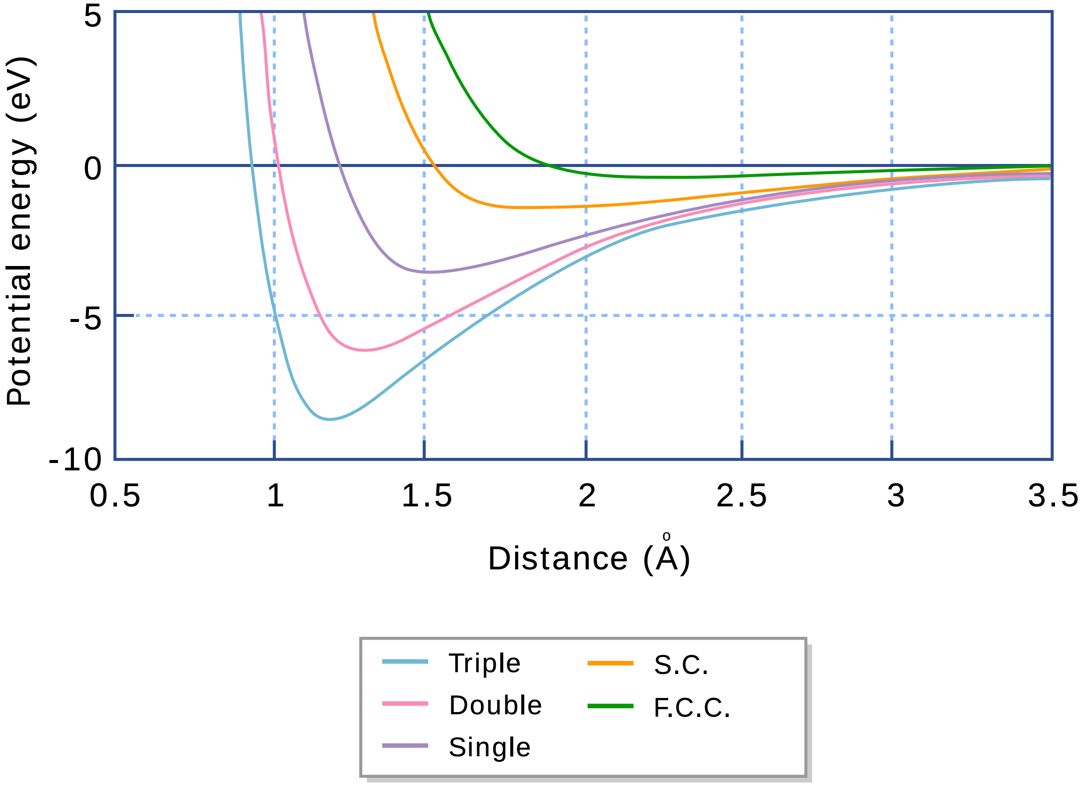
Effective pair-interactions for various C-C (Carbon) bonds

Image by MIT OpenCourseWare.

$$k(r) \sim k_0 M_{ij}(Z,\delta)$$

Changes in spring constant as function of bond order
Continuous change possible
= **continuous energy landscape during chemical reactions**

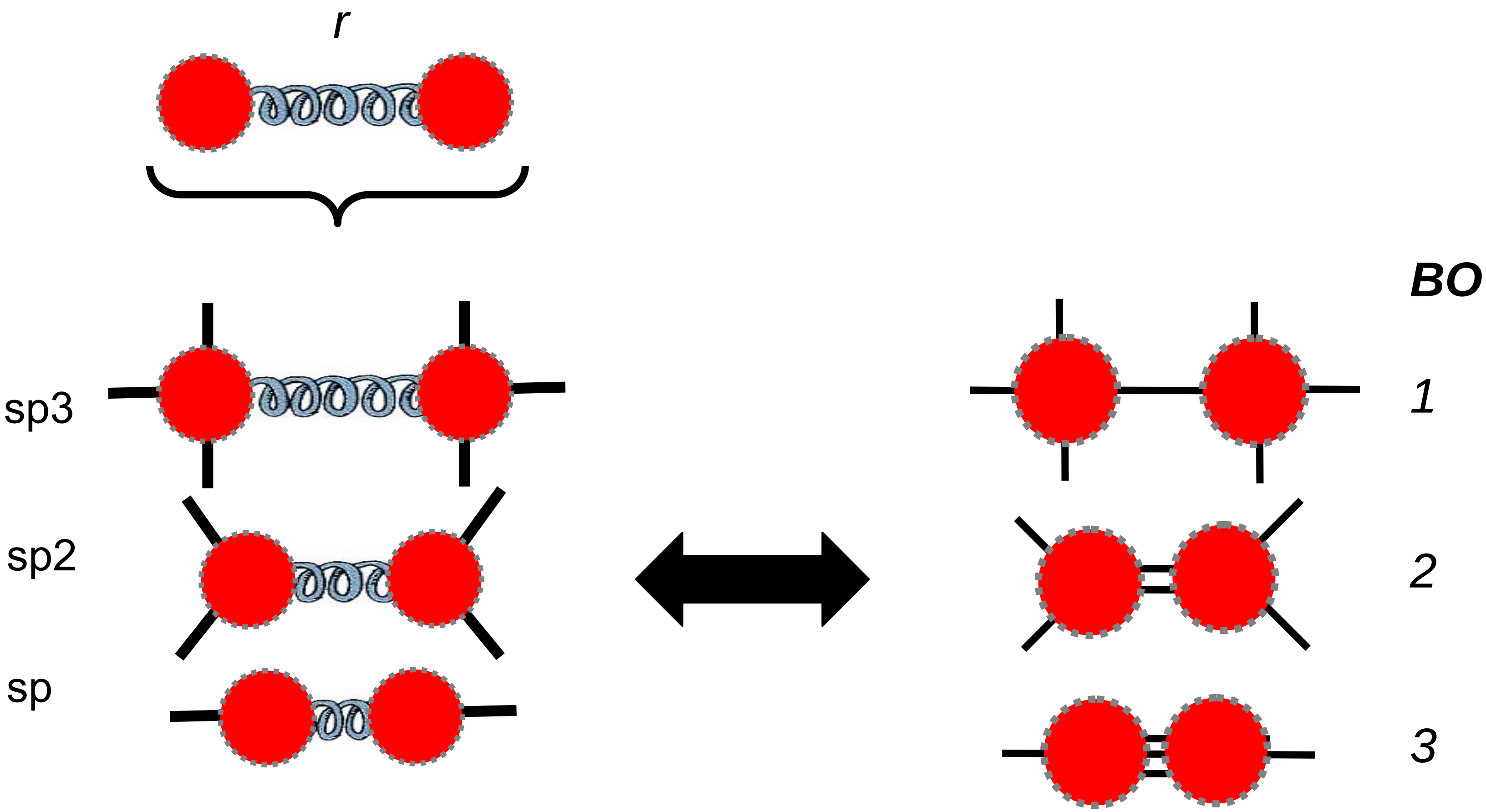
Theoretical basis: bond order potential



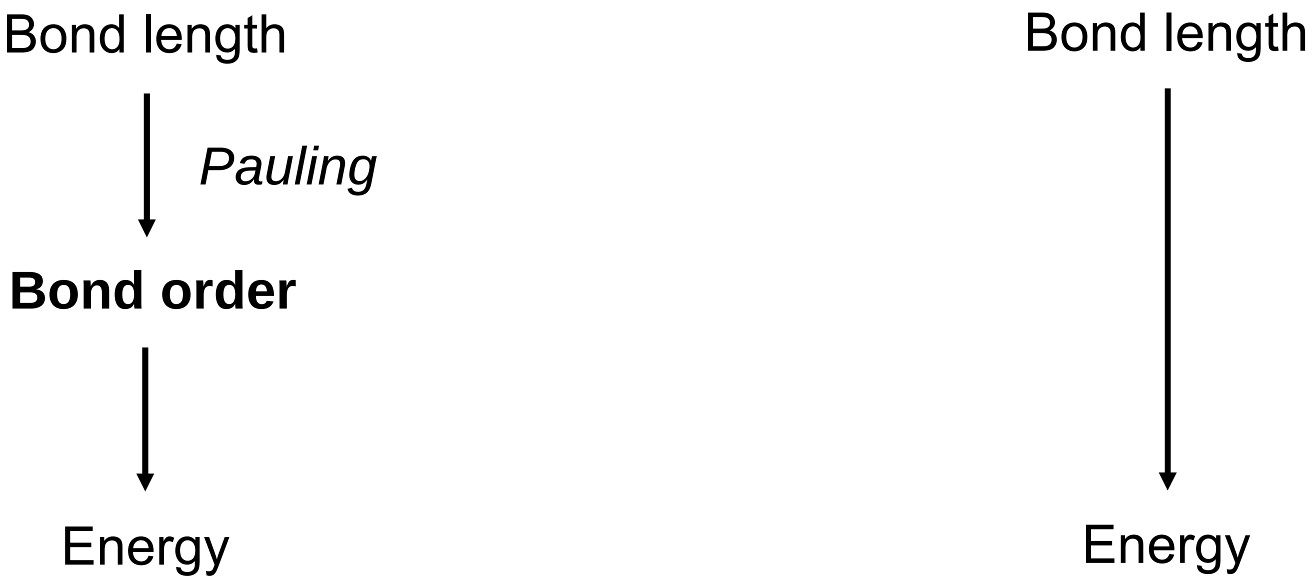
Effective pair-interactions for various C-C (Carbon) bonds

Image by MIT OpenCourseWare.

Concept of bond order (BO)



Bond order based energy landscape



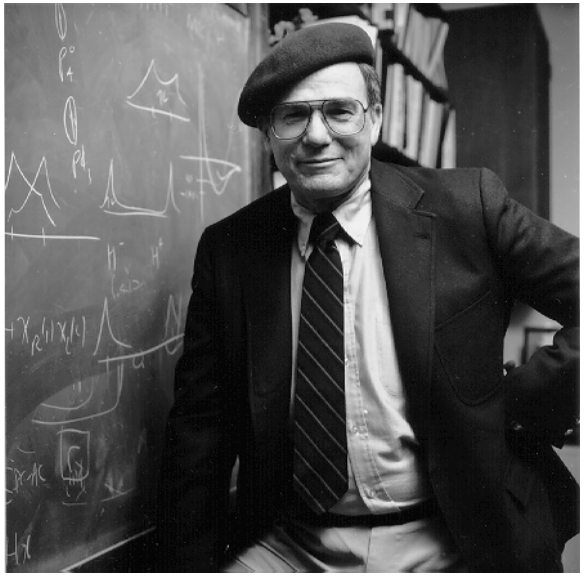
Bond order potential
Allows for a more general
description of chemistry
All energy terms dependent
on bond order

Conventional potential
(e.g. LJ, Morse)

Historical perspective of reactive bond order potentials

- 1985: Abell: General expression for binding energy as a sum of near nieghbor pair interactions moderated by local atomic environment
- 1990s: Tersoff, Brenner: Use Abell formalism applied to silicon (successful for various solid state structures)
- 2000: Stuart et al.: Reactive potential for hydrocarbons
- 2001: Duin, Godddard et al.: Reactive potential for hydrocarbons “ReaxFF”
- 2002: Brenner et al.: Second generation “REBO” potential for hydrocarbons
- 2003-2005: Extension of ReaxFF to various materials including metals, ceramics, silicon, polymers and more in Goddard‘s group

Example: ReaxFF reactive force field



William A. Goddard III
California Institute of Technology

Courtesy of Bill Goddard. Used with permission.

Adri C.T. v. Duin
California Institute of Technology

ReaxFF: A reactive force field

$$E_{system} = \underbrace{E_{bond} + E_{vdWaals} + E_{Coulomb}}_{\text{2-body}} + \underset{\text{3-body}}{E_{val,angle}} + \underset{\text{4-body}}{E_{tors}}$$

$$+ \underbrace{E_{over} + E_{under}}_{\text{multi-body}}$$

Total energy is expressed as the sum of various terms describing individual chemical bonds

All expressions in terms of bond order

All interactions calculated between ALL atoms in system…

No more atom typing: Atom type = chemical element

Example: Calculation of bond energy

$$E_{system} = \boxed{E_{bond}} + E_{vdWaals} + E_{Coulomb} + E_{val,angle} + E_{tors} + E_{over} + E_{under}$$

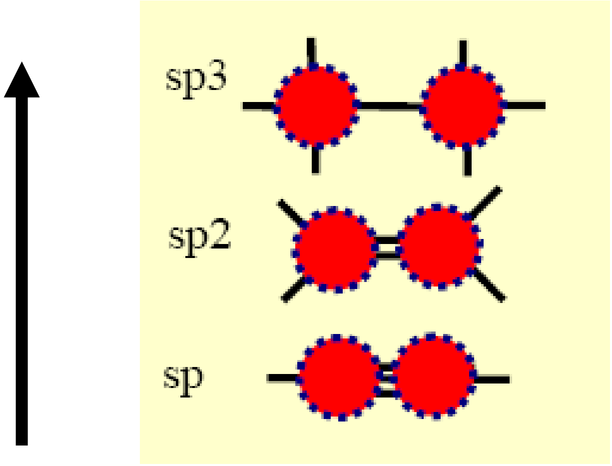
$$E_{\mathrm{bond}} = -D_{\mathrm{e}} \cdot \mathrm{BO}_{ij} \cdot \exp\left[p_{\mathrm{be},1} \left(1 - \mathrm{BO}_{ij}^{p_{\mathrm{be},1}} \right) \right]$$

Bond energy between atoms *i* and *j* does not depend on bond distance

Instead, it depends on bond order

Bond order functions

BO goes smoothly from 3-2-1-0



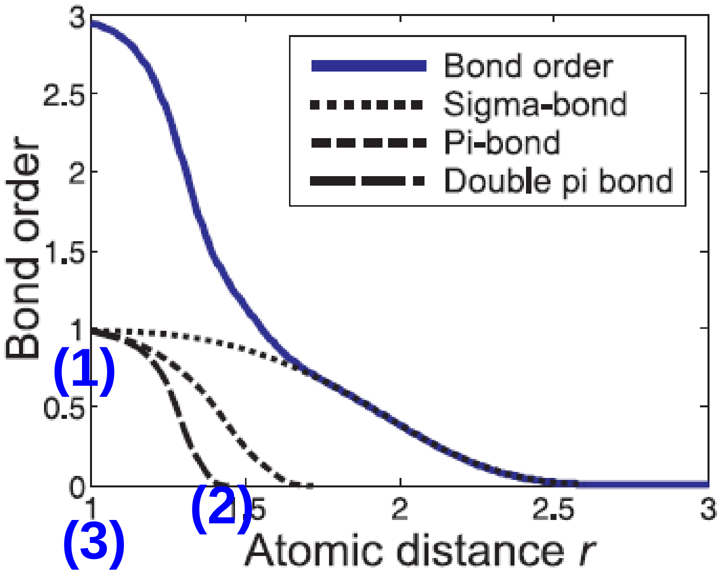


Fig. 2.21c in Buehler, Markus J. *Atomistic Modeling of Materials Failure*. Springer, 2008. © Springer. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.

$$\mathrm{BO}_{ij} = \overset{(1)}{\exp\left[\alpha_\sigma \cdot \left(\frac{r_{ij}}{r_0}\right)^{\beta_\sigma}\right]} + \overset{(2)}{\exp\left[\alpha_\pi \cdot \left(\frac{r_{ij}^{\pi}}{r_0}\right)^{\beta_\pi}\right]} + \overset{(3)}{\exp\left[\alpha_{\pi\pi} \cdot \left(\frac{r_{ij}^{\pi\pi}}{r_0}\right)^{\beta_{\pi\pi}}\right]}$$

Characteristic bond distance

All energy terms are expressed as a function of bond orders

Illustration: Bond energy

$$E_{bond} = -D_e^{\sigma} \cdot BO_{ij}^{\sigma} \cdot f(BO_{ij}^{\sigma}) - D_e^{\pi} \cdot BO_{ij}^{\pi} - D_e^{\pi\pi} \cdot BO_{ij}^{\pi\pi}$$

Image removed due to copyright restrictions.
Please see slide 10 in van Duin, Adri. "Dishing Out the Dirt on ReaxFF."
http://www.wag.caltech.edu/home/duin/FFgroup/Dirt.ppt.

vdW interactions

$$E_{system} = E_{bond} + E_{vdWaals} + E_{Coulomb} + E_{val,angle} + E_{tors} + E_{over} + E_{under}$$

- Accounts for short distance repulsion (Pauli principle orthogonalization) and attraction energies at large distances (dispersion)
- Included for all atoms with shielding at small distances

$$E_{\mathrm{vdWaals}} = D_{ij} \cdot \left\{ \exp\left[\alpha_{ij} \cdot \left(1 - \frac{f_{13}(r_{ij})}{r_{\mathrm{vdW}}} \right) \right] - 2 \cdot \exp\left[\frac{1}{2} \cdot \alpha_{ij} \cdot \left(1 - \frac{f_{13}(r_{ij})}{r_{\mathrm{vdW}}} \right) \right] \right\}$$

$$f_{13}(r_{ij}) = \left[r_{ij}^{\lambda_{29}} + \left(\frac{1}{\lambda_w} \right)^{\lambda_{28}} \right]^{1/\lambda_{28}}$$

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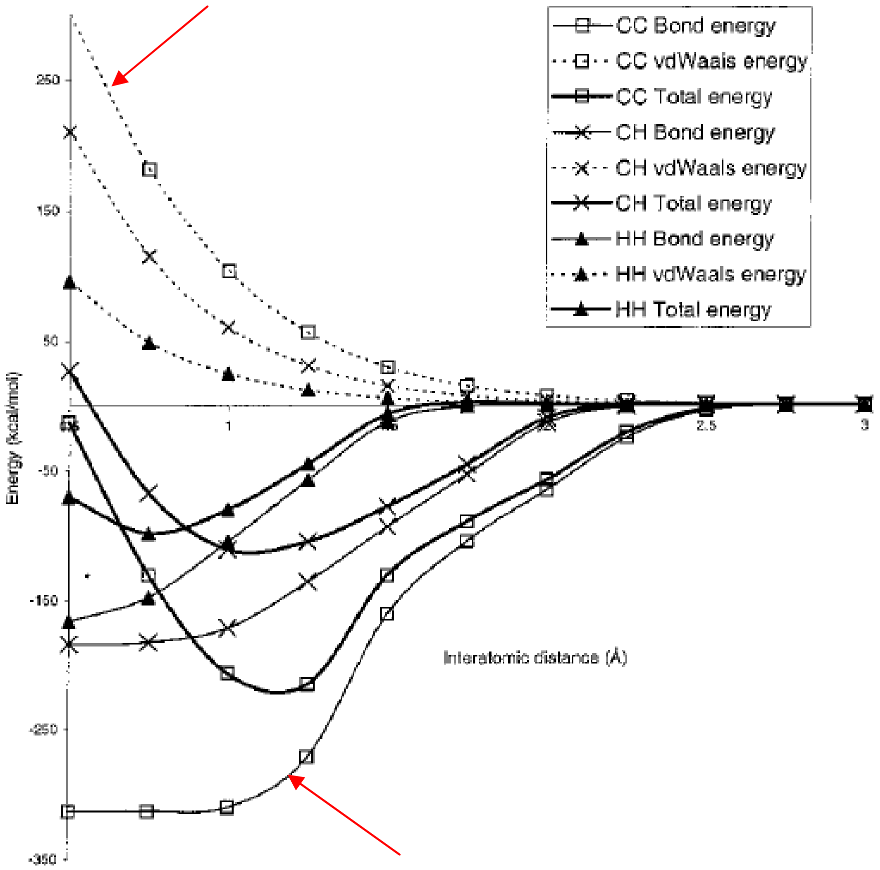
Please see slide 11 in van Duin, Adri. "Dishing Out the Dirt on ReaxFF." http://www.wag.caltech.edu/home/duin/FFgroup/Dirt.ppt.

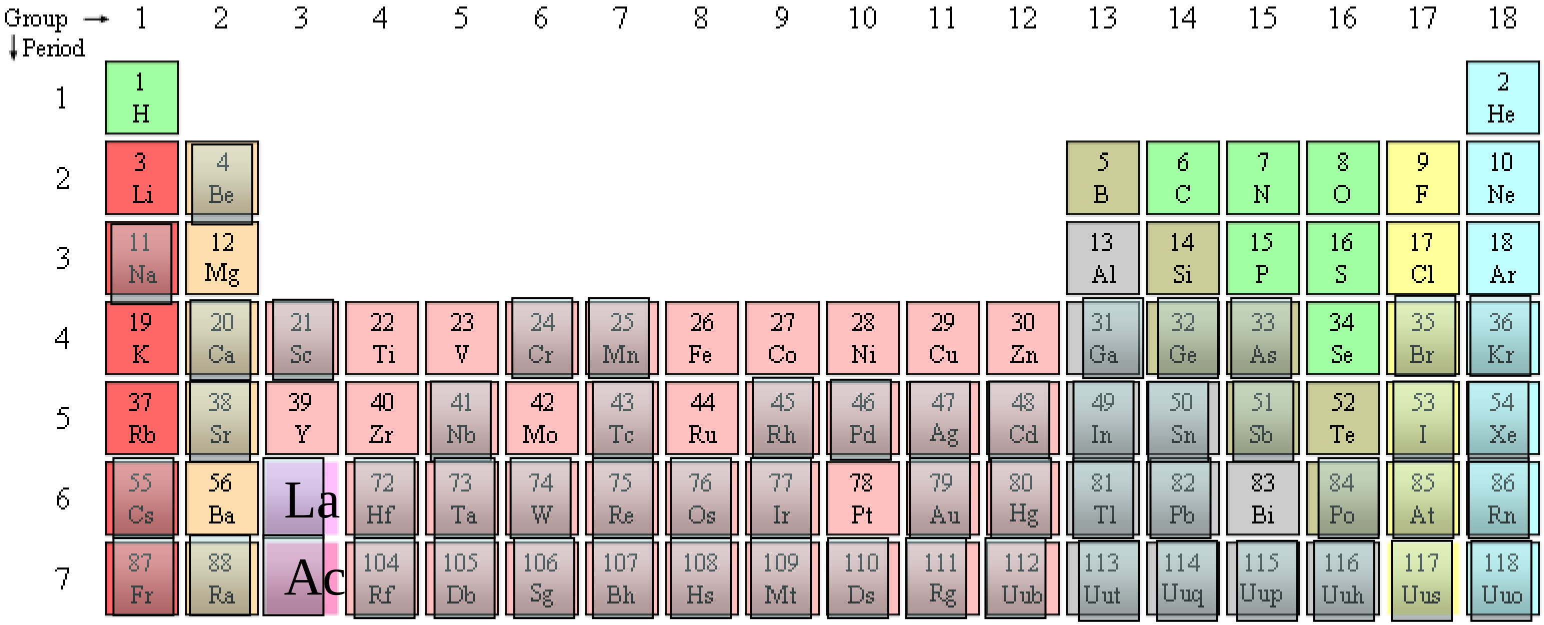
Resulting energy landscape



Contribution of E_{bond} and vdW energy

Source: van Duin, C. T. Adri, et al. "ReaxFF: A Reactive Force Field for Hydrocarbons." *Journal of Physical Chemistry A* 105 (2001).

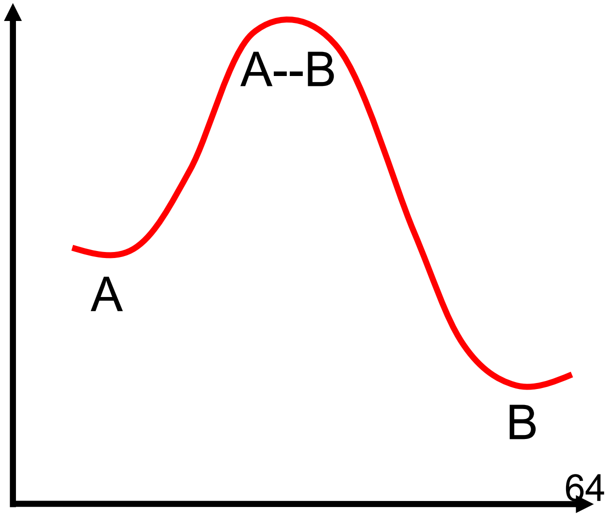
Current development status of ReaxFF



Group → ↓Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

▨ : not currently described by ReaxFF

Allows to interface metals, ceramics with organic chemistry: Key for complex materials, specifically biological materials



Periodic table courtesy of Wikimedia Commons.

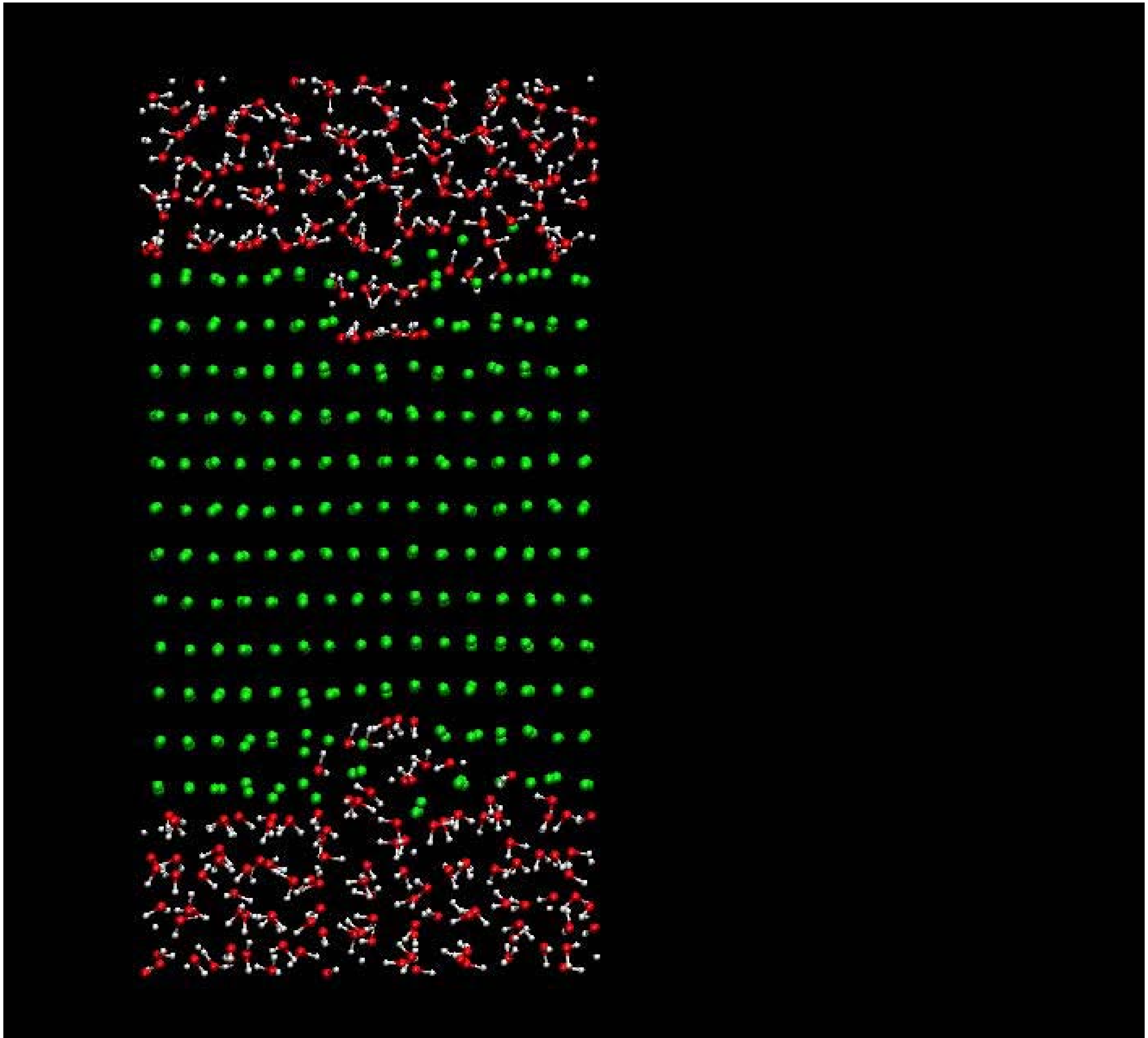
Mg-water interaction: How to make fire with water

Video stills removed due to copyright restrictions; watch the video now: http://www.youtube.com/watch?v=QTKivMVUcqE.

Mg

http://video.google.com/videoplay?docid=4697996292949045921&q=magnesium+water&total=46&start=0&num=50&so=0&type=search&plindex=0

Mg – water interaction – ReaxFF MD simulation



3.021J / 1.021J / 10.333J / 18.361J / 22.00J Introduction to Modeling and Simulation
Spring 2012