Atomistic simulations of fracture in silicon

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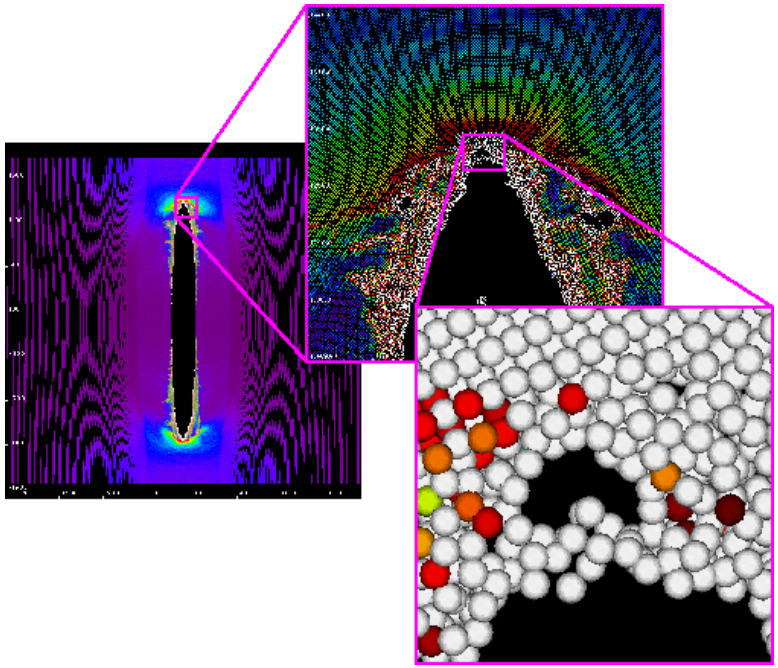

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OVERVIEW

Fracture: the canonical multiscale materials problem
- brittle vs. ductile fracture

Coupling of length scales

CLS: first approach
- method
- results
- lessons learned

DCET: new approach
- method
- results

Conclusions

FRACTURE

Structural materials: keep their shape under mechanical load

What happens when load is too large? Failure . . .

Technologically important:

- Can we predict failure (*ab initio*) ?
- How can we control failure properties?

Scientifically interesting:

Why do materials break in the way they do?

MODES OF FAILURE

Real materials aren't continuous

Atomistic details control action at crack tip

Two possible failure modes:

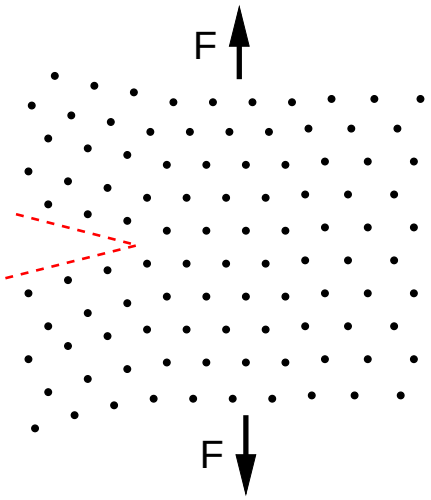
Brittle:

- Crack remains sharp
- Singularity at crack tip remains
- No damage except crack
- Minimal amount of energy dissipated

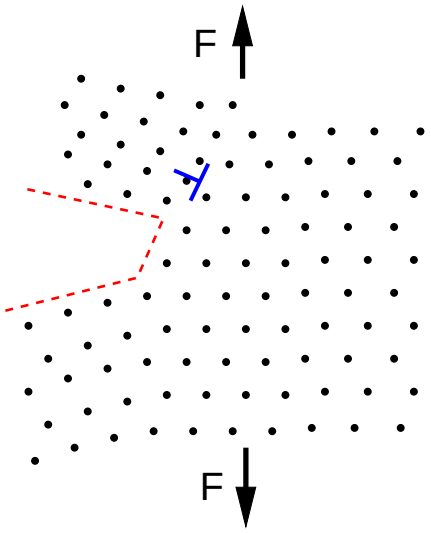
Ductile:

- Crack becomes blunt
- Material deforms non-reversibly ($\equiv$ plasticity)
- Dislocations propagate into material
- A lot of energy dissipated

brittle



ductile



EXPERIMENT VS. SIMULATION

What we want: **microscopic understanding of processes**

What we can get from experiment:

- crack speed as a function of loading (critical loading)
- morphology of exposed surface (fractography)
- atomic configuration (only at surface, very slow cracks)

What can't we get from experiment:

- perfect system (defect free, pure loading)
- view of atoms during dynamic fracture

Can simulations help?

- Perfect material, loading
- Perfect resolution view (in space, in time)
- System size, time scale
- Description of interatomic interactions

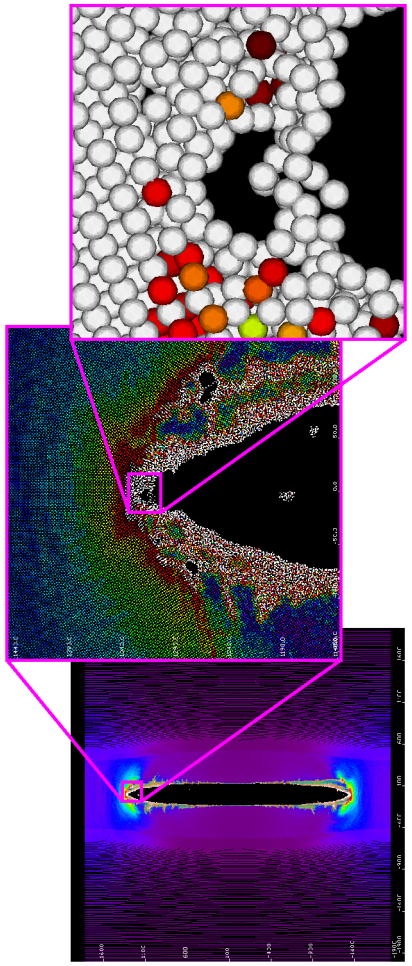
COUPLING OF LENGTH SCALES

Material properties controlled by processes over many length scales

Different processes best described by different models

Example: fracture

- Short scale – 10^2 atoms
  - breaking atomic bonds
  - classical nuclei, quantum-mechanical bonds
- Medium scale – 10^4 atoms
  - highly strained bonds
  - classical nuclei, empirical interactions
- Long scale – 10^{23} atoms
  - elastic deformation
  - continuum mechanics

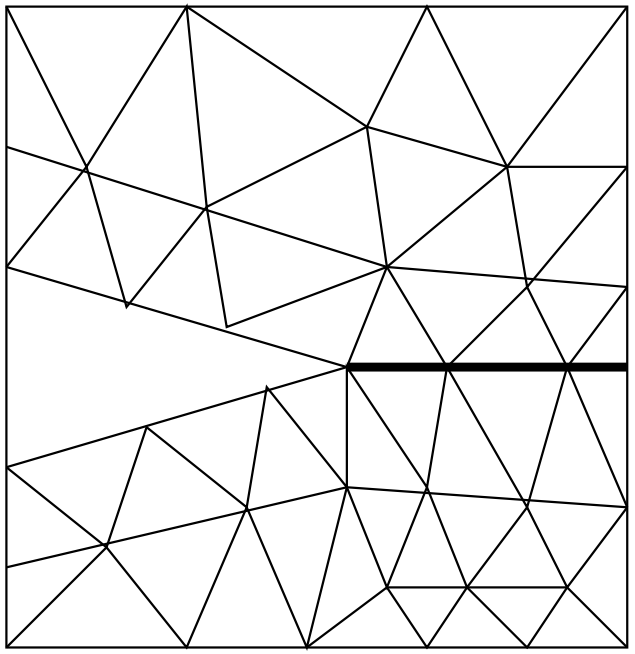


How can you treat all of these aspects?

SEQUENTIAL COUPLING

Fast method: continuum mechanics

- very fast, accurate but fails at crack tip
- cohesive zone: rule for behavior at crack tip
- parameters: elastic constants, surface energy



Slow method: first-principles calculations

- very slow
- accurate, rarely fails

Advantages:

- length scale much larger than atomistics
- *time scale much longer than atomistics*

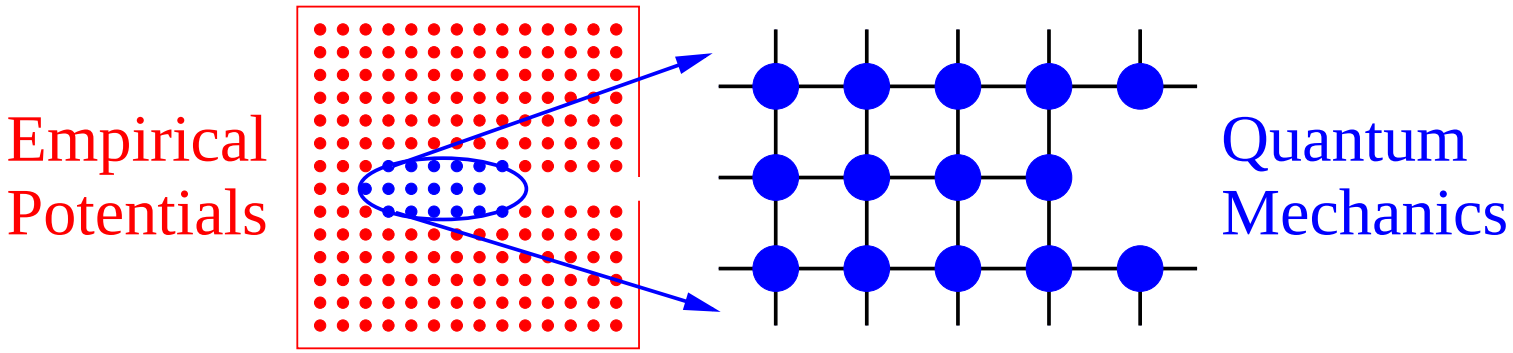
Limits: assumptions

- type of fracture (e.g. brittle)
- process at crack tip known
- *More generally: coarse-grain theory is known*

CONCURRENT COUPLING

Concurrent: large system with a fast method, limited applicability
where needed, use a slower, more accurate method

- Fracture: QM for crack tip, bulk sample with empirical potentials
- Friction: QC for surface interaction, elasticity for contact forces



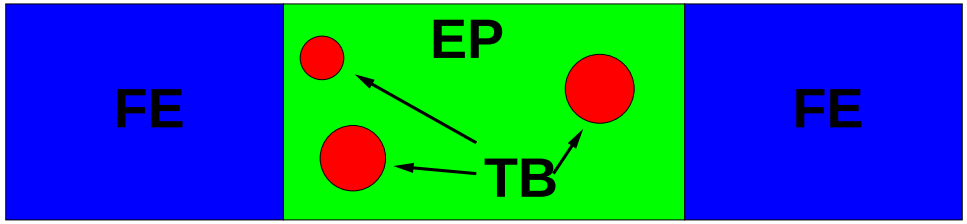
Need

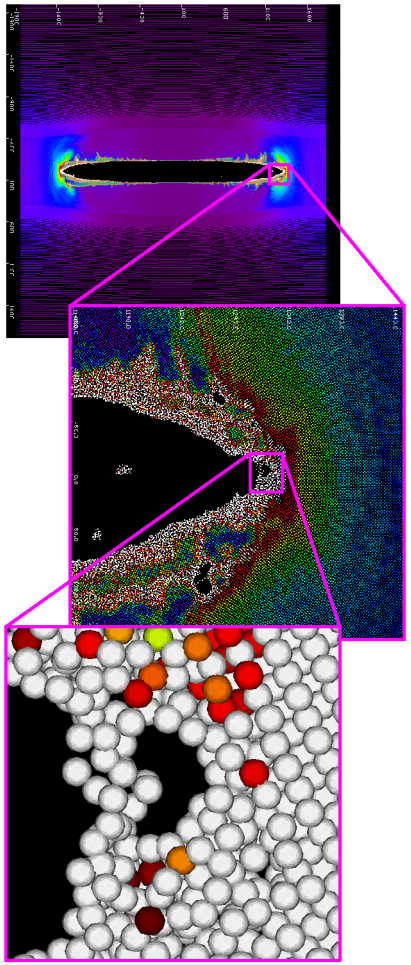
- localized region for slower method

Especially important for dynamics, changing boundary conditions

ORIGINAL CLS METHOD

Three regions, three methods



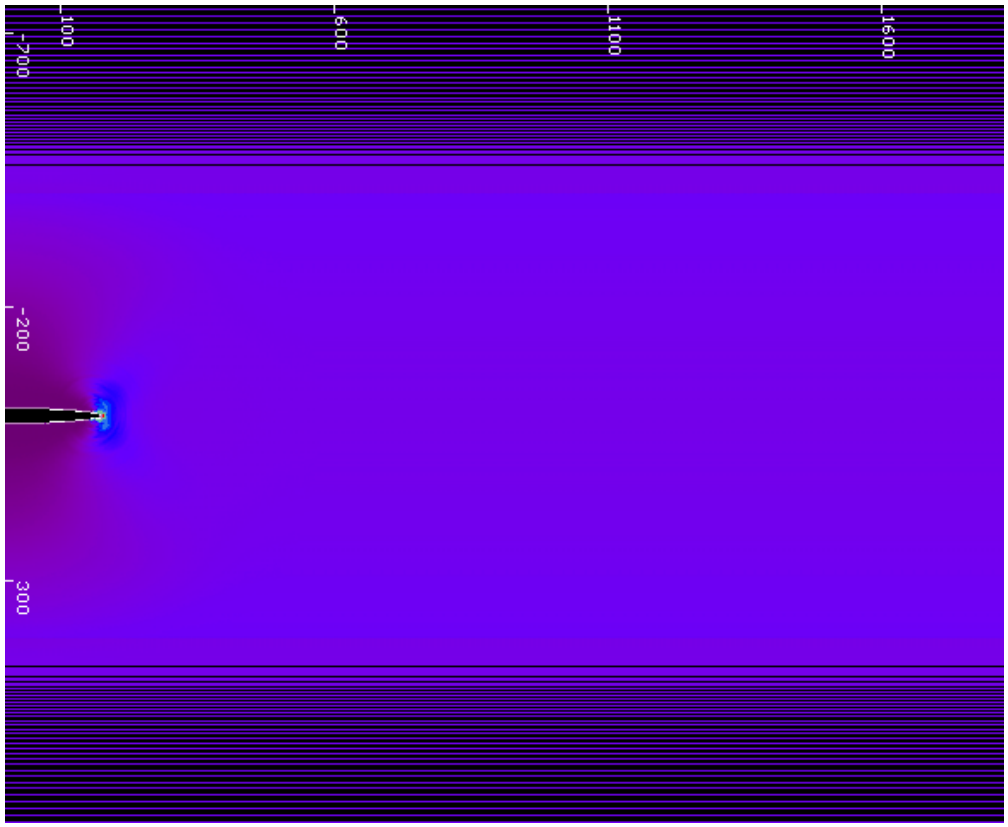


- V_{FE} Continuum elasticity finite elements
- V_{EP} Empirical potential molecular dynamics
- V_{TB} Tight-binding molecular dynamics
  Force law: simple QM (approx. solution overlapping passivated clusters)

Stability: well defined total energy,
dynamics for each region in sync

(Abraham *et al.* Comp. in Phys. 1998, Abraham *et al.* Europhys. Lett. 1998, Broughton *et al.* PRB 1999)

ORIGINAL CLS RESULTS



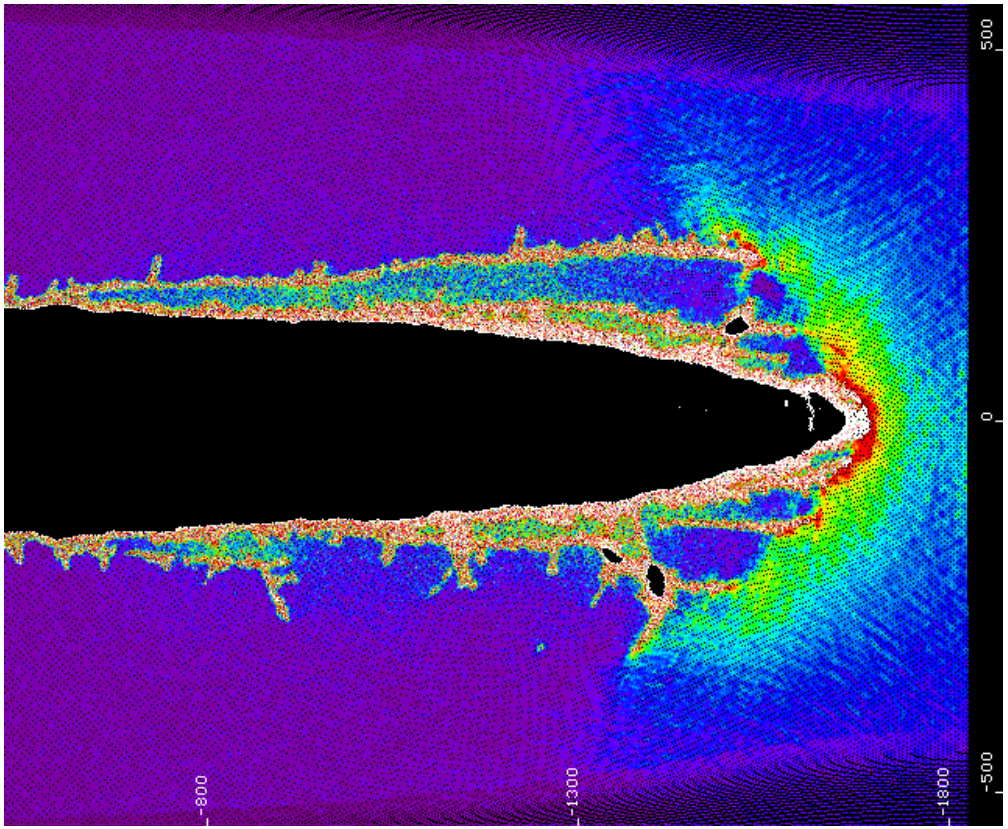
4000 Å $\times$ 3600 Å $\times$ 11 Å

About 1.5×10^6 atoms

About 3×10^5 FE nodes

$\Leftrightarrow$ 7.7×10^6 atoms

ORIGINAL CLS RESULTS



4000 Å $\times$ 3600 Å $\times$ 11 Å
About 1.5×10^6 atoms
About 3×10^5 FE nodes
$\Leftrightarrow$ 7.7×10^6 atoms

Elastic waves
Voids
Amorphous tendrils
(dislocations)

Not brittle
No effect from TB

Crititcal energy release rate G for fracture:
simulation: 8–130 J/m^3 (Marder *et al.*, Abaraham *et al.*)
experiment: $\approx$2.5 J/m^3 (Hauch *et al.*)

Experiment: not much energy for dislocations/voids/disorder

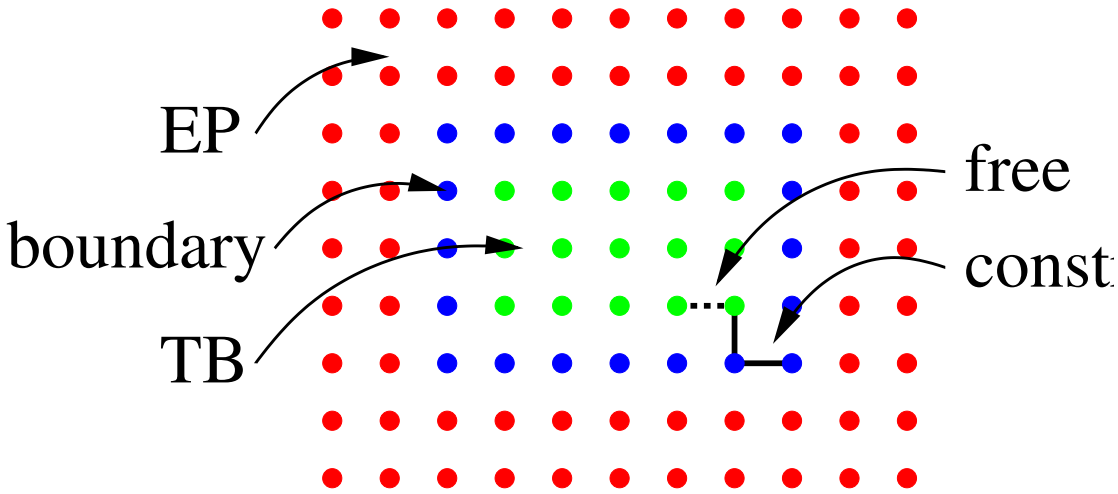
DCET

(No finite elements continuum, just molecular dynamics)

TB forces from constrained electronic Green's function

Mechanical coupling:

- EP atoms: included in EP calculation, forces from EP
- TB atoms: included in TB calculation, forces from TB
- boundary atoms: included in both calculations, forces from EP



No well defined total energy. (Bernstein Europhys. Lett. 2001)

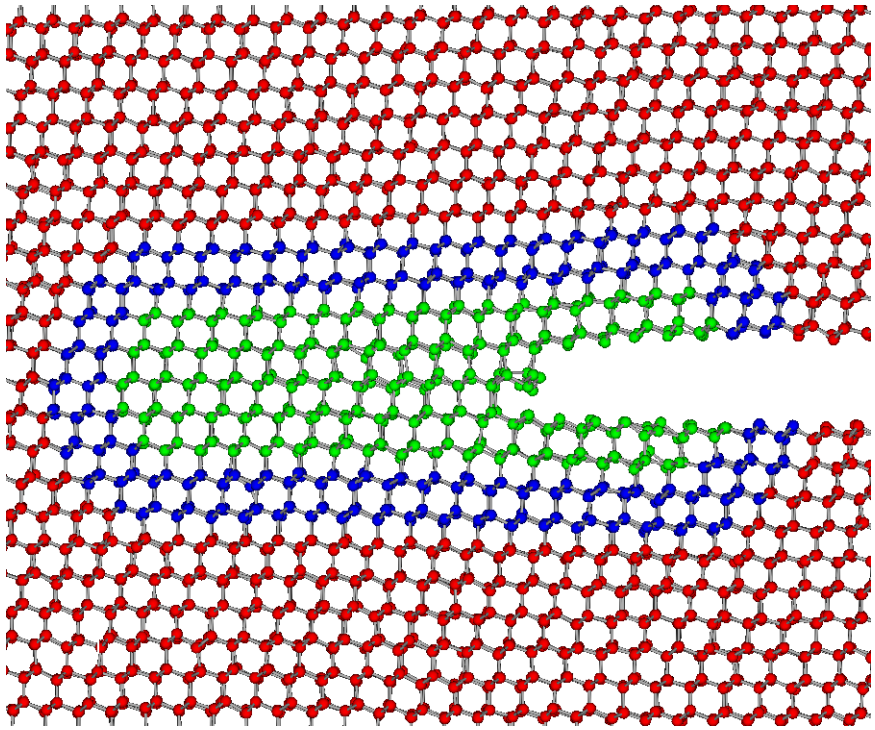
FRACTURE WITH TB

Couple empirical potential (EDIP) and TB

Continuum solution for fixed strain, top/bottom boundary fixed

$\sim$50000 EP atoms $\sim$1000 TB atoms

400 Å $\times$ 250 Å $\times$ 12 Å, (80 Å $\times$ 65 Å shown)



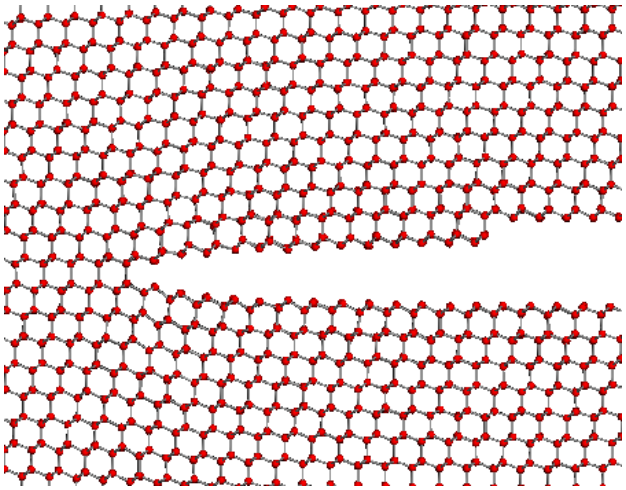
Red: EP

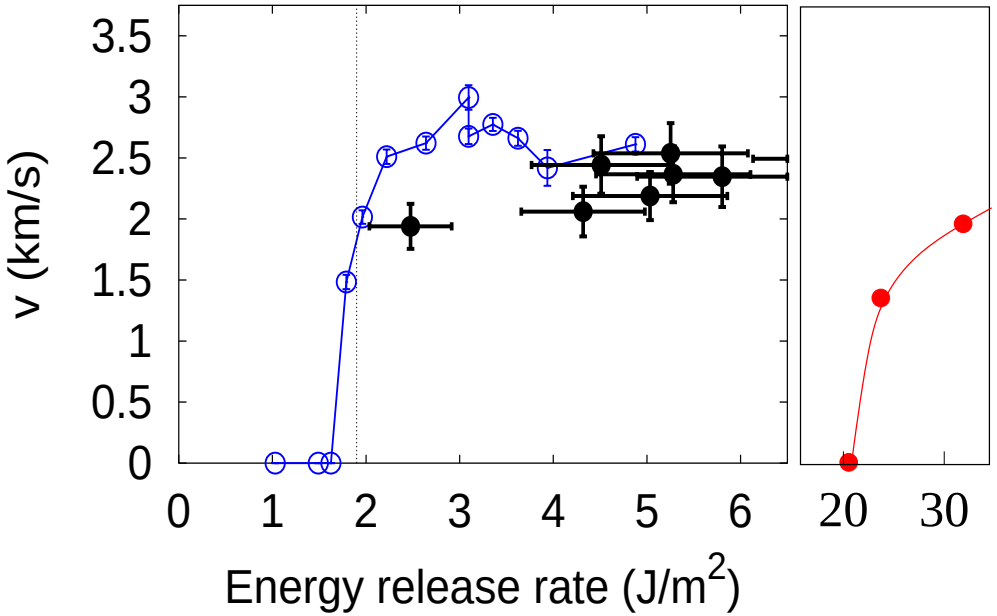
Green: TB

Blue: Boundary

(Bernstein and Hess PRL 2003)

BRITTLE FRACTURE





Blue: sim., Black: exper. (Hauch *et al.* PRL **82**), Red: EP (approx.)

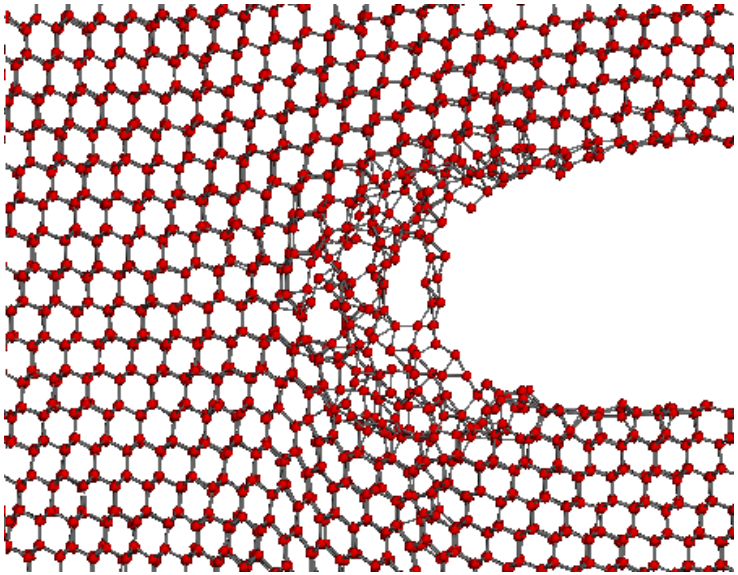
Vertical line: Griffith criterion for brittle fracture

Onset approximately at Griffith criterion

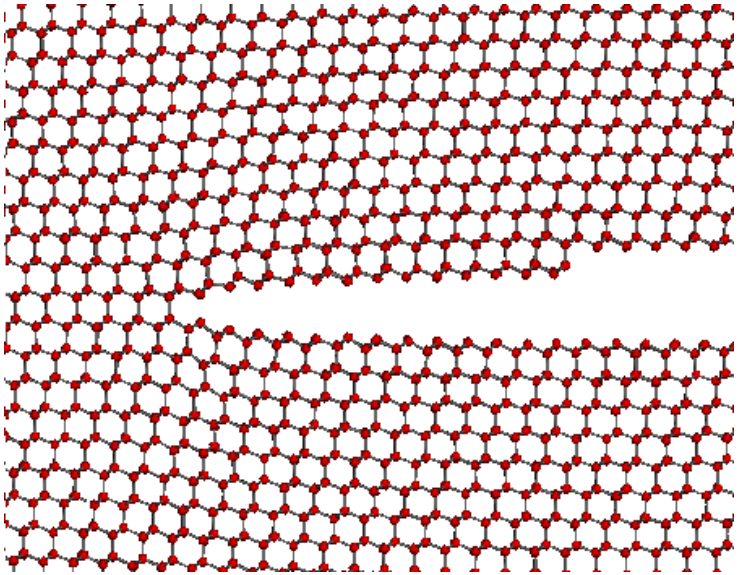
Limiting speed is $\approx 1/2$ Rayleigh speed

DISCUSSION

EDIP/SW/?



EDIP+TB



What's different?

I.e. what are the fundamental materials parameters that control the nature of fracture?

ENERGIES . . .

Energetic view of brittle vs. ductile: Rice criterion

Griffith: brittle fracture when energetically favored

Rice: emit dislocations when energetically favored

Process (cleavage, dislocation emission) with lower critical load wins

- γ_s surface energy : make new crack surface
- γ_{us} unstable stacking fault energy : make dislocations

	LDA	BK-TB	EDIP	SW
c_{11}	166	145	175	162
c_{12}	63.3	84.5	65	82
c_{44}	79.3	53.4	71	60
γ_s (111) ideal	1.7	1.0	1.1	1.4
γ_{us} glide relaxed	1.9	2.5	1.9	3.1
γ_{us} shuffle relaxed	1.7	1.1	1.3	0.8
γ_s/γ_{us} (glide)	0.90	**0.40**	0.59	**0.45**
γ_s/γ_{us} (shuffle)	1.02	**0.90**	**0.85**	1.71

Apparently not Rice criterion

(LDA from Kaxiras and Duesbery, EDIP and SW from Justo *et al.*)

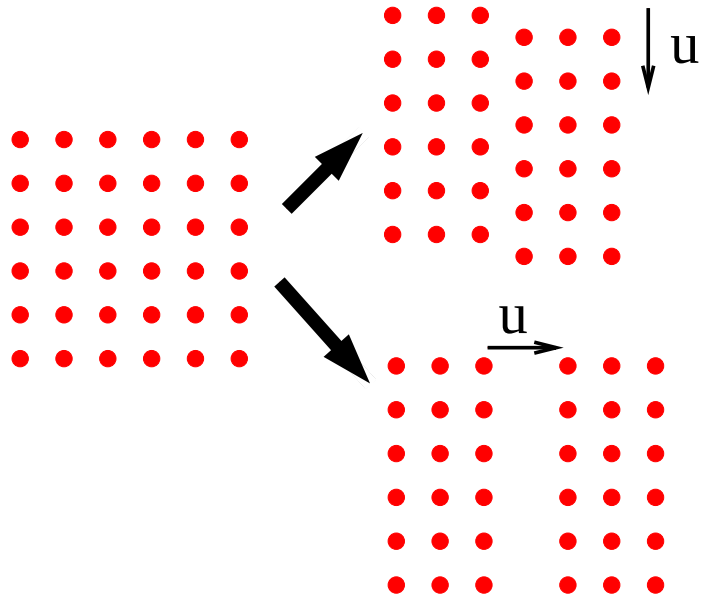
. . . VS. FORCES

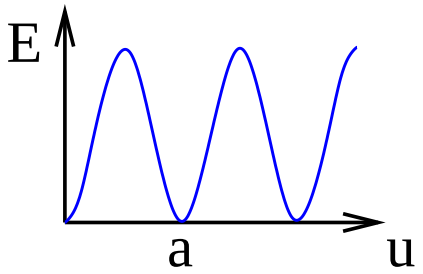
(Abraham, Marder)

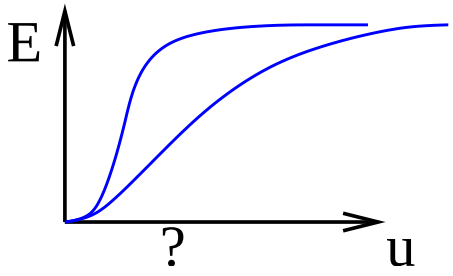
Force depends on energy/distance

Dislocations (γ_{us}): distance set by lattice, same for all models
Surfaces (γ_s): distance set by range of interactions in model

- Determined by physics (covalent vs. Coulomb)
- Restricted by model (DFT vs. empirical potentials)







WHAT CAUSES THE DIFFERENCE?

Energetics: **NO**

- Rice criterion comparable

clue: first failure of EPs (before onset of ductile fracture):

Just above Griffith criterion:

- EP crack won't propagate
- TB crack does

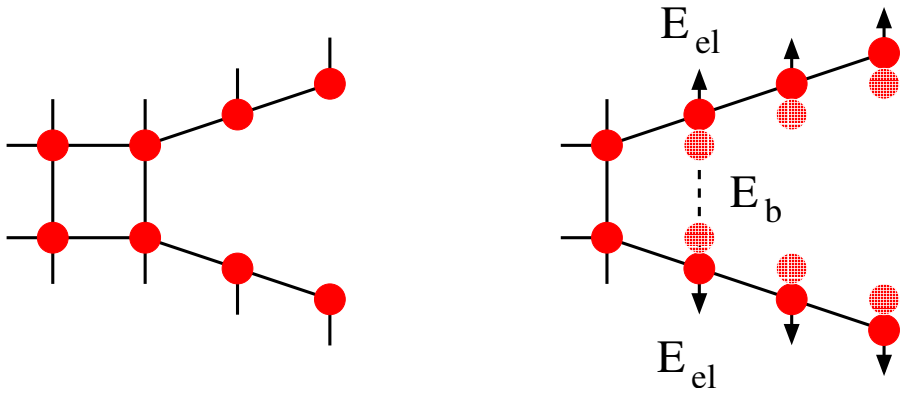
Stress induced lattice trapping:

- Brittle fracture in EP definitely supressed
- Why doesn't this happen in TB?

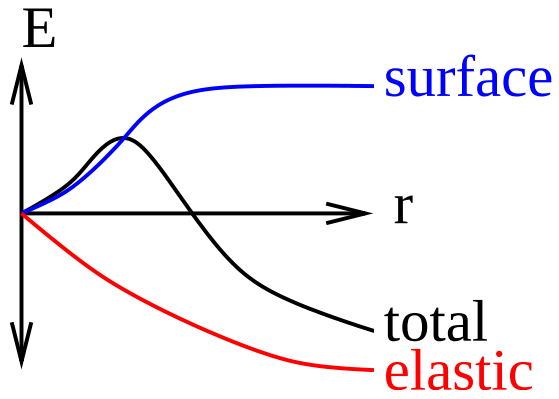
MODEL FOR LATTICE TRAPPING

(Curtin, Gumbsch and Perez)

As crack is propagating forward one lattice spacing:
separate: surface energy (increasing), elastic energy (decreasing)



- Calculate actual energy barrier for propagation (elastic band)
- Subtract decohesion energy (from separation of slabs)
- Extract elastic energy contribution (normalized)



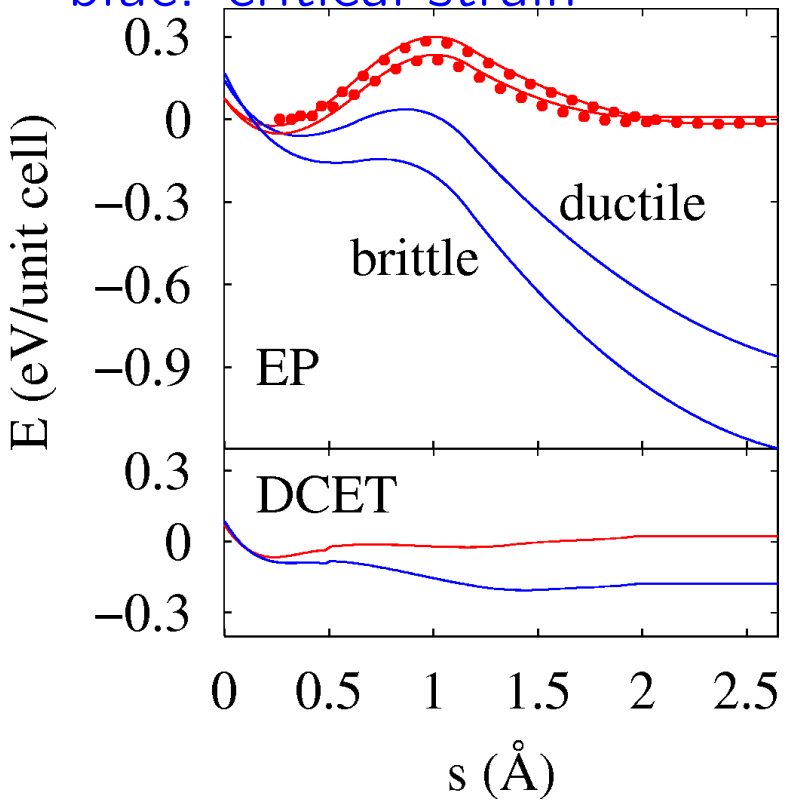
RESULTS OF MODEL

Fit elastic energy to empirical potentials:
Good fit to all EPs after rescaling

Results:

- Energy barrier is apparent
- Brittle models:
  fracture when barrier goes to zero
- Ductile models:
  barrier at dislocation nucleation load

red: Griffith strain
blue: critical strain



Model works – predicts load for onset of brittle fracture
applies to EP and TB

IMPLICATIONS OF MODEL

Separation into elastic energy, decohesion terms works

- bond breaking process is "local"
  i.e. unaffected by strain gradient, asymetry
- (scaled) elastic energy is model independent
  i.e. linear elasticity holds except for crack tip shape

Usual view: one length scale – interaction range

Two length scales

- bond breaking distance (TB 2–3 times larger vs. EP)
- elastic relaxation length (TB 25–40% smaller vs. EP)

Both length scales conspire to reduce barrier for TB

CONCLUSIONS

Concurrent coupling of length scales:
Benefits: combination of accuracy and speed

Insight into fracture mechanics:

- Energies matter
- Energy barriers at crack tip are essential
  - range of interaction
  - detailed shape of crack tip

Future directions

Finite temperature effects

Fracture in more complex, techn. relevant systems (metals?)

Friction and stiction: (NSF NIRT – JHU, Naval Academy)

- Big limitation for MEMS
- Interaction between surface chemistry and mechanical loading