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

Part I – Continuum and particle methods

Reactive potentials and applications (cont'd)

Lecture 9

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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** (EAM, a bit of ReaxFF—chemical reactions)
- **Lecture 7: Application – MD simulation of materials failure**
- **Lecture 8: Application – Reactive potentials and applications**
- **Lecture 9: Application – Reactive potentials and applications (cont'd)**

Lecture 9: Reactive potentials and applications (cont'd)

Outline:

1. Notes on fracture application
2. Closure: ReaxFF force field
3. Hybrid multi-paradigm fracture models

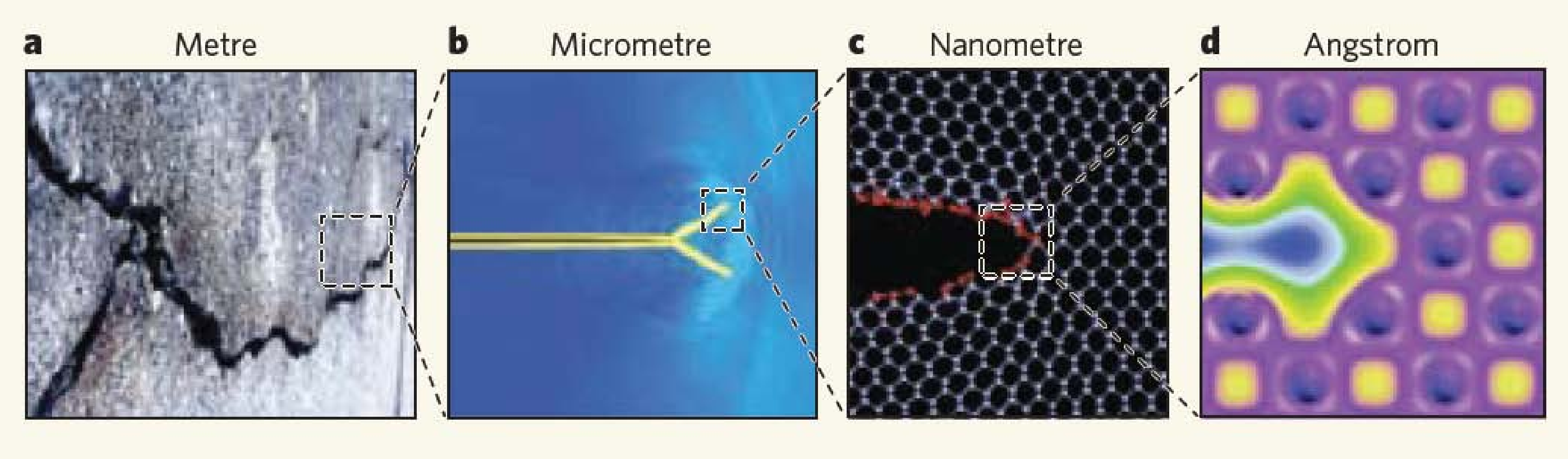
Goal of today's lecture:

- Remarks: Modeling of fracture and relation to diffusion problem
- New potential: ReaxFF, to describe complex chemistry (bond breaking and formation)
- Application in hybrid simulation approaches (combine different force fields)

1. Notes on fracture application

Consider for pset #2

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



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Source: Buehler, M., and Z. Xu. "Materials Science: Mind the Helical Crack." *Nature* 464, no. 7285 (2010): 42-3. © 2010.

Limiting speeds of cracks: linear elastic continuum theory

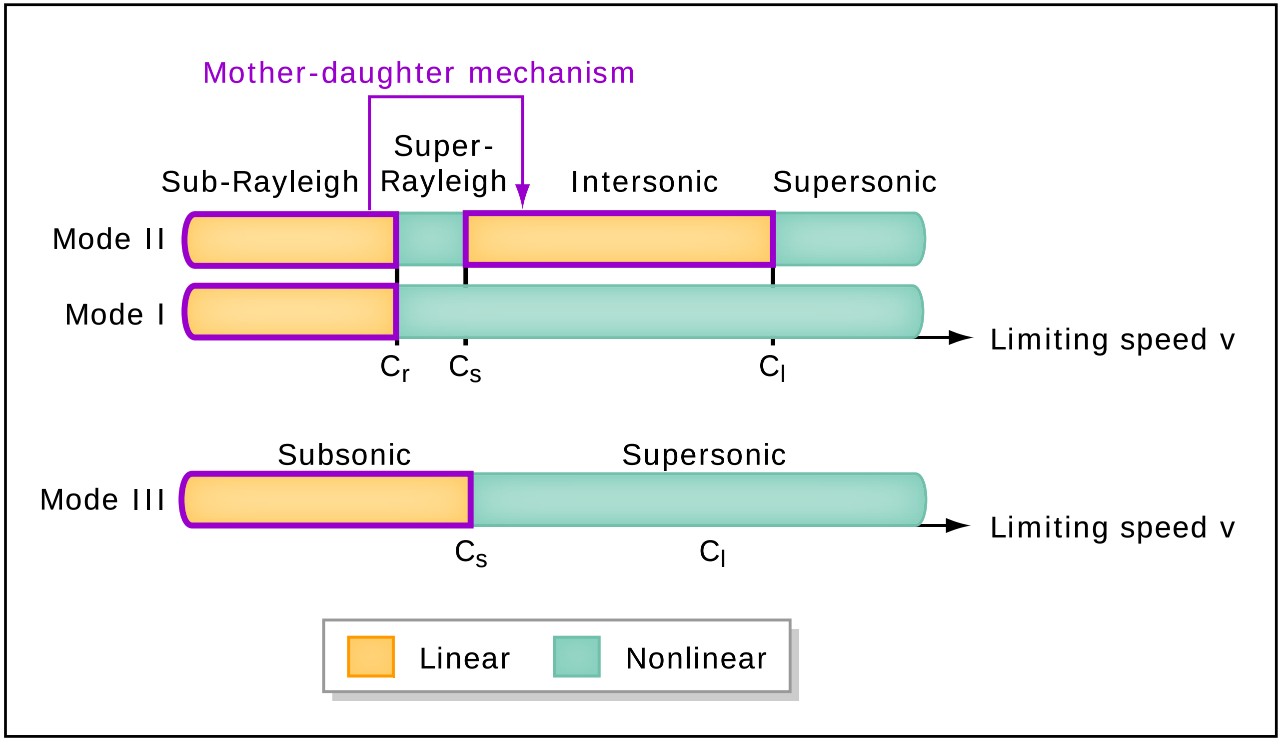


Image by MIT OpenCourseWare.

$$c_l = \sqrt{\frac{9}{8}\frac{E}{\rho}} \sim \sqrt{E}$$

$$c_s = \sqrt{\frac{3}{8}\frac{E}{\rho}} \sim \sqrt{E}$$

$$c_r = 0.92 c_s$$

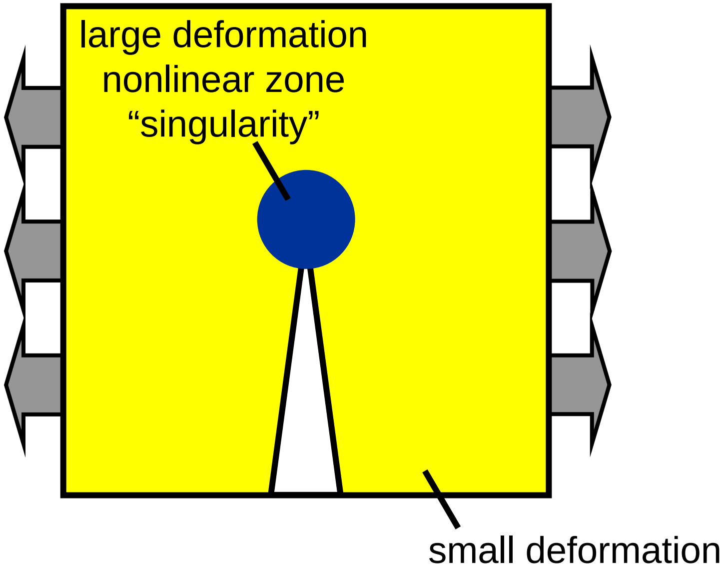
- Cracks **can not exceed** the limiting speed given by the corresponding wave speeds **unless material behavior is nonlinear**
- Cracks that exceed limiting speed would produce energy (physically impossible - ***linear elastic continuum theory***)

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

Deformation field near a crack $\sigma(r) \sim \frac{1}{\sqrt{r}}$

$E_{\text{large (stiff)}}$



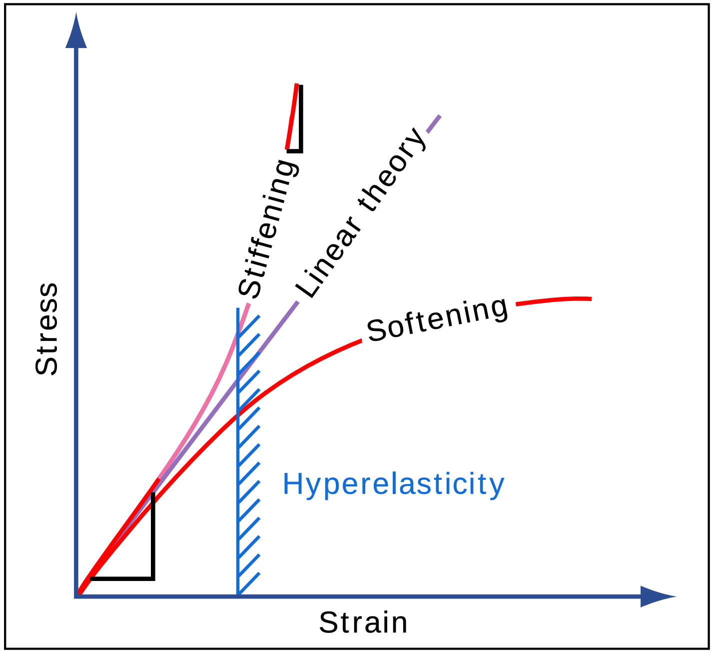


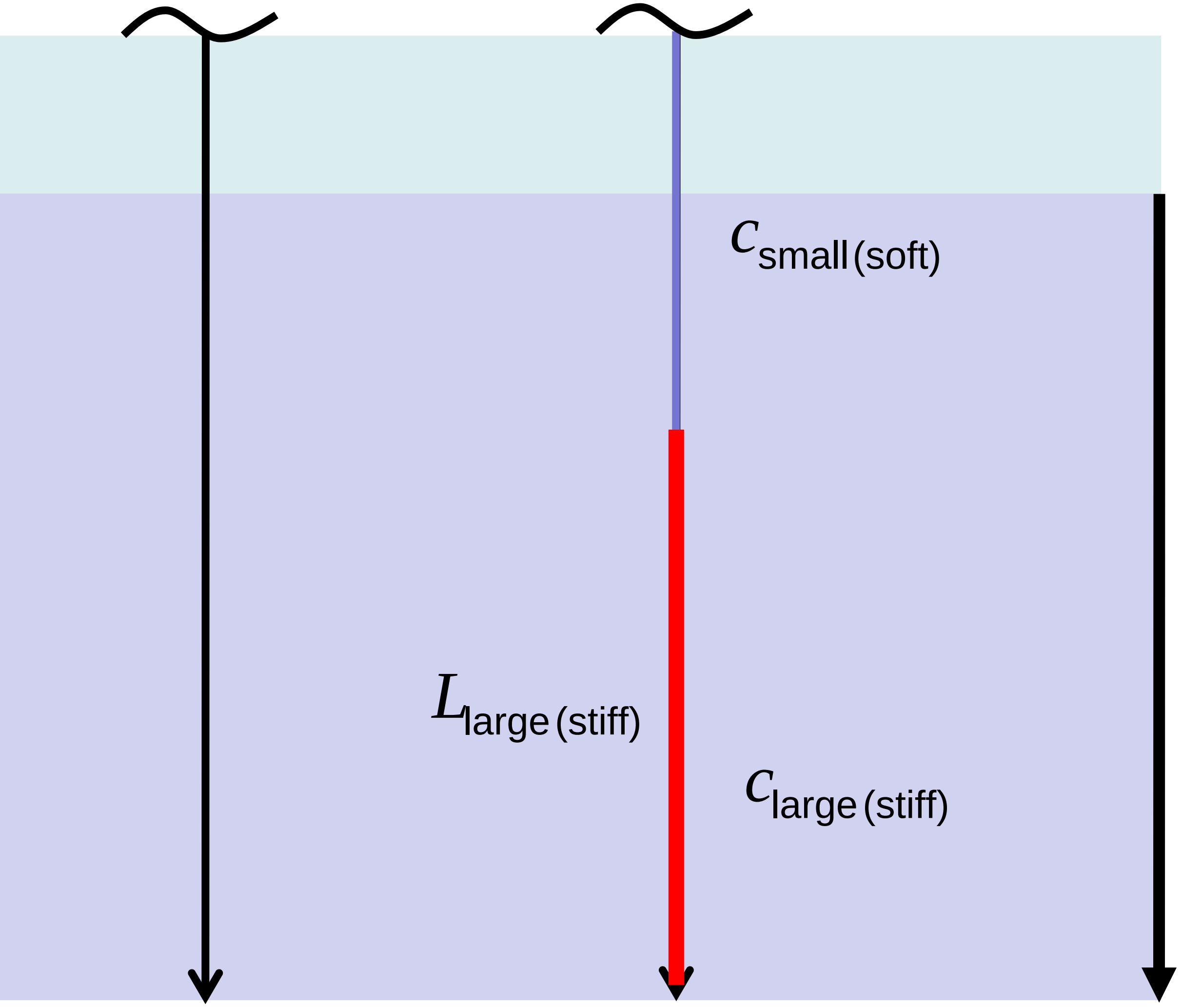
Image by MIT OpenCourseWare.

$$c_l = \sqrt{\frac{9}{8}\frac{E}{\rho}} \sim \sqrt{E}$$

$E_{\text{small (soft)}}$

Energy flux concept

Far away from crack tip



$c_{\text{small (soft)}}$

$L_{\text{large (stiff)}}$

$c_{\text{large (stiff)}}$

Crack tip

L_{energy}

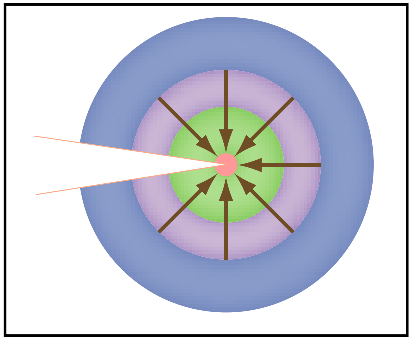
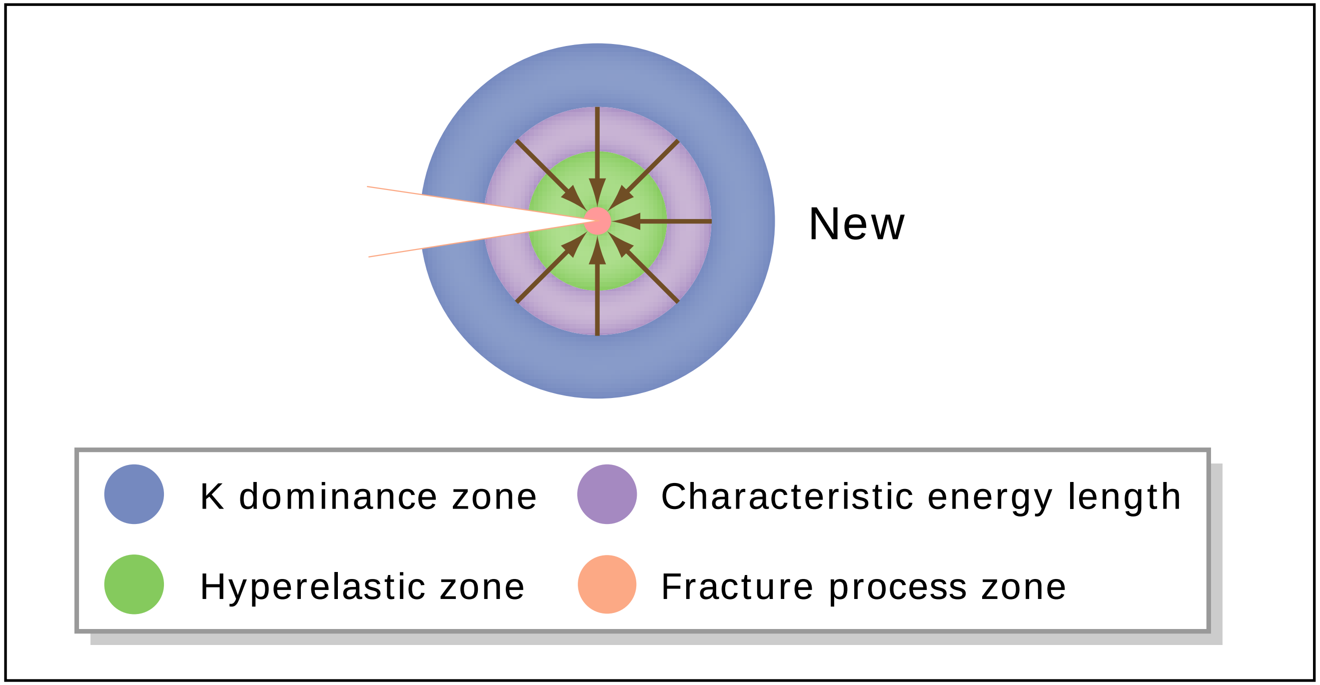


Image by MIT OpenCourseWare.

Characteristic energy length (energy from this distance needs to flow to the crack tip)

$$\frac{L_{\text{large (stiff)}}}{L_{\text{energy}}} \approx 1$$ → Supersonic cracking

Energy flux reduction/enhancement



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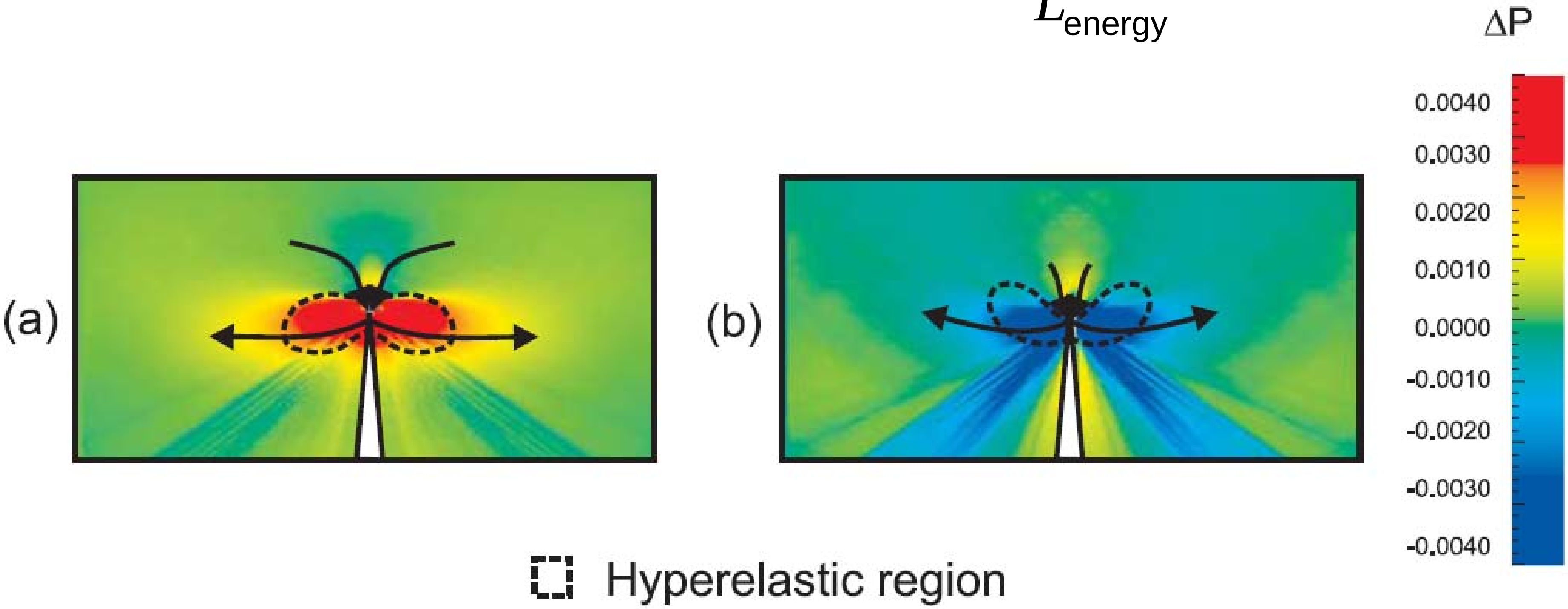
$$L_{\text{energy}}$$

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

L_{energy}



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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.

Buehler *et al*., *Nature*, 2003

Diffusion problem

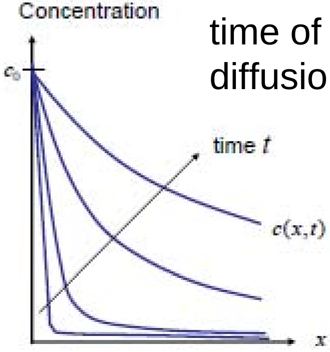
Fracture problem

Continuum approach (distinct PDE)

$$\frac{\partial c}{\partial t} = D\frac{d^2c}{dx^2}$$

PDE
(Fick's law)

Integration
(BCs, ICs)



Characteristic time of diffusion

$$\begin{aligned}
\frac{\partial\sigma_{11}}{\partial x_1}+\frac{\partial\sigma_{12}}{\partial x_2}+\frac{\partial\sigma_{13}}{\partial x_3}+\rho(g_1-a_1) &= 0\\
\frac{\partial\sigma_{21}}{\partial x_1}+\frac{\partial\sigma_{22}}{\partial x_2}+\frac{\partial\sigma_{23}}{\partial x_3}+\rho(g_2-a_2) &= 0\\
\frac{\partial\sigma_{31}}{\partial x_1}+\frac{\partial\sigma_{32}}{\partial x_2}+\frac{\partial\sigma_{33}}{\partial x_3}+\rho(g_3-a_3) &= 0
\end{aligned}$$

PDE (continuum equilibrium)

Integration
(BCs, ICs)

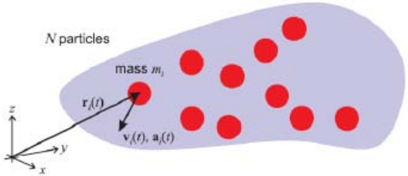
$$c_l = \sqrt{\frac{3\mu}{\rho}} \qquad c_s = \sqrt{\frac{\mu}{\rho}} \qquad \boxed{c_R \approx \beta c_s} \qquad \beta \approx 0.923$$

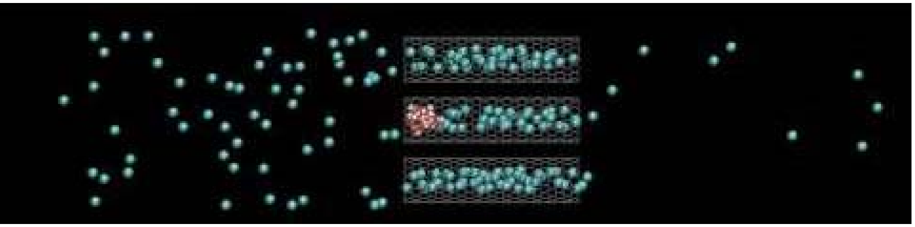
Crack limiting speed

Atomistic approach (same PDE)

$$f = m\frac{d^2x}{dt^2} = ma$$

Integration
(BCs, ICs)

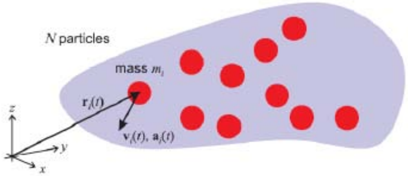


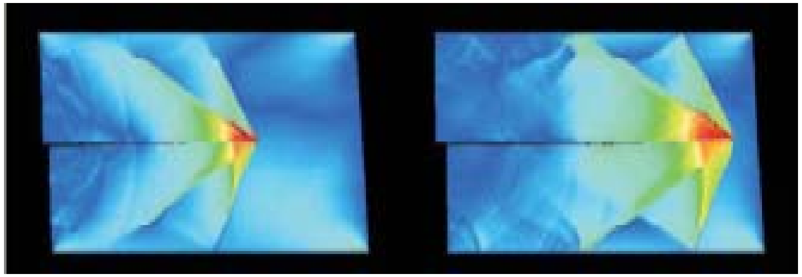


Characteristic time of diffusion

$$f = m\frac{d^2x}{dt^2} = ma$$

Integration
(BCs, ICs)





Crack limiting speed

2. Closure: ReaxFF force field

Potential energy expressions for more complex materials/chemistry, including bond formation and breaking

Review: atomic interactions – different types of chemical bonds

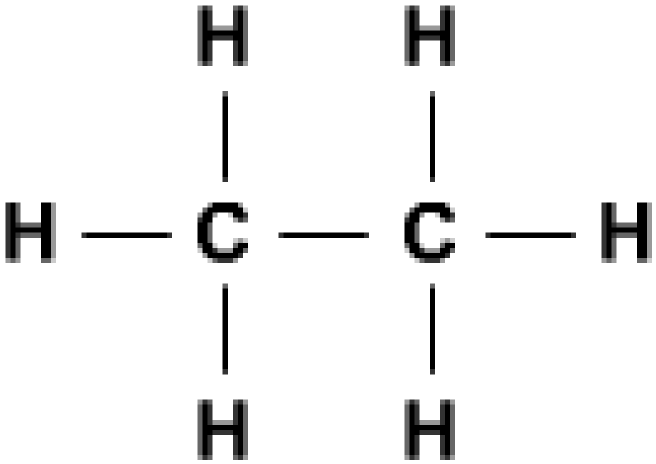
- **Primary bonds ("strong")**
  - Ionic (ceramics, quartz, feldspar - **rocks**)
  - Covalent (**silicon**)
  - Metallic (copper, nickel, **gold**, silver)
    (high melting point, 1000-5,000K)

- **Secondary bonds ("weak")**
  - Van der Waals (**wax**, low melting point)
  - Hydrogen bonds (proteins, **spider silk**)
    (melting point 100-500K)

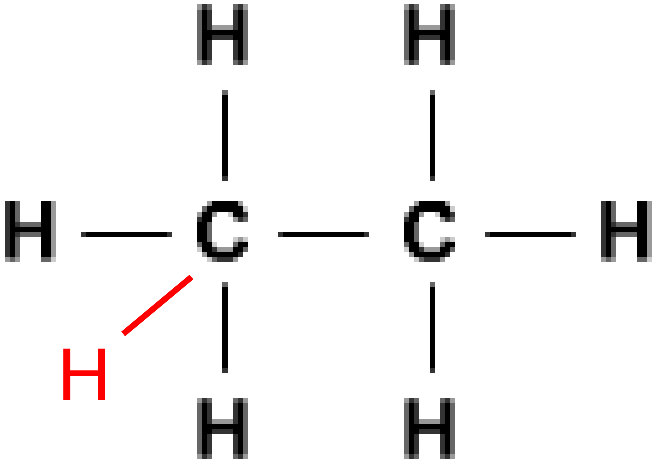
- Ionic: Non-directional (point charges interacting)
- Covalent: Directional (bond angles, torsions matter)
- Metallic: Non-directional (electron gas concept)

Difference of material properties originates from different atomic interactions

But…are all bonds the same? - valency in hydrocarbons



Ethane C_2H_6
(stable configuration)

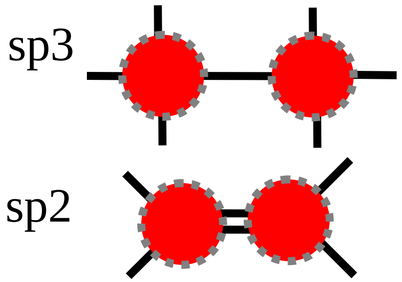


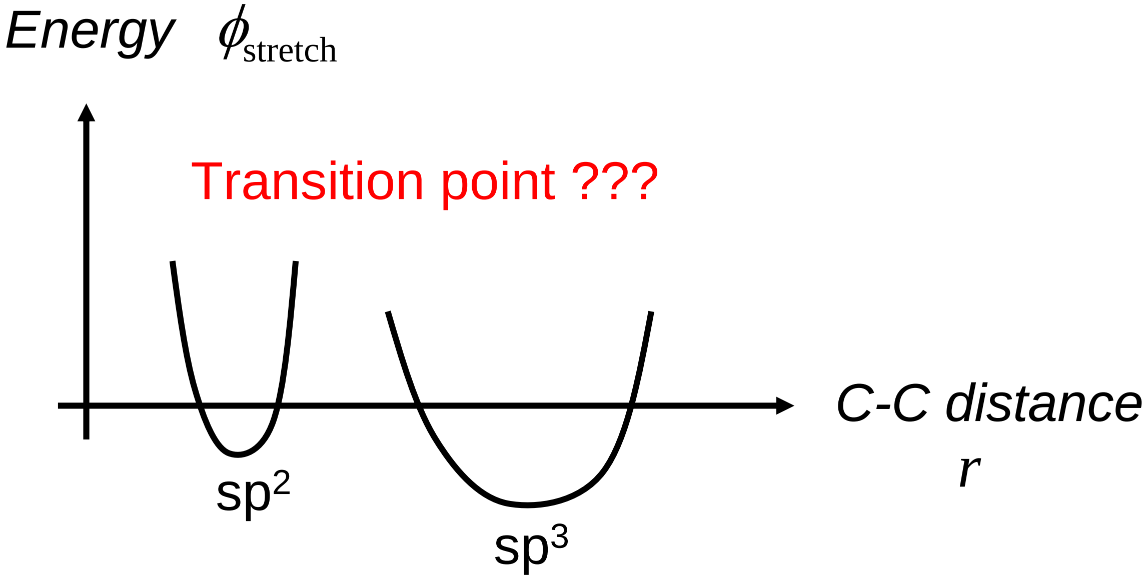
All bonds are not the same!

Adding another H is not favored

Bonds depend on the environment!

Another challenge: chemical reactions





Simple pair potentials can not describe chemical reactions

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

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

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*

Theoretical basis: bond order potential

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

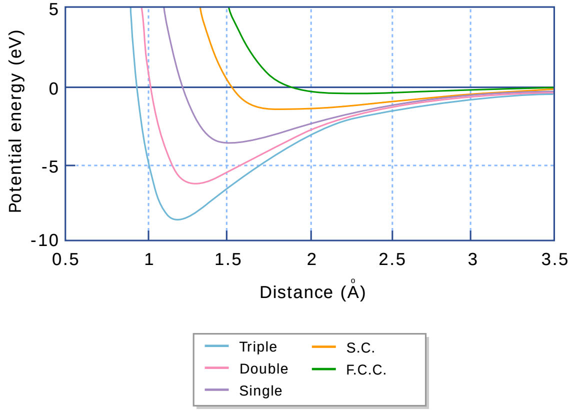
$$\phi(r_{ij}) = \phi_{\mathrm{R}}(r_{ij}) - M_{ij}\phi_A(r_{ij})$$

↓

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

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

Abell, Tersoff



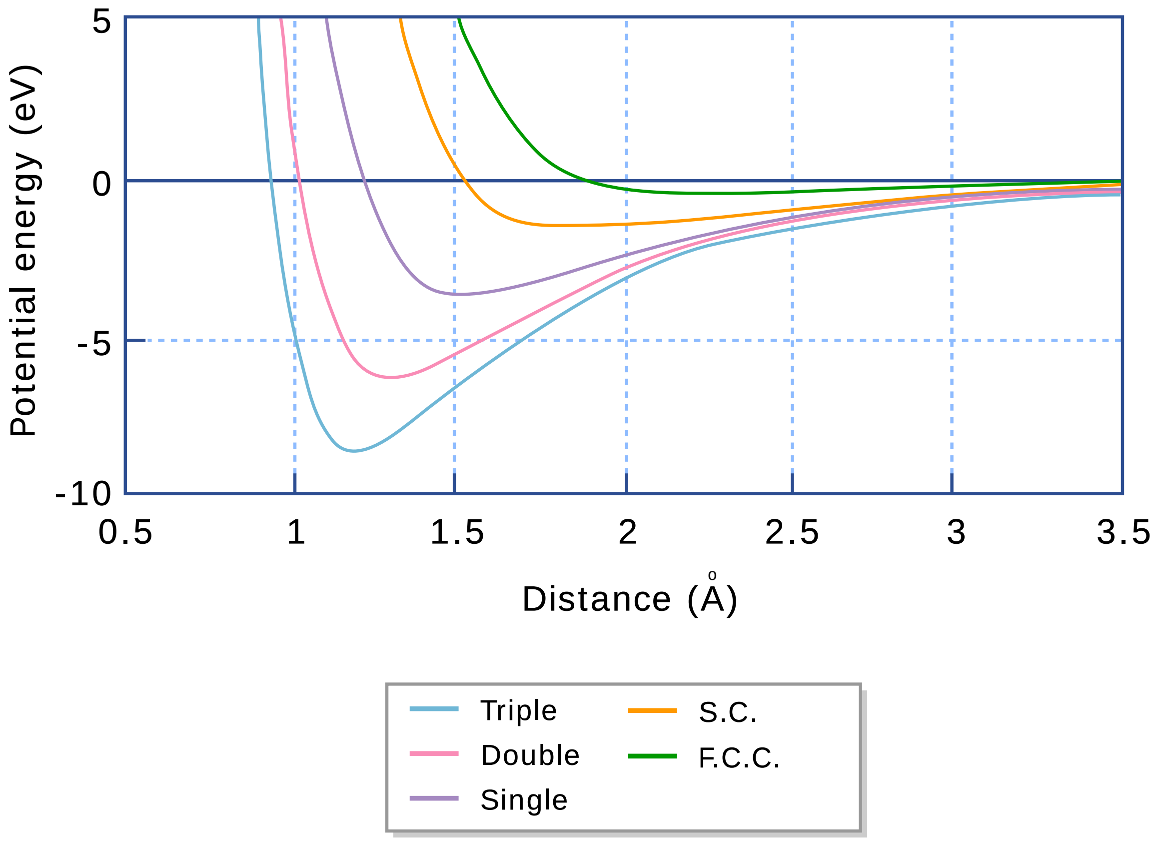
Effective pair-interactions for various C-C (Carbon) bonds

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

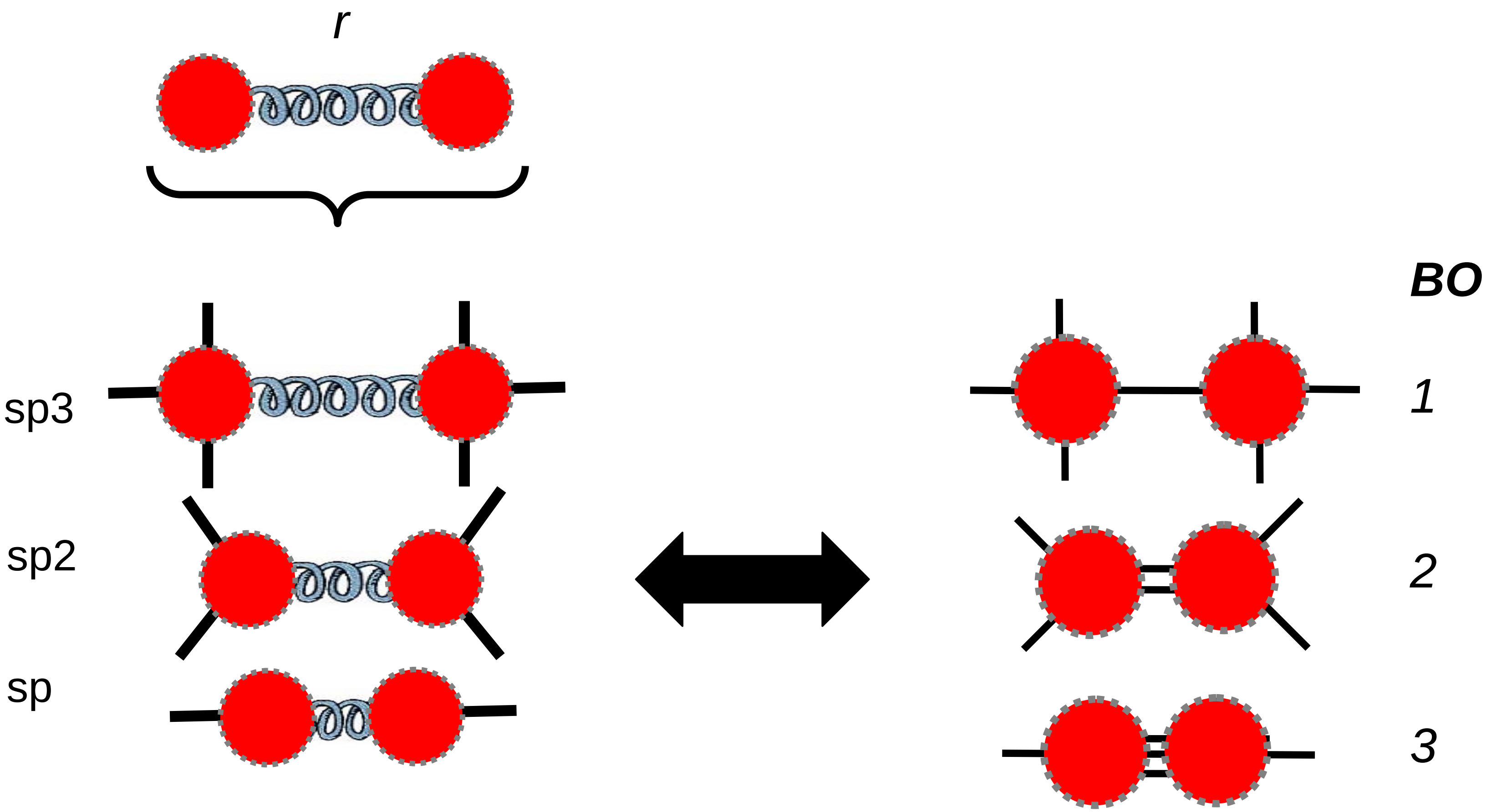


Effective pair-interactions for various C-C (Carbon) bonds

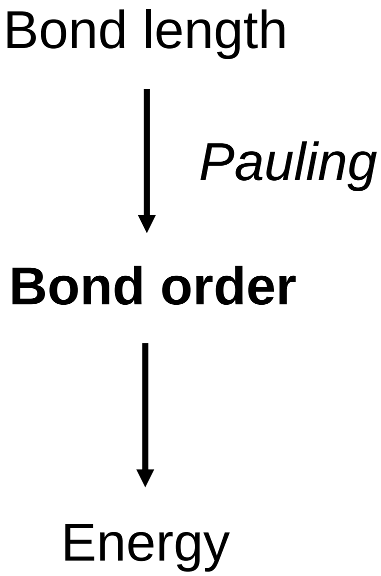
Image by MIT OpenCourseWare.

D. Brenner, 2000

Concept of bond order (BO)



Bond order based energy landscape



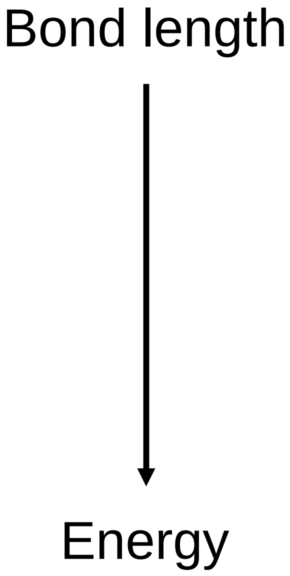
Bond length

Pauling

Bond order

Energy

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



Bond length

Energy

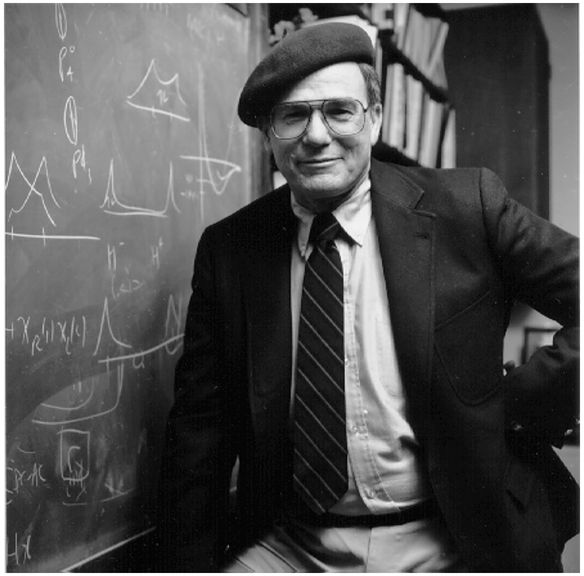
Conventional potential (e.g. LJ, Morse)

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

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

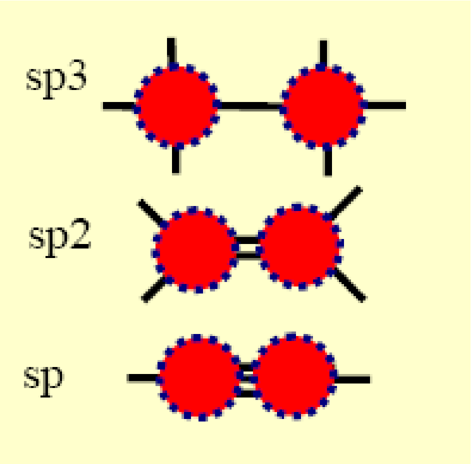
$$E_{\text{bond}} = -D_{\text{e}} \cdot \text{BO}_{ij} \cdot \exp\left[p_{\text{be},1} \left(1 - \text{BO}_{ij}^{p_{\text{be},1}} \right) \right]$$

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



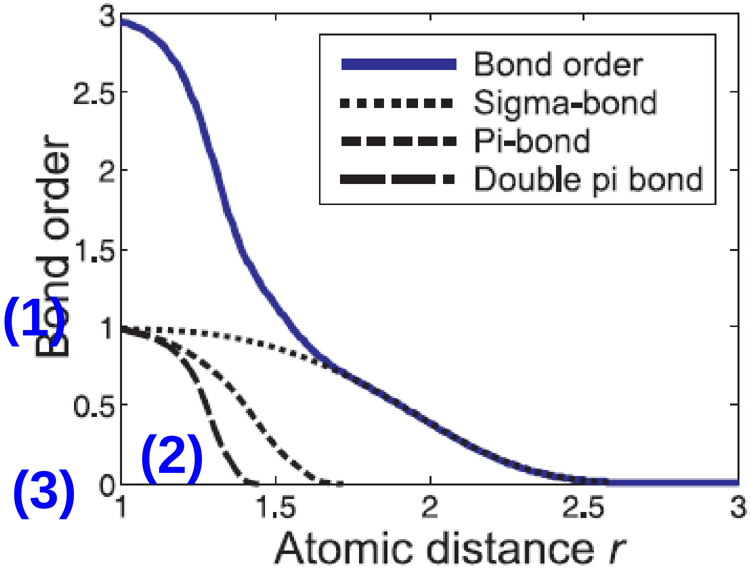


Fig. 2.21c in Buehler, Markus J. *Atomistic Modeling of Materials Failure*. Springer, 2008. © Springer. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.

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

Characteristic bond distance

All energy terms are expressed as a function of bond orders

Illustration: Bond energy

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

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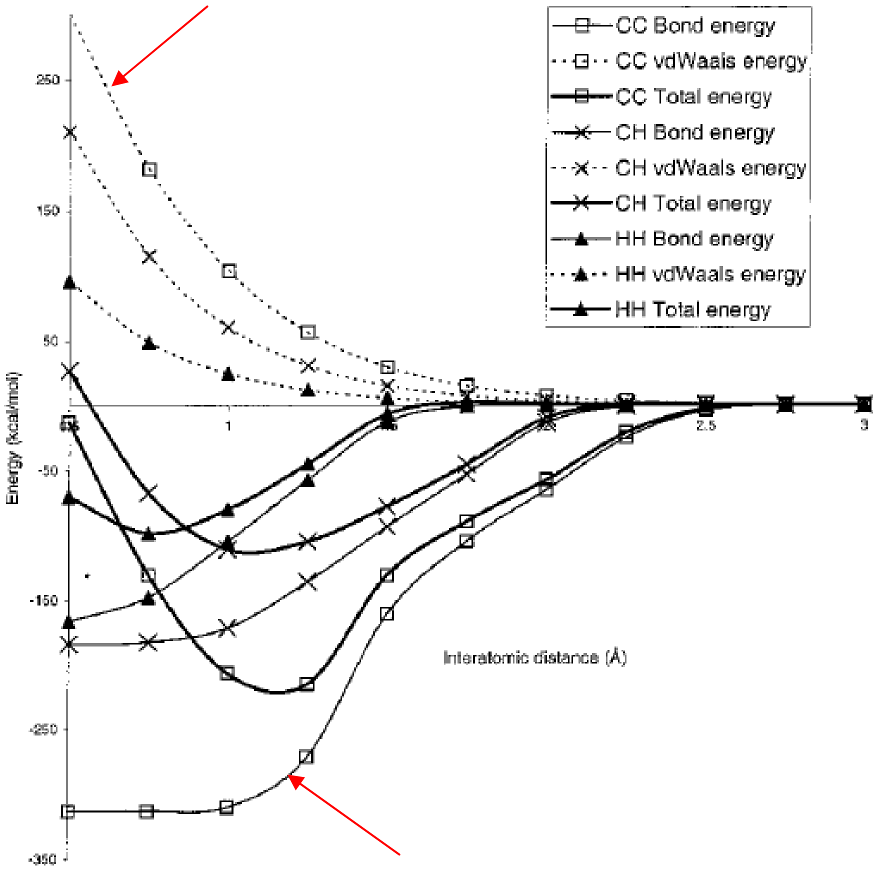
Please see slide 11 in van Duin, Adri. "Dishing Out the Dirt on ReaxFF."
http://www.wag.caltech.edu/home/duin/FFgroup/Dirt.ppt.

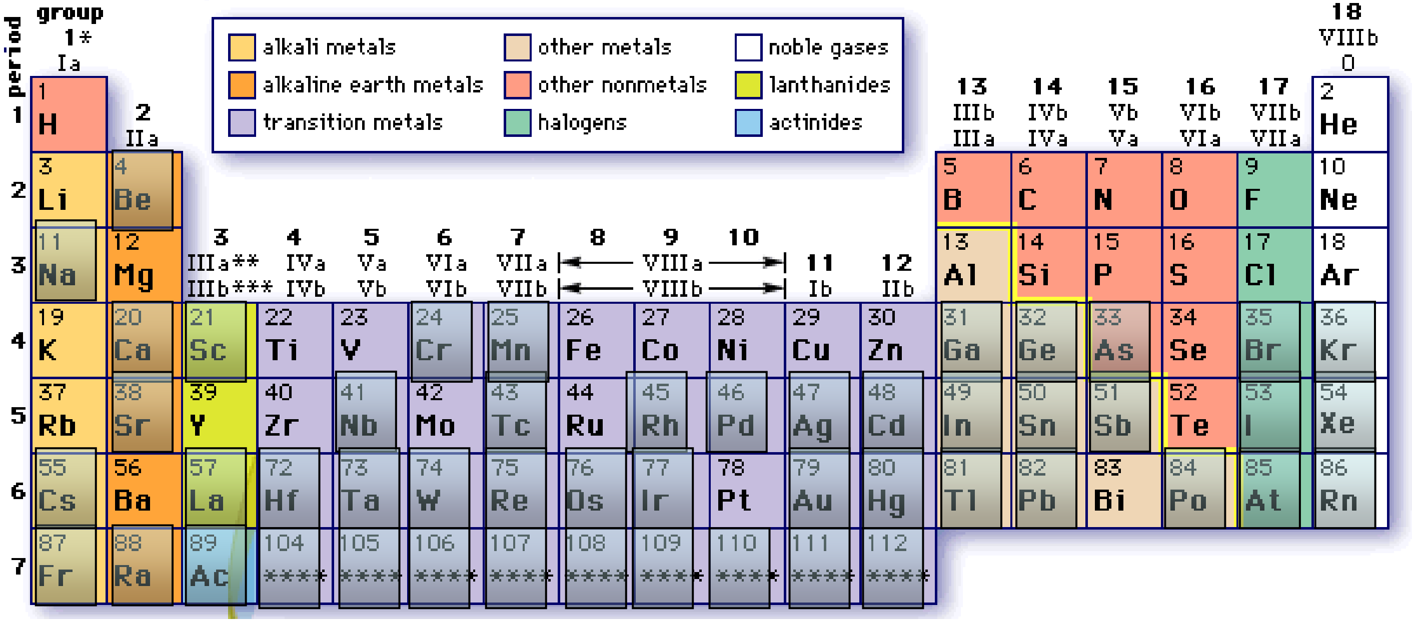
Resulting energy landscape



Contribution of E_{bond} and vdW energy

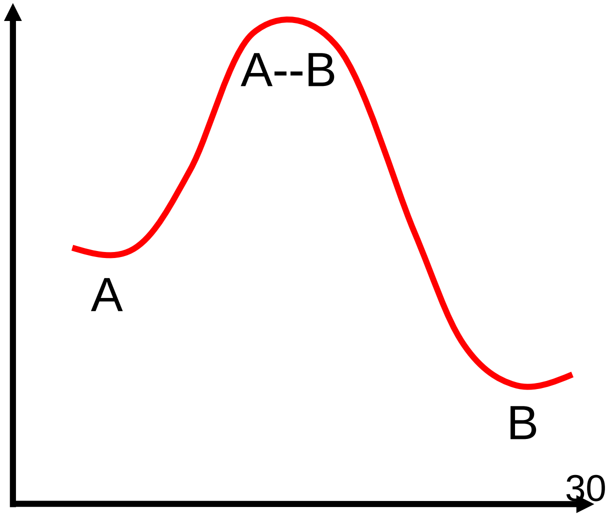
Source: van Duin, C. T. Adri, et al. "ReaxFF: A Reactive Force Field for Hydrocarbons." *Journal of Physical Chemistry A* 105 (2001). © American Chemical Society. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.

Current development status of ReaxFF



▨ : 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.

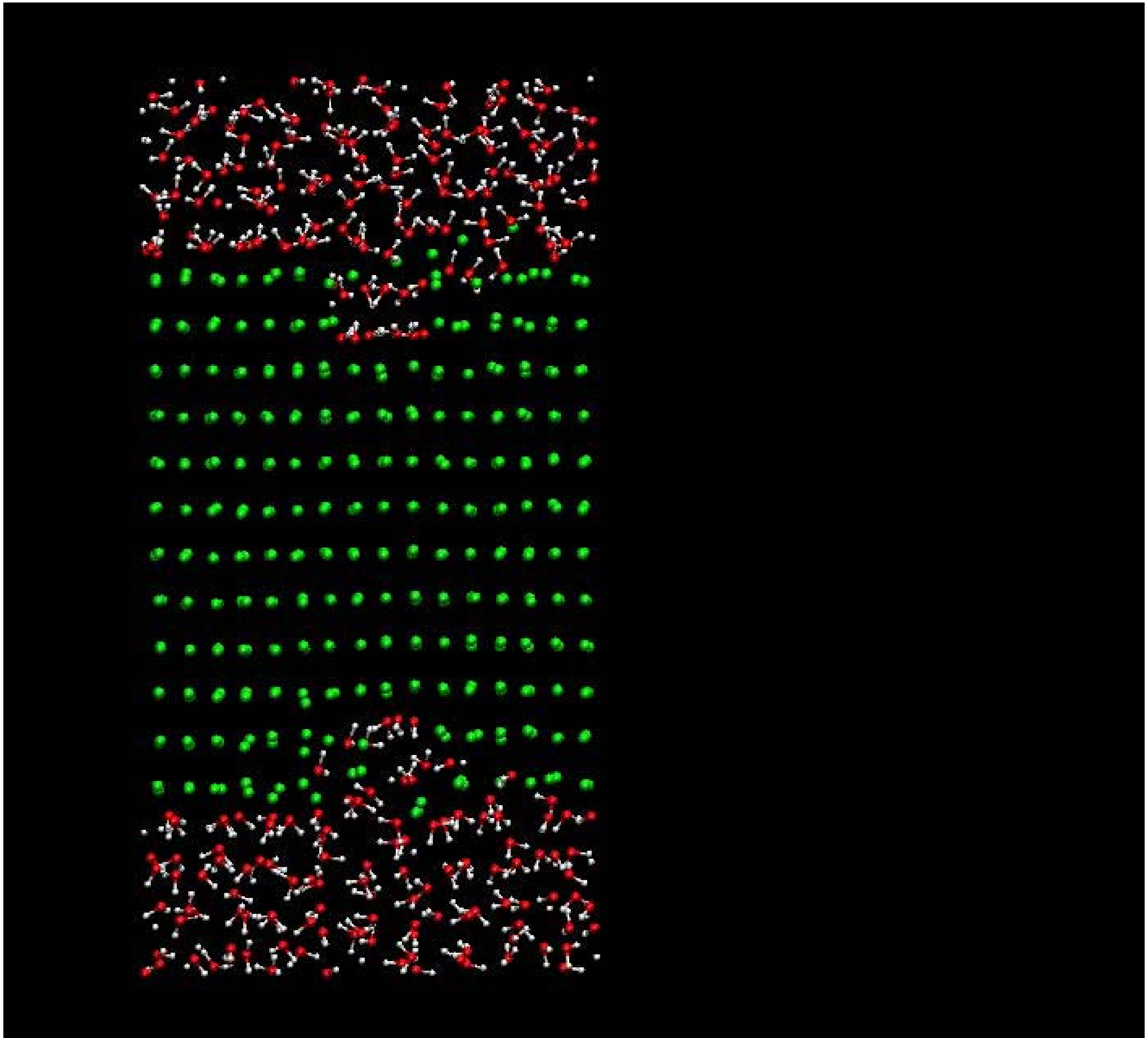
Mg-water interaction: How to make fire with water

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. Hybrid multi-paradigm fracture models

Focus: *model particular fracture properties of silicon (chemically complex material)*

Fracture of silicon: problem statement

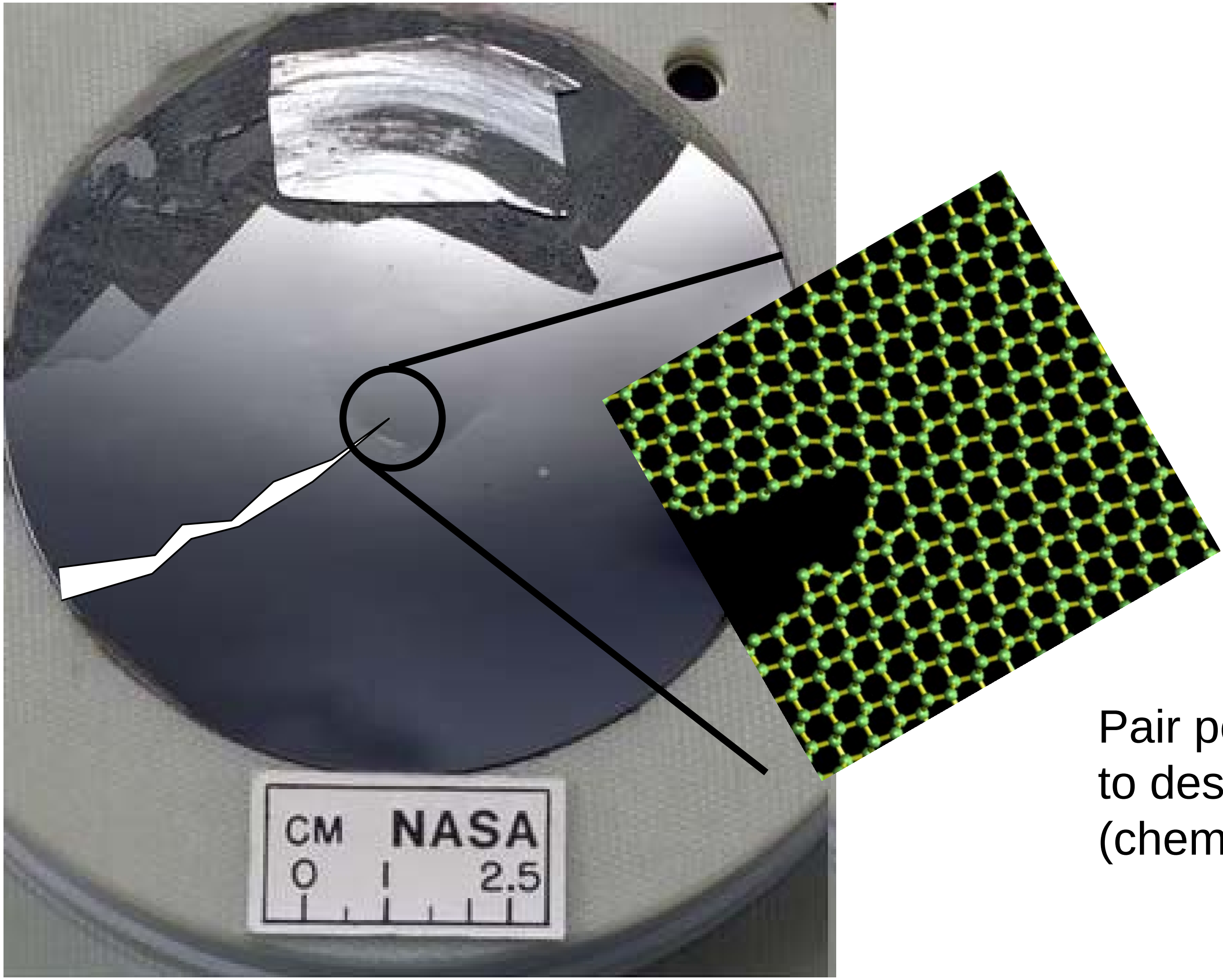


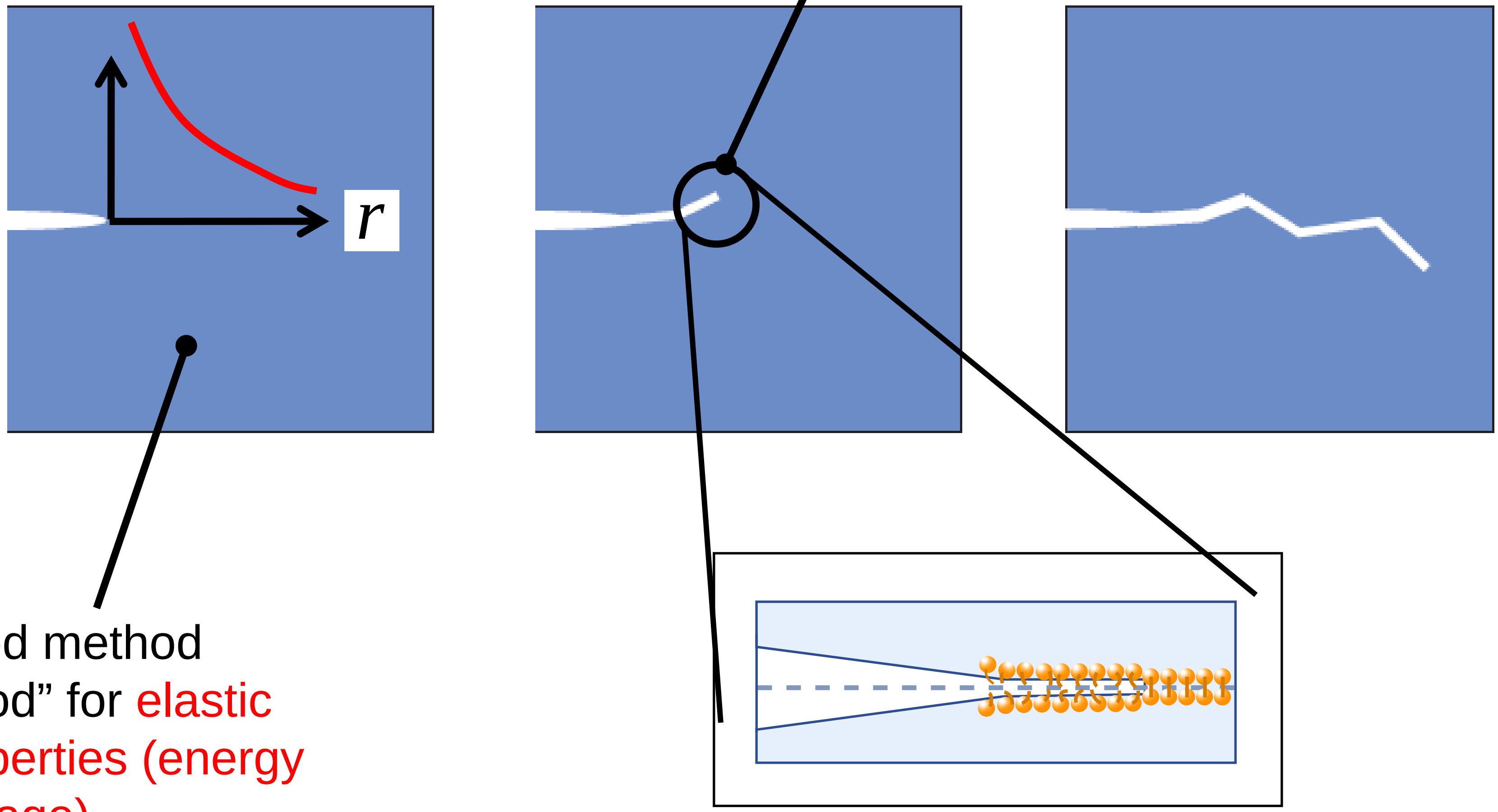
Image courtesy of NASA.

Pair potential insufficient to describe bond breaking (chemical complexity)

Multi-paradigm concept for fracture

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

Need method “good” for describing rupture of chemical bonds



Need method “good” for elastic properties (energy storage)

Image by MIT OpenCourseWare.

What about combining different potentials?

Computational efficiency

Increased accuracy & **"transferability"**

- Empirical models: mathematical functions with parameters (fitted to experiment or quantum mechanics)
    - Pair potentials (LJ, Morse, Buck., harmonic) **(lecture 5)**
    - Embedded atom models/effective medium theories
    - Multi-body potentials (e.g. Tersoff, CHARMM, etc.) **(lecture 9 and following)**
    - Reactive potentials (ReaxFF) **(lecture 9)**
- Semi-empirical models (explicitly note electronic structure)
    - Tight binding
    - MINDO (=Modified Intermediate Neglect of Differential Overlap), NINDO (=Intermediate Neglect of Differential Overlap)
- Quantum mechanical models: Start from Schroedinger's equation (and make approximations to be able to solve it)
    - Quantum chemistry (Hartree-Fock)
    - Density Functional Theory
    - Quantum Monte Carlo

"good" for elastic properties (energy storage)

+

"good" for describing rupture of chemical bonds

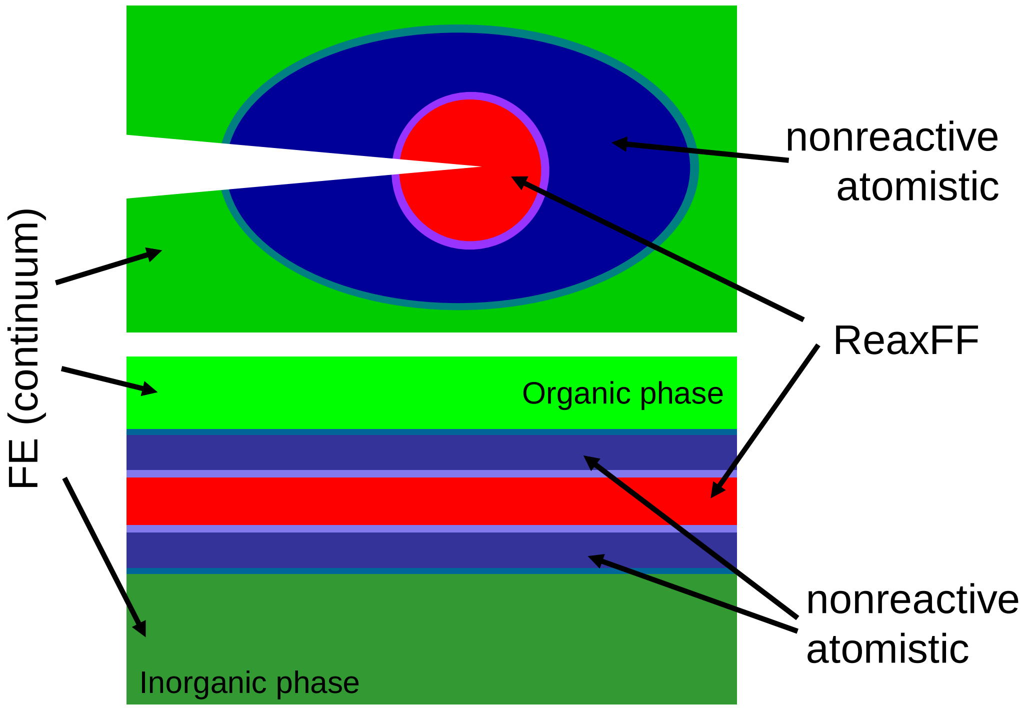
=

"multi-paradigm model"

After: G. Ceder

Concept: concurrent multi-paradigm simulations

Crack tips, defects (dislocations)



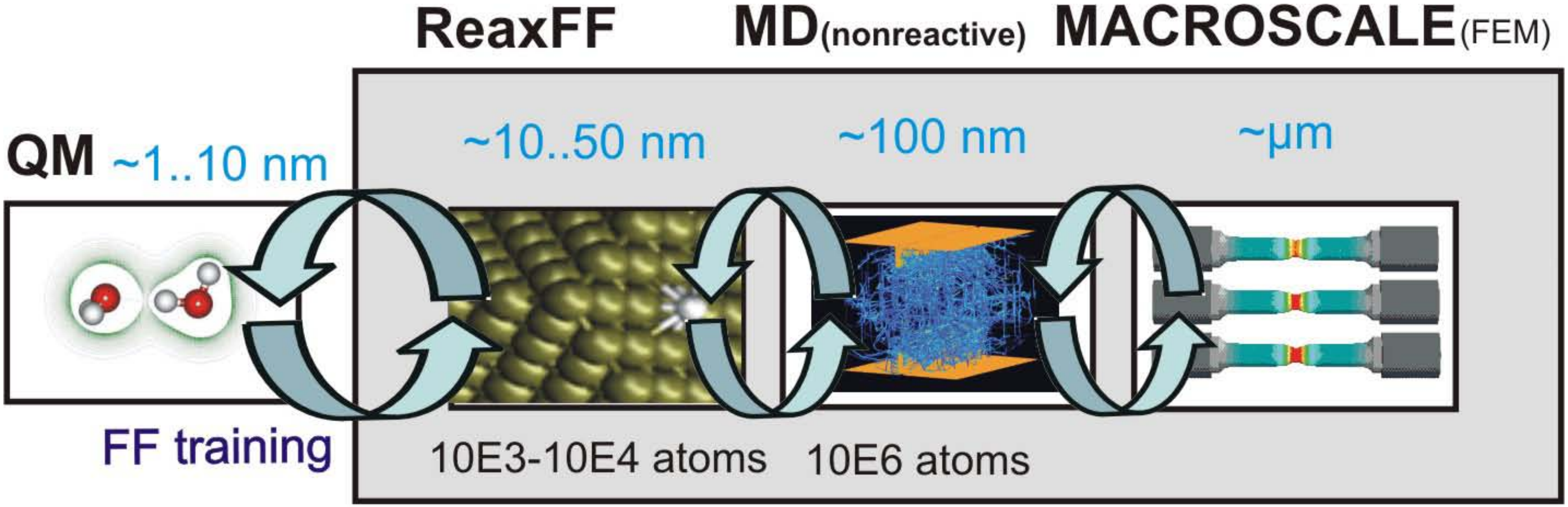
Interfaces (oxidation, grain boundaries,..)

- **Multi-paradigm approach**: combine different computational methods (different resolution, accuracy..) in a single computational domain

- **Decomposition of domain** based on suitability of different approaches

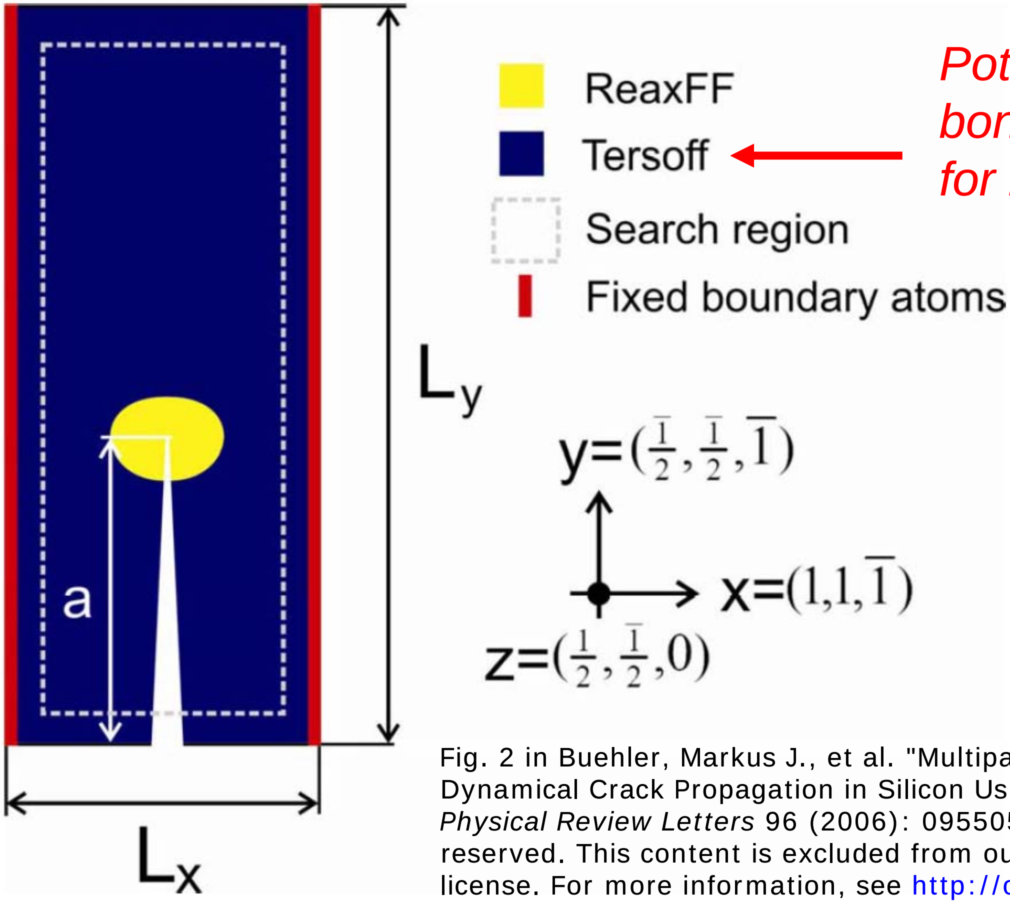
- **Example**: concurrent FE-atomistic-ReaxFF scheme in a crack problem (crack tip treated by ReaxFF) and an interface problem (interface treated by ReaxFF).

Concurrent multi-paradigm simulations: link nanoscale to macroscale



Concurrent coupling: use of multiple force fields within one simulation domain

Simulation Geometry: Cracking in Silicon



Potential for covalent bonds, not suitable for bond breaking

Fig. 2 in Buehler, Markus J., et al. "Multiparadigm Modeling of Dynamical Crack Propagation in Silicon Using a Reactive Force Field." *Physical Review Letters* 96 (2006): 095505. © APS. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.

- Consider a crack in a silicon crystal under mode I loading.

- Periodic boundary conditions in the *z*-direction (corresponding to a plane strain case).

Cracking in Silicon: Hybrid model versus Tersoff based model

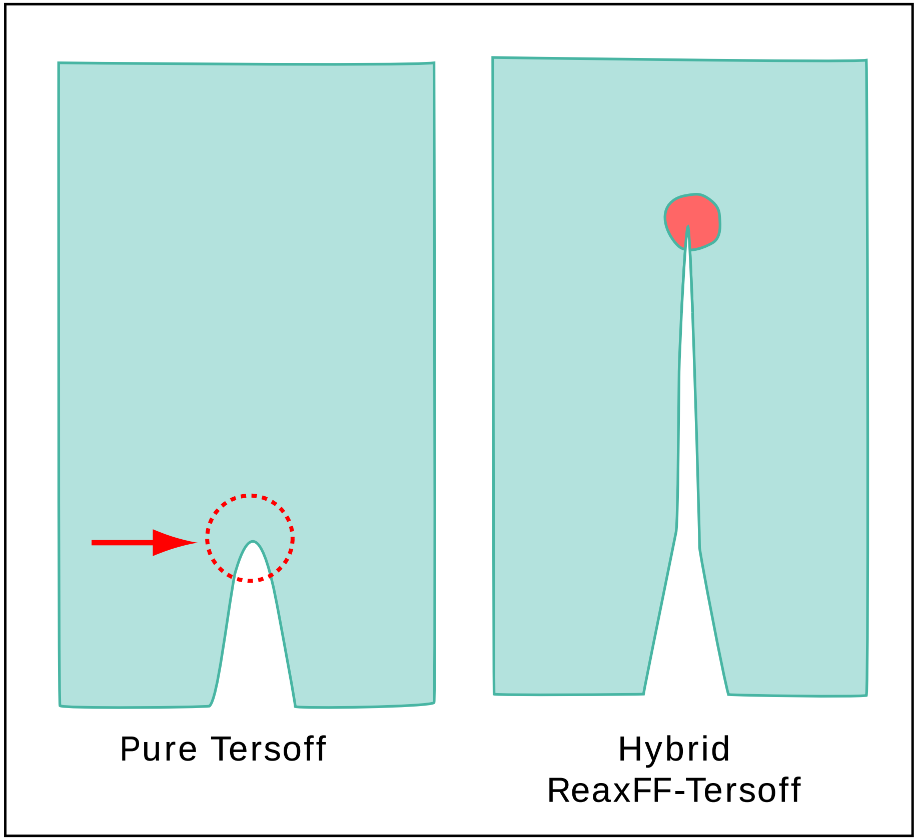


Image by MIT OpenCourseWare.

Conclusion: Pure Tersoff can not describe correct crack dynamics

How is the handshaking achieved?

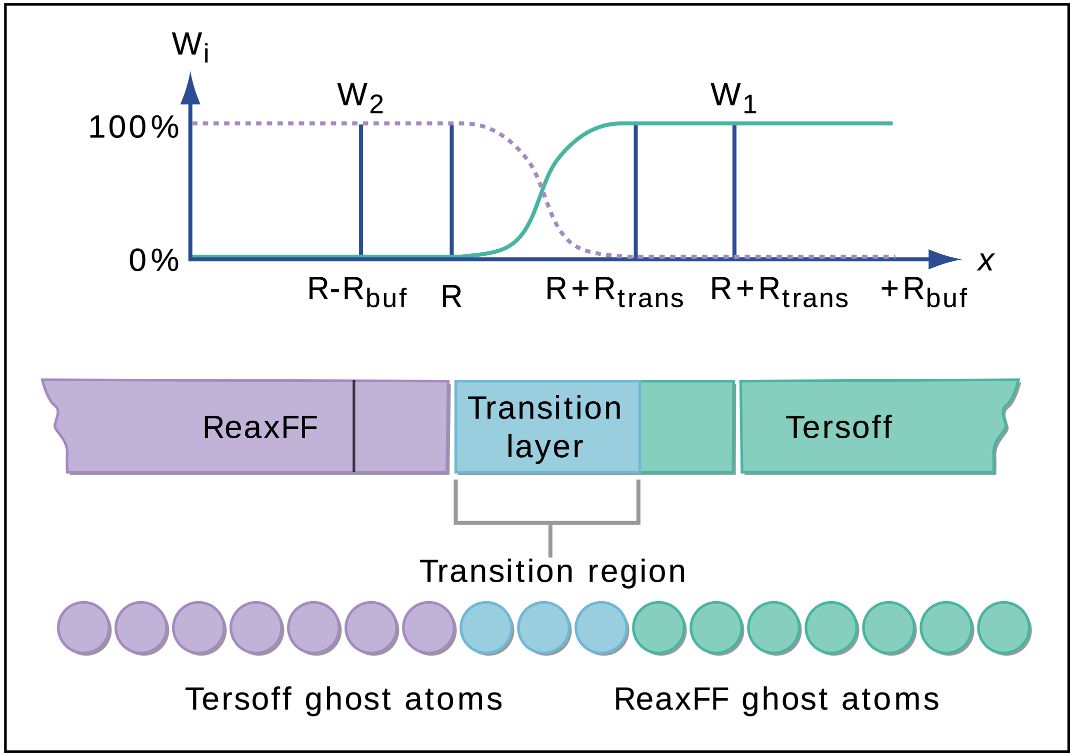
Hybrid potential energy model (Hamiltonian)

Weights = describe how much
a particular FF counts (assigned to each atom)

To obtain forces:

$$F = -\frac{\partial U_{tot}(x)}{\partial x}$$

need potential energy



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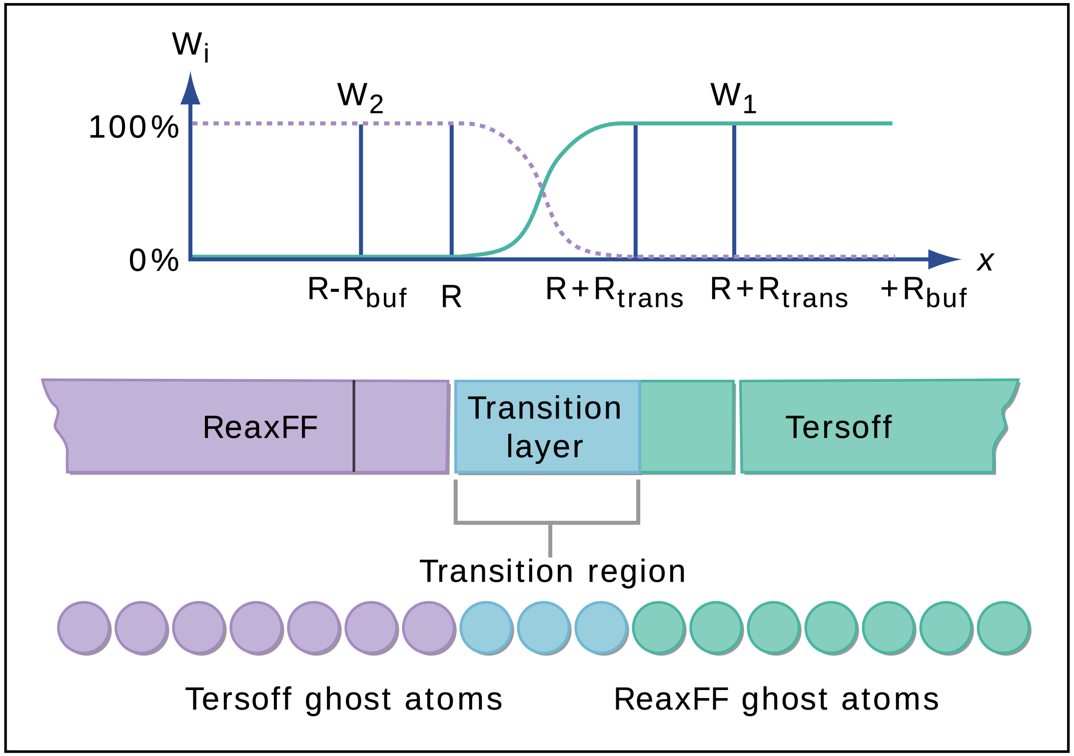
Approach: handshaking via mixed Hamiltonians

$$U_{tot} = U_{\text{ReaxFF}} + U_{\text{Tersoff}} + \overbrace{U_{\text{ReaxFF-Tersoff}}}^{\textit{transition region}}$$

Assigning weights to atoms



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Percentage ReaxFF	100%	…	100%	70%	30%	0%	…	0%
Percentage Tersoff	0%	…	0%	30%	70%	100%	…	100%

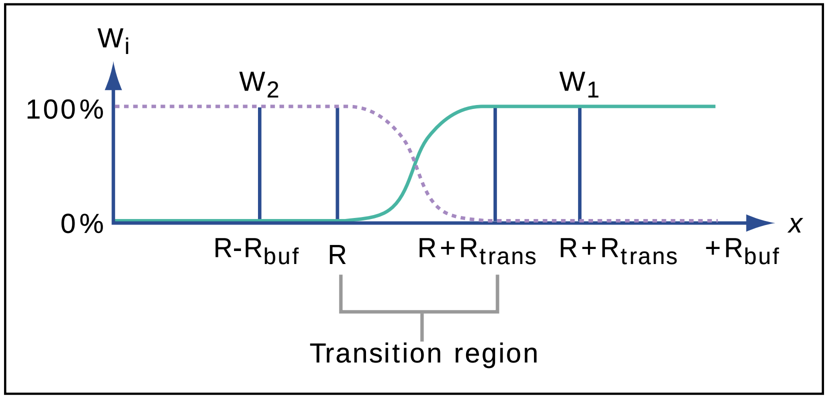
(relative contribution to total energy)

Force calculation

Potential energy

$$U_{tot} = U_{\text{ReaxFF}} + U_{\text{Tersoff}} + U_{\text{ReaxFF}-\text{Tersoff}}$$

$$U_{\text{ReaxFF}-\text{Tersoff}} = w_{\text{ReaxFF}}(x) U_{\text{ReaxFF}} + (1 - w_{\text{ReaxFF}}) U_{\text{Tersoff}}$$



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Recall: $F = -\dfrac{\partial U}{\partial x}$

$$w_{\text{ReaxFF}}(x) + w_{\text{Tersoff}}(x) = 1 \qquad \forall x$$

w_{ReaxFF} is the weight of the reactive force field in the handshaking region.

$$F_{\text{ReaxFF}-\text{Tersoff}} = -\left[\left(w_{\text{ReaxFF}}(x) F_{\text{ReaxFF}} + (1 - w_{\text{ReaxFF}}) F_{\text{Tersoff}} \right) - \frac{\partial w_{\text{ReaxFF}}}{\partial x} \left(U_{\text{ReaxFF}} - U_{\text{Tersoff}} \right) \right]$$

D. Sen and M. Buehler, *Int. J. Multiscale Comput. Engrg*., 2007

Hybrid Hamiltonians – force calculation

$$F_{\text{ReaxFF}-\text{Tersoff}} = -\left[\left(w_{\text{ReaxFF}}(x)F_{\text{ReaxFF}} + (1-w_{\text{ReaxFF}})F_{\text{Tersoff}}\right) - \underset{\approx 0}{\cancel{\frac{\partial w_{\text{ReaxFF}}}{\partial x}}}\,\overset{}{\underset{}{\cancel{\left(U_{\text{ReaxFF}} - U_{\text{Tersoff}}\right)}}}\xrightarrow{}\approx 0\right]$$

Slowly varying weights (wide transition region): $\partial w_{\text{ReaxFF}} / \partial x \approx 0$

If $U_{\text{ReaxFF}} - U_{\text{Tersoff}} \approx 0$ (*i.e.*, both force fields have similar energy landscape)

Simplified result: can interpolate forces from one end to the other

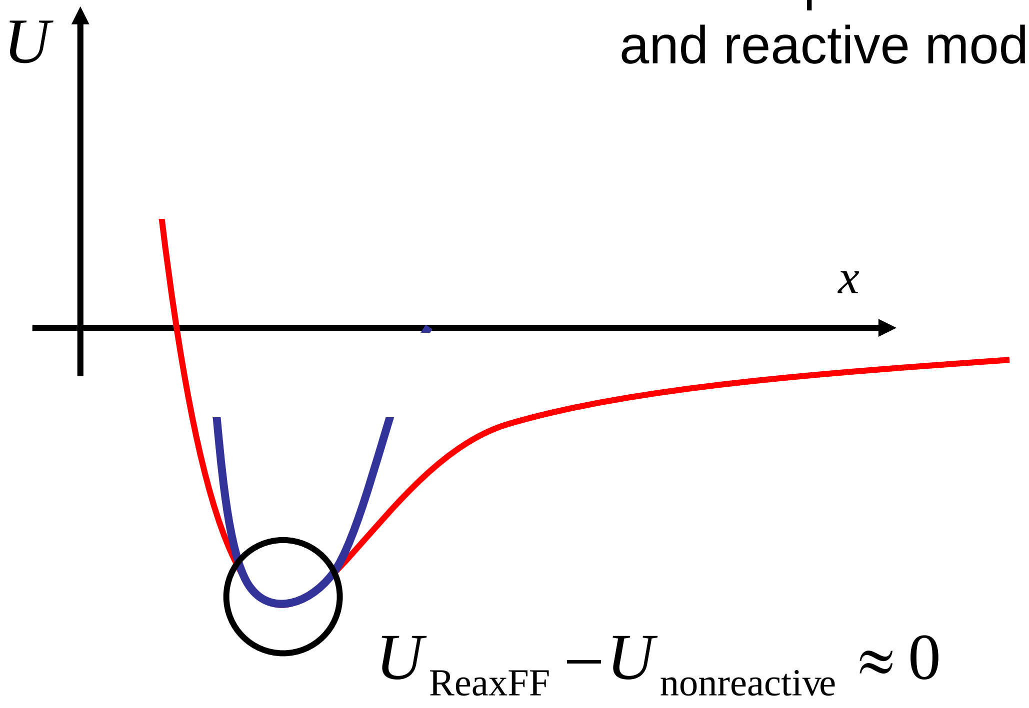
$$\boxed{F_{\text{ReaxFF}-\text{Tersoff}} = \left(w_{\text{ReaxFF}}(x)F_{\text{ReaxFF}} + (1-w_{\text{ReaxFF}})F_{\text{Tersoff}}\right) \quad\Big|\quad w_{\text{ReaxFF}}(x) + w_{\text{Tersoff}}(x) = 1 \qquad \forall x}$$

D. Sen and M. Buehler, *Int. J. Multiscale Comput. Engrg.*, 2007

Energy landscape of two force fields

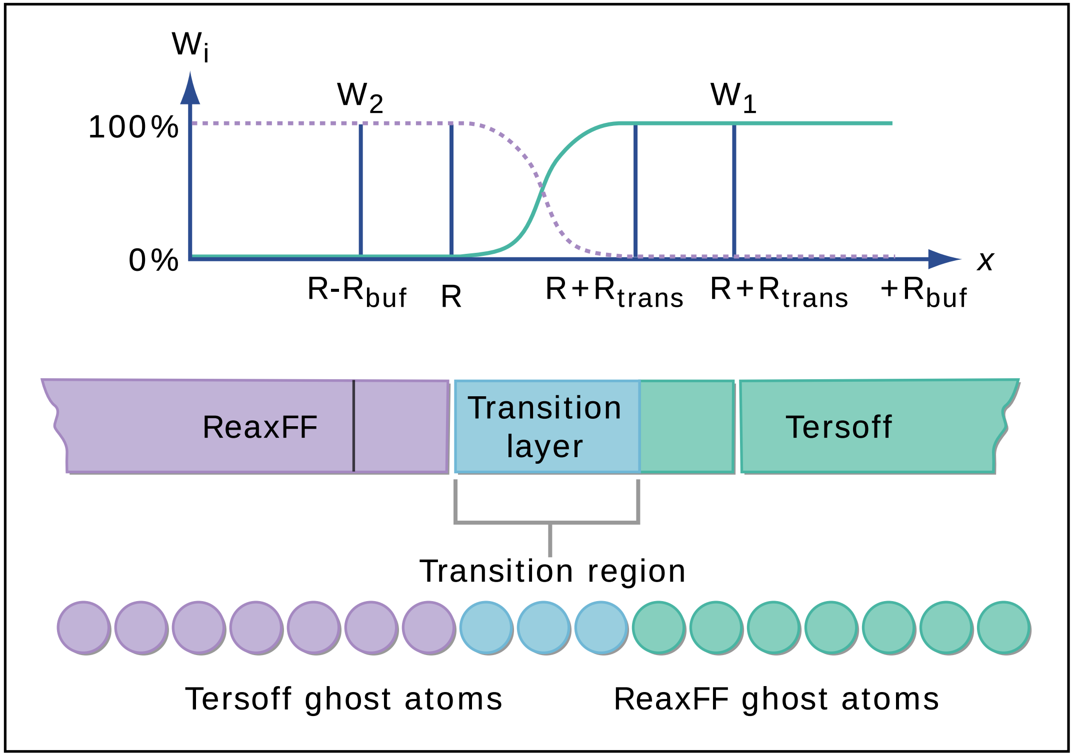
- Schematic showing the coupling of reactive and nonreactive potentials

- At small deviations, energy landscape is identical in nonreactive and reactive models



$$U_{\mathrm{ReaxFF}} - U_{\mathrm{nonreactive}} \approx 0$$

Summary: hybrid potential energy model



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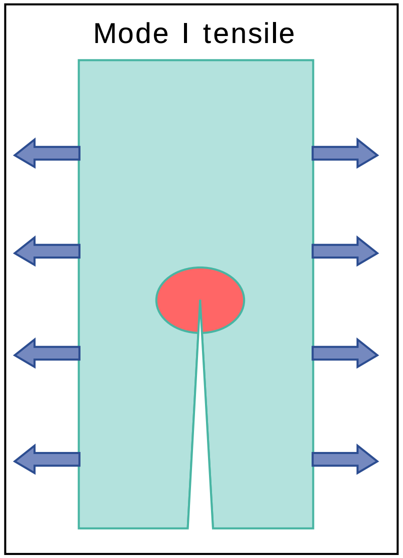
$$F_{\text{ReaxFF}-\text{Tersoff}} = \left(w_{\text{ReaxFF}}(x) F_{\text{ReaxFF}} + (1 - w_{\text{ReaxFF}}) F_{\text{Tersoff}} \right)$$

$$w_{\text{ReaxFF}}(x) + w_{\text{Tersoff}}(x) = 1 \qquad \forall x$$

Fracture of silicon single crystals

Use multi-paradigm scheme that combines the Tersoff potential and ReaxFF



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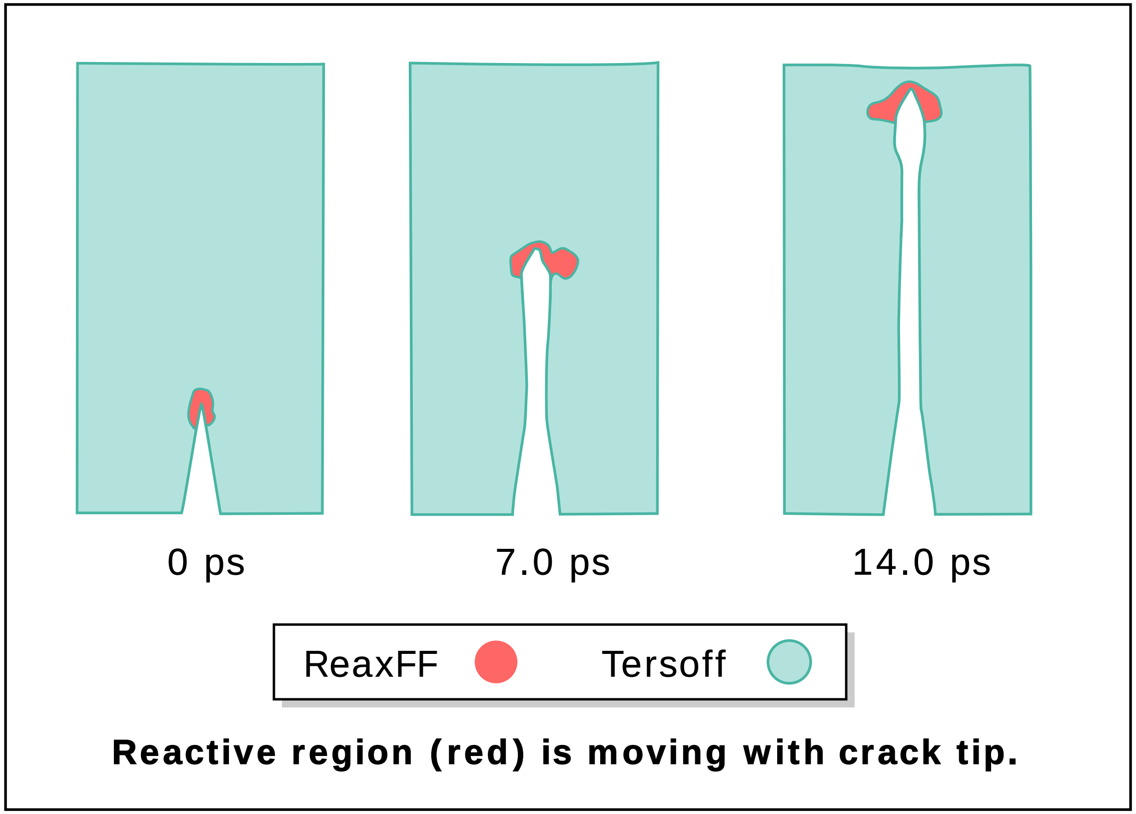
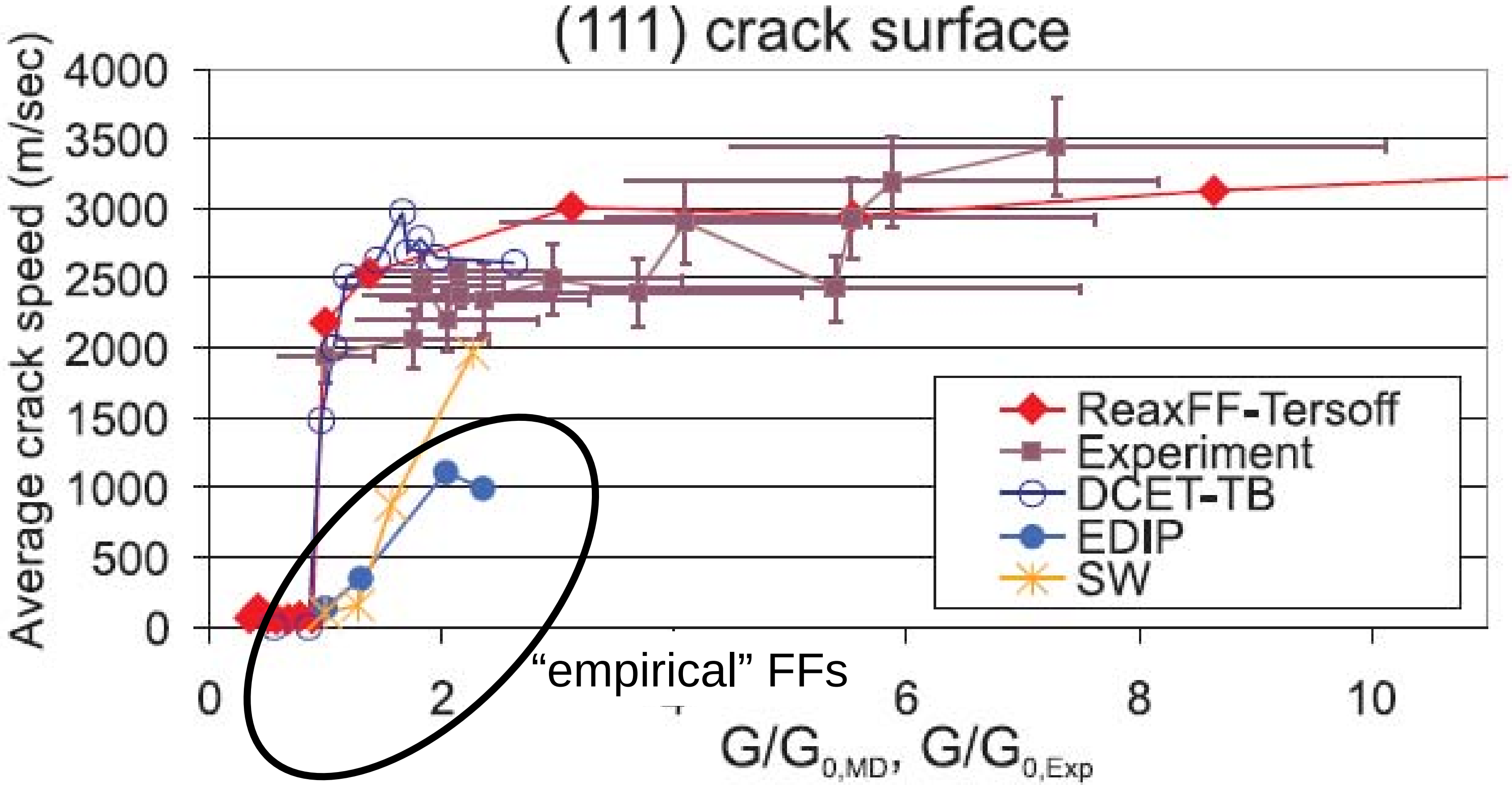


Reactive region (red) is moving with crack tip.

Image by MIT OpenCourseWare.

Quantitative comparison w/ experiment



“empirical” FFs

Fig. 1c in Buehler, M., et al. "Threshold Crack Speed Controls Dynamical Fracture of Silicon Single Crystals." *Physical Review Letters* 99 (2007). © APS. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.

Load: normalized by critical energy release rate to initiate fracture

Crack dynamics

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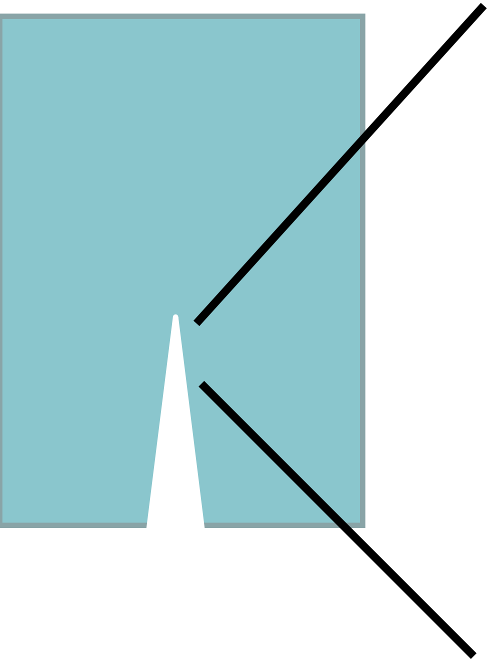
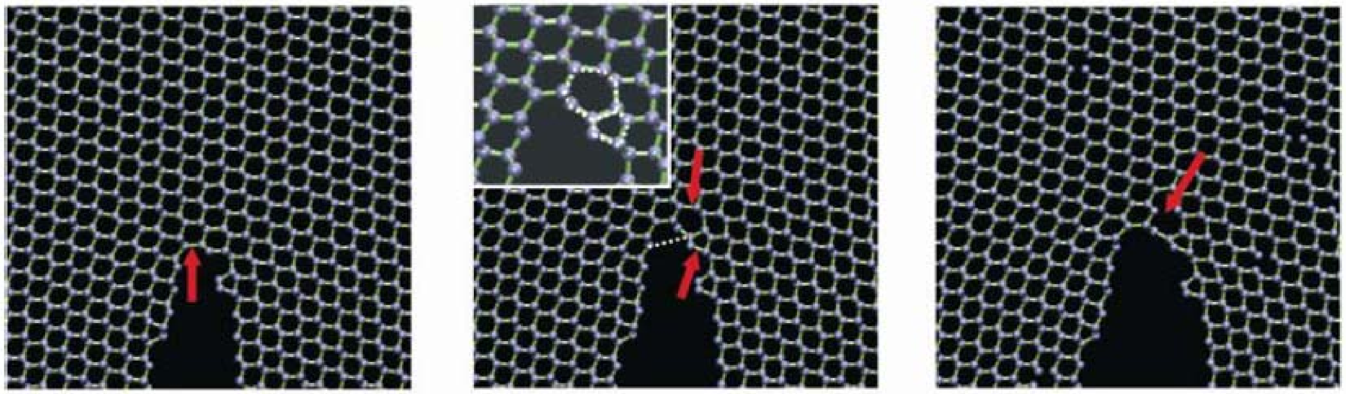
Crack speed: O(km/sec)

=O(nm/ps) (well in reach with MD)

Atomistic fracture mechanism

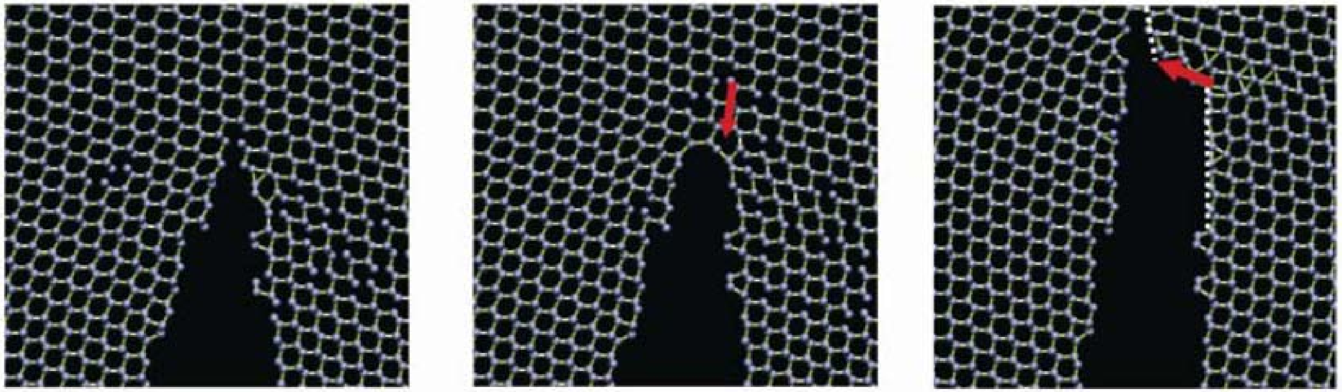




Initial crack

Formation of 7-5 ring defect

Rupture ahead of 7 membered ring

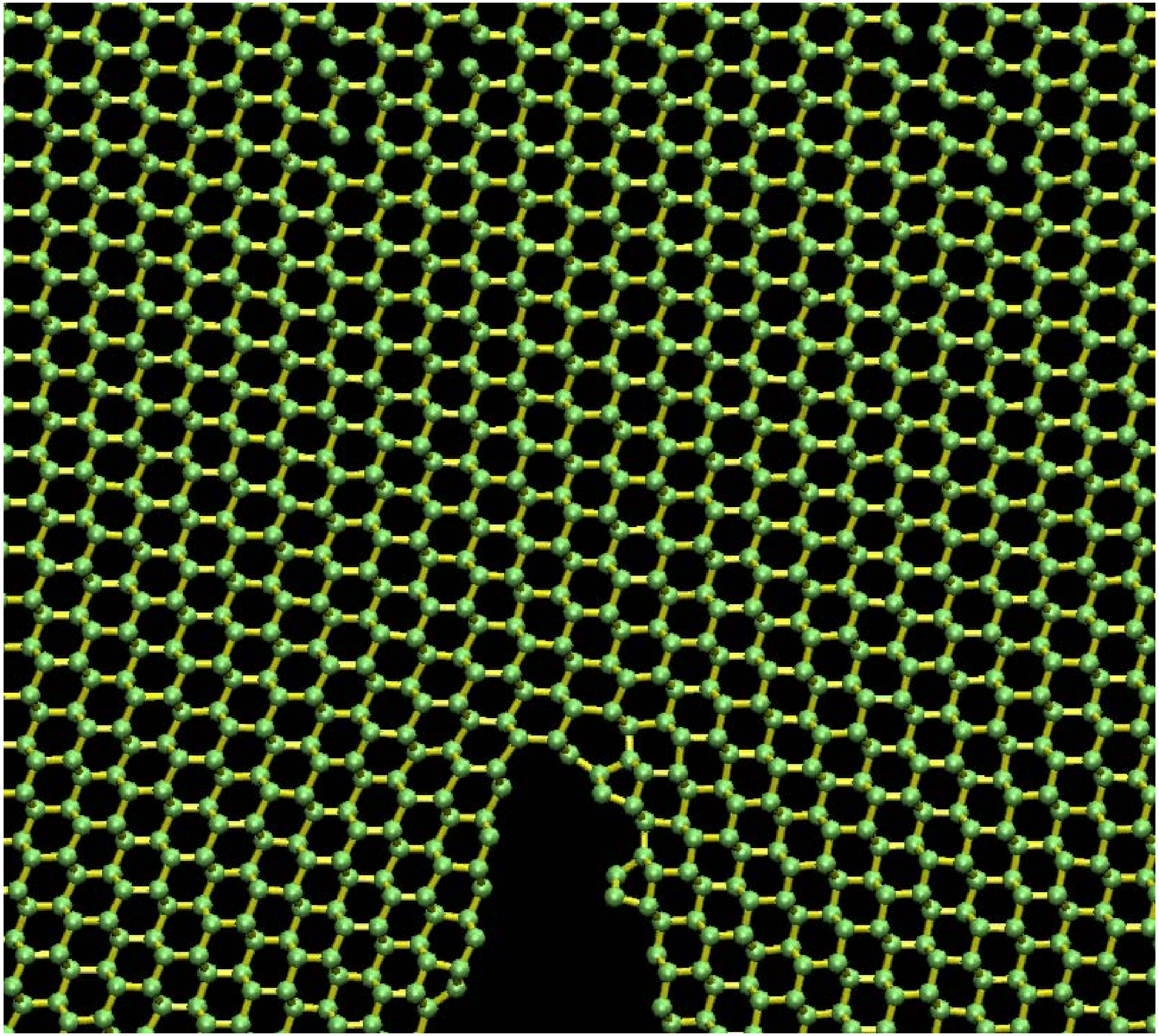


Crack propagation (smooth surface)

Formation of another 7-5 ring defect

7-5 ring leads to change in crack direction
Creates surface step

Fracture initiation and instabilities



Fracture mechanism: tensile vs. shear loading

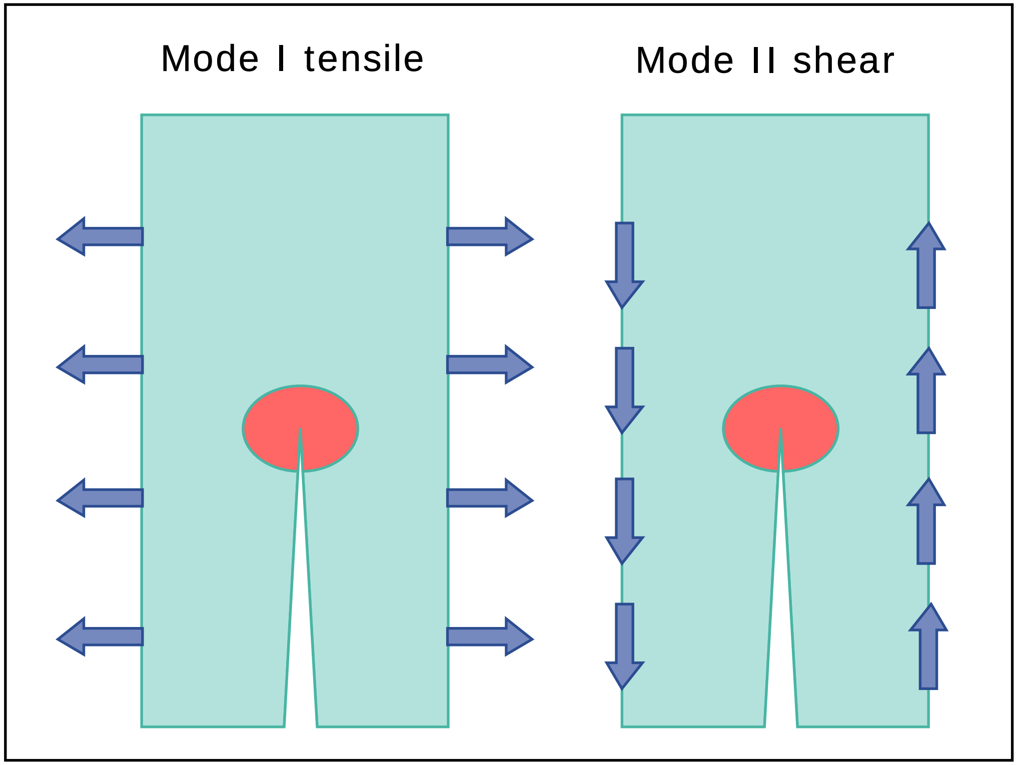


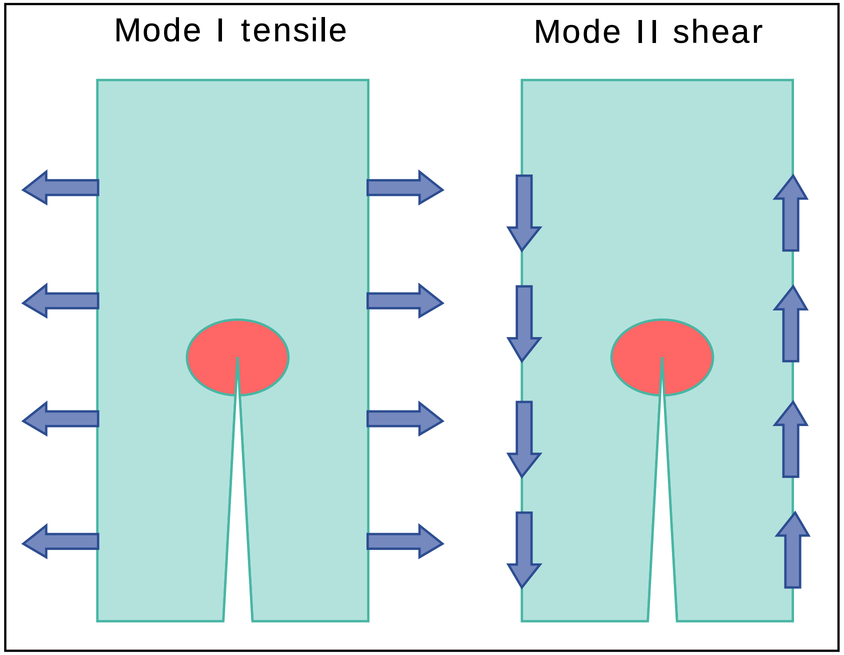
Image by MIT OpenCourseWare.

Shear (mode II) loading:
Crack branching

Tensile (mode I) loading:
Straight cracking

M.J. Buehler, A. Cohen, D. Sen, *Journal of Algorithms and Computational Technology*, 2008

Fracture mechanism: tensile vs. shear loading



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Shear (mode II) loading: Crack branching
Tensile (mode I) loading: Straight cracking

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Please see figures in Buehler, M. J., A. Cohen, and D. Sen. "Multi-paradigm Modeling of Fracture of a Silicon Single Crystal Under Mode II Shear Loading."*Journal of Algorithms and Computational Technology* 2 (2008): 203-21.

Summary: main concept of this section

- Can **combine different force fields** in a single computational domain = **multi-paradigm modeling**
- Enables one to **combine the strengths of different force fields**
- Simple approach by **interpolating force contributions** from individual force fields, use of weights (sum of weights = 1 at all points)
- **ReaxFF based models quite successful**, e.g. for describing fracture in silicon, quantitative agreement with experimental results

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