Stressed-Out Metals: Predicting their Response from the Bottom Up

Emily A. Carter
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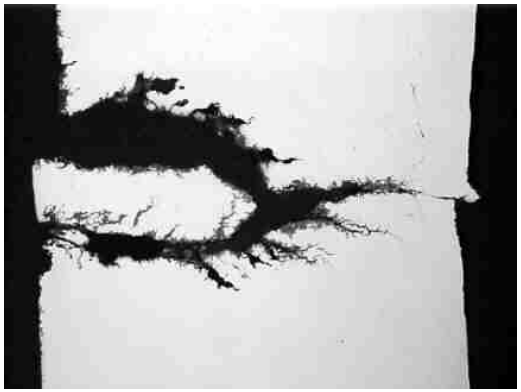
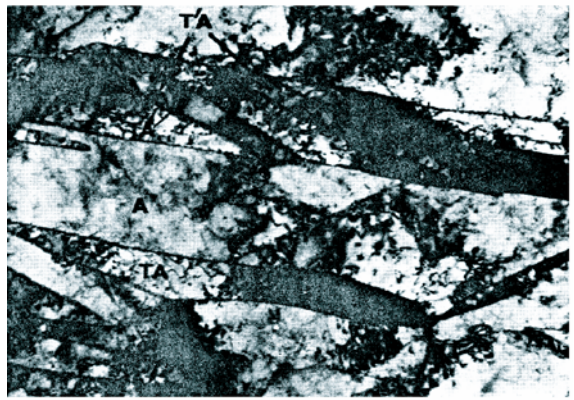




Stress corrosion cracking of steel

Stressed and Embrittled Fe:
Predict **fracture behavior as a function of applied tension and impurity concentration**

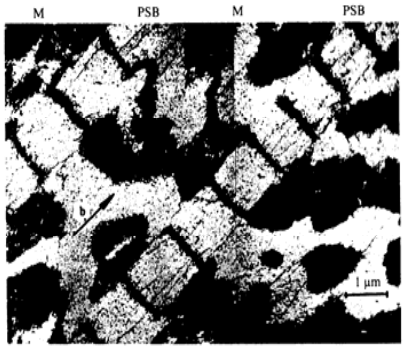
Shocked Fe:
Predict **microstructure and transition pressure as a function of applied compression and shear**

Team: Robin L. Hayes, De-en Jiang, Kyle Caspersen, E. A. Carter (UCLA/Princeton)
Santiago Serebrinsky, Adrian Lew, M. Ortiz (Caltech)
Funding: DoD-MURI, ARO, & DoE-ASCI

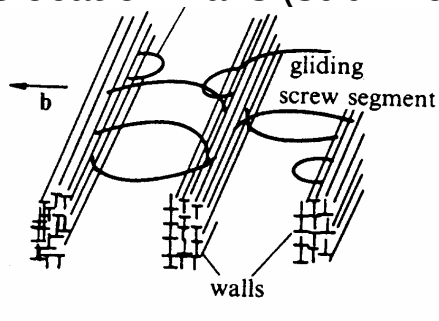
Response of Materials to External Stresses (Chemical or Physical) involves Multiple Length Scales

"Plastic Flow" (~1- 0.1 mm)

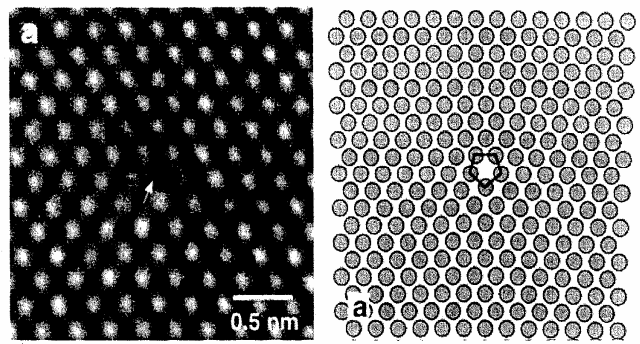
Persistent slip bands (1-10 μ)



Dislocation walls (sub-micron)



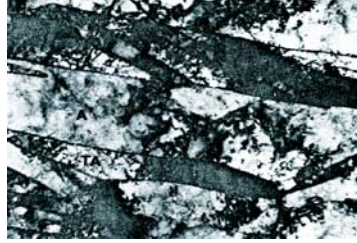
Atomic dislocation structure (Å)



- Difficult and expensive to measure
- Simulations only as reliable as assumed physical laws and input parameters…

Goal: *predictive* tools for insight into materials behavior and ultimately design…
Requires input from lower scales down to atoms/electrons…

Challenges for Quantum-Mechanics-Based Multiscale Modeling



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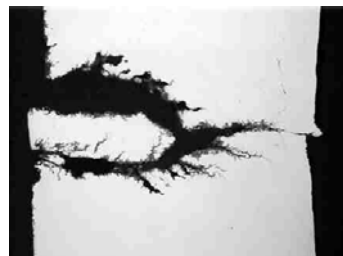
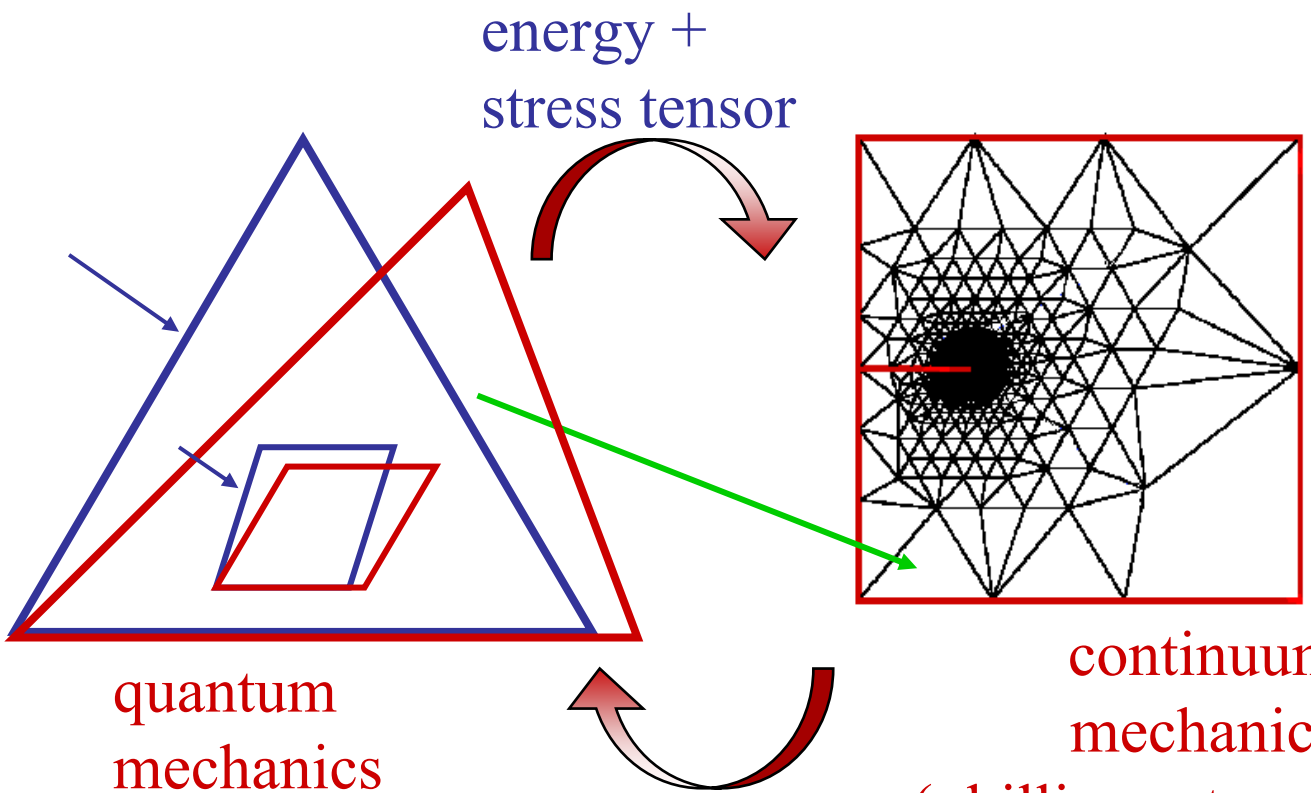
- **Stressed Al:**
  Predict **onset of plasticity during nanoindentation via on-the-fly coupling of orbital-free density functional theory to the local quasicontinuum method**
  (Hayes, Fago, Ortiz, and EAC, PRB, 2004; MMS, in press)
- **Ductile Fracture of Al under Shock:**
  Predict **kinetics of vacancy coalescence, void formation, and spall via orbital-free DFT rates coupled to kinetic Monte Carlo simulations**
  (Ong, Serebrinsky, Caspersen, Ho, Ortiz, and EAC)
- **Shocked Fe:**
  Predict **microstructure as a function of applied compression and shear via quantum-mechanically-informed sequential lamination model**
  (Caspersen, Lew, Ortiz, and EAC, PRL, 2004)
- **Stressed and Embrittled Fe:**
  Predict **fracture behavior as a function of applied tension and impurity concentration via quantum-mechanically-informed cohesive zone model (Serebrinsky, Jiang, Hayes, Ortiz, and EAC, PRB, 2004; Acta Materialia, 2004; JMPS, 2004)**



Funding: DoD-MURI, ARO, & DoE-ASCI

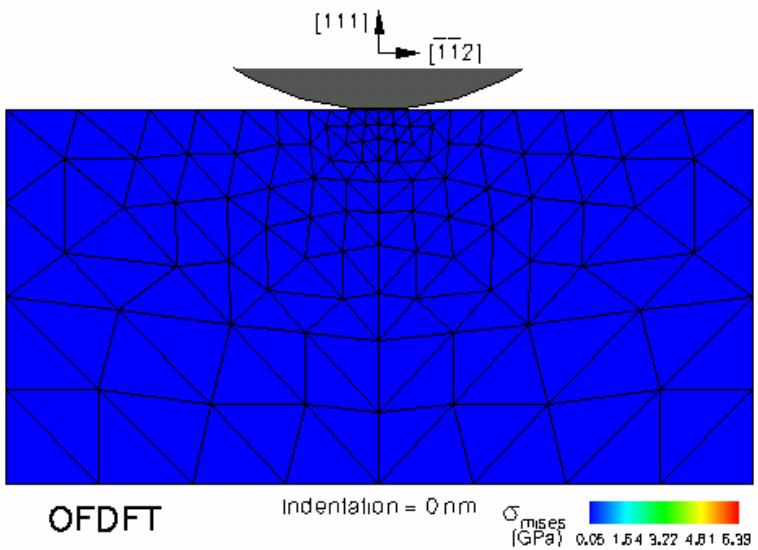
Quantum Mechanics and Local Quasicontinuum Coupling

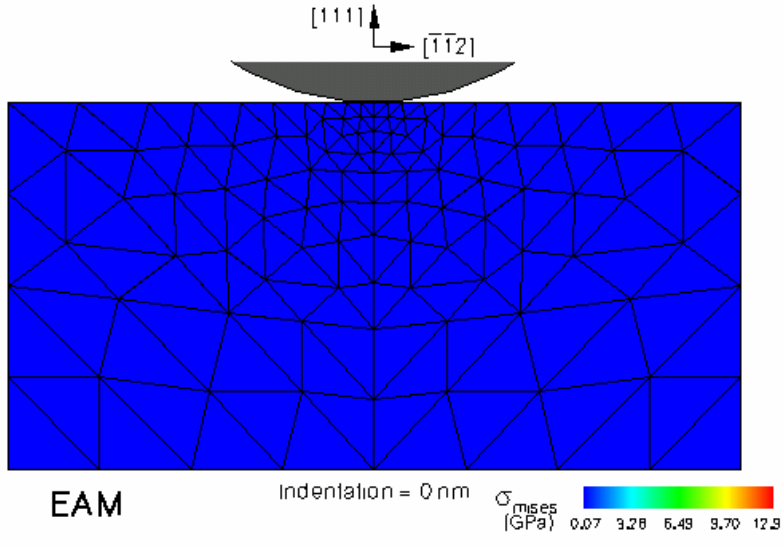
Quantum-derived stress tensor for representative unit cells
↳ stress on nodes in each finite element



Hayes, Fago, Ortiz, EAC, PRB 04

Comparison OFDFT-LQC to EAM-LQC for Nanoindentation of Al(111) for identification of first dislocation





Dislocation location and orientation completely different between the two models…

Fago, Hayes, et al. PRB 2004

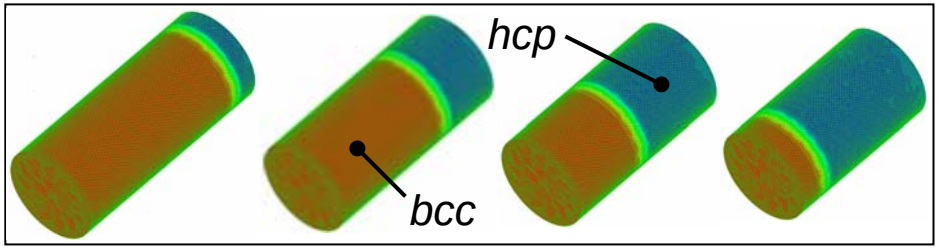
- *OFDFT-LQC provides an efficient on-the-fly coupling between quantum and continuum mechanics*

- Current Challenges:
  - generality and accuracy of OFDFT
  - Nature of quantum wave functions => difficult to extend LQC to nonlocal QC

- Current Approaches:
  - Bulk-derived LPSs for all elements
  - KEDFs based on real material (interacting electron) response functions
  - Multigrid real space OFDFT with density matching boundary conditions…

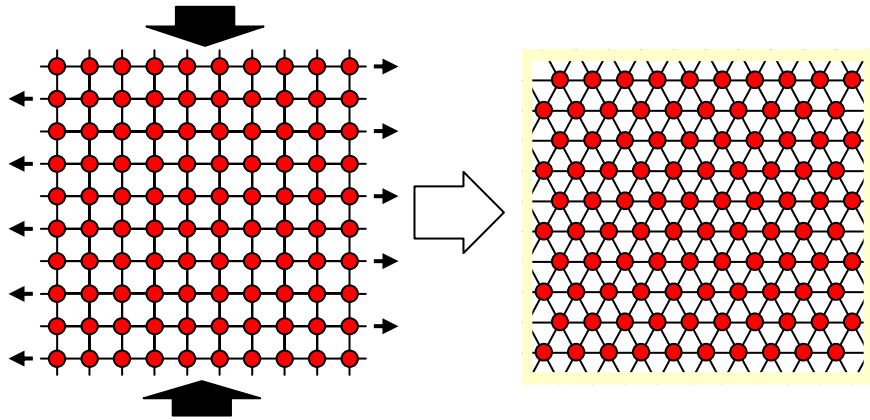
  => *fully nonlocal QC for any material someday…*

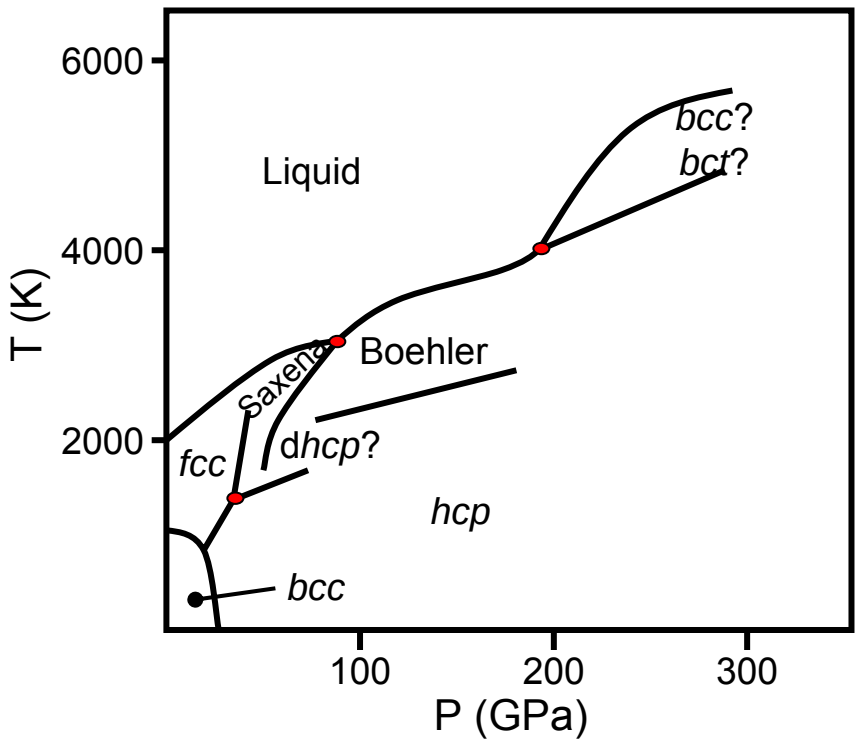
Shocked Iron



Ground state *bcc* undergoes a martensitic phase transformation to *hcp* at ~13 GPa.

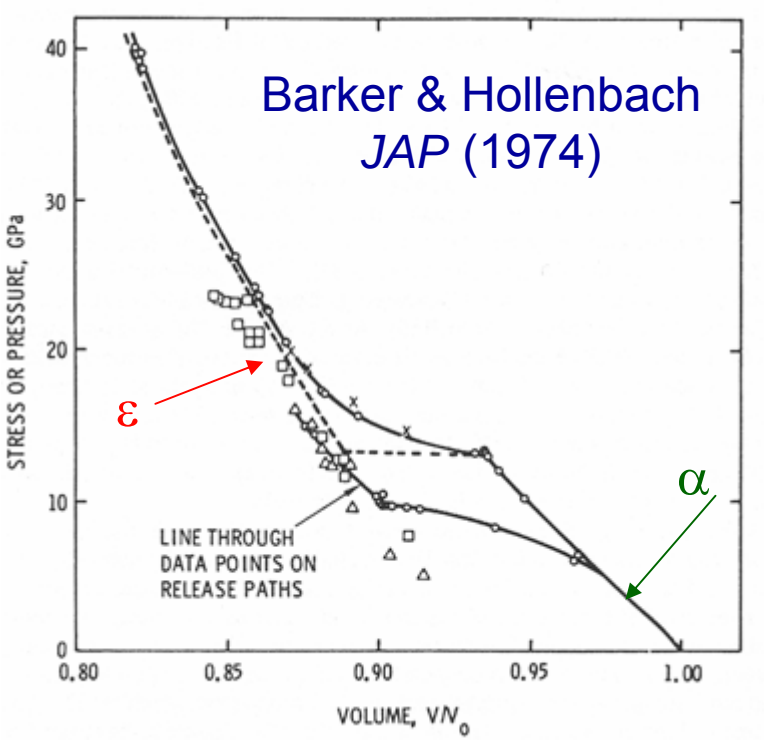
Strong shocks induce phase transitions involving complicated microstructures.





The transformation displays considerable hysteresis and a large range of transition pressures.

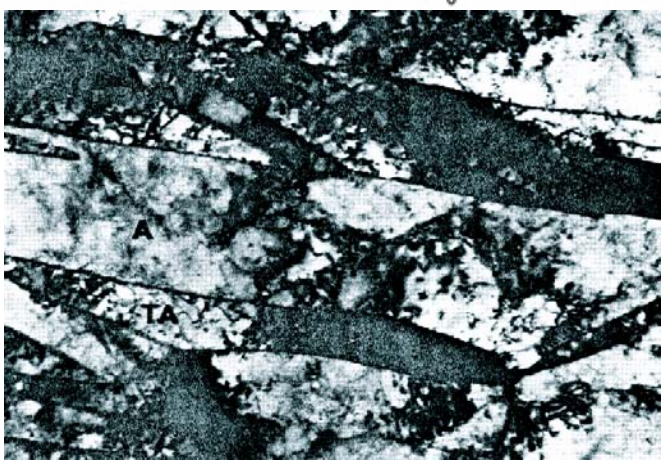
Shock Hugoniot and Microstructure of α-Iron



Hysteresis loop observed in P-V curve: bcc (α) transforms to hcp (ε) at higher pressure than reverse…

G. Ravichandran et al., 2004

Laminate microstructure observed in shocked Fe

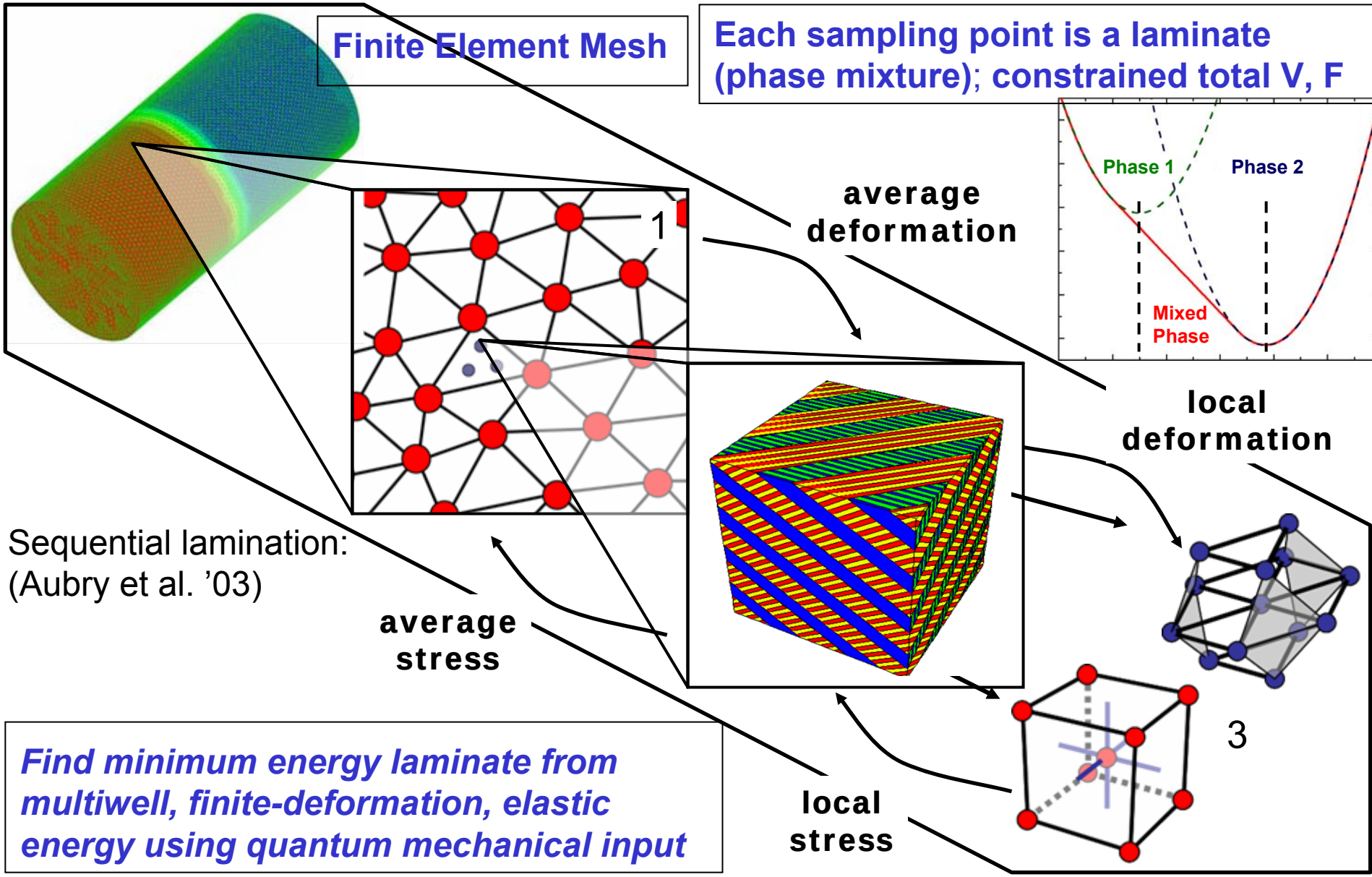


Bowden and Kelly, 1967

GOALS:

- *Understand* the origin of the hysteresis and experimental scatter in transition pressures.
- *Predict* detailed microstructures.

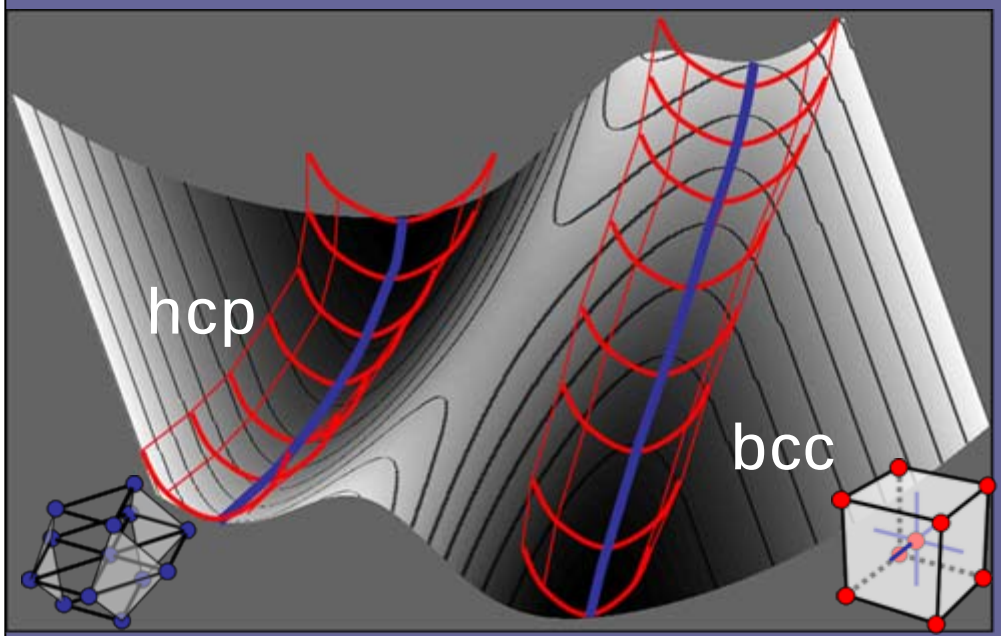
Multiscale Iron Model: on-the-fly Microstructures



Energy Approximation for Each Phase

Too expensive to calculate from first principles on the fly. Instead construct non-linear elastic energy using input from QM.

Must assume each deformed variant at given volume "close" to the minimum energy deformation for that volume.



iso-volume manifolds

transformation strains at different volumes

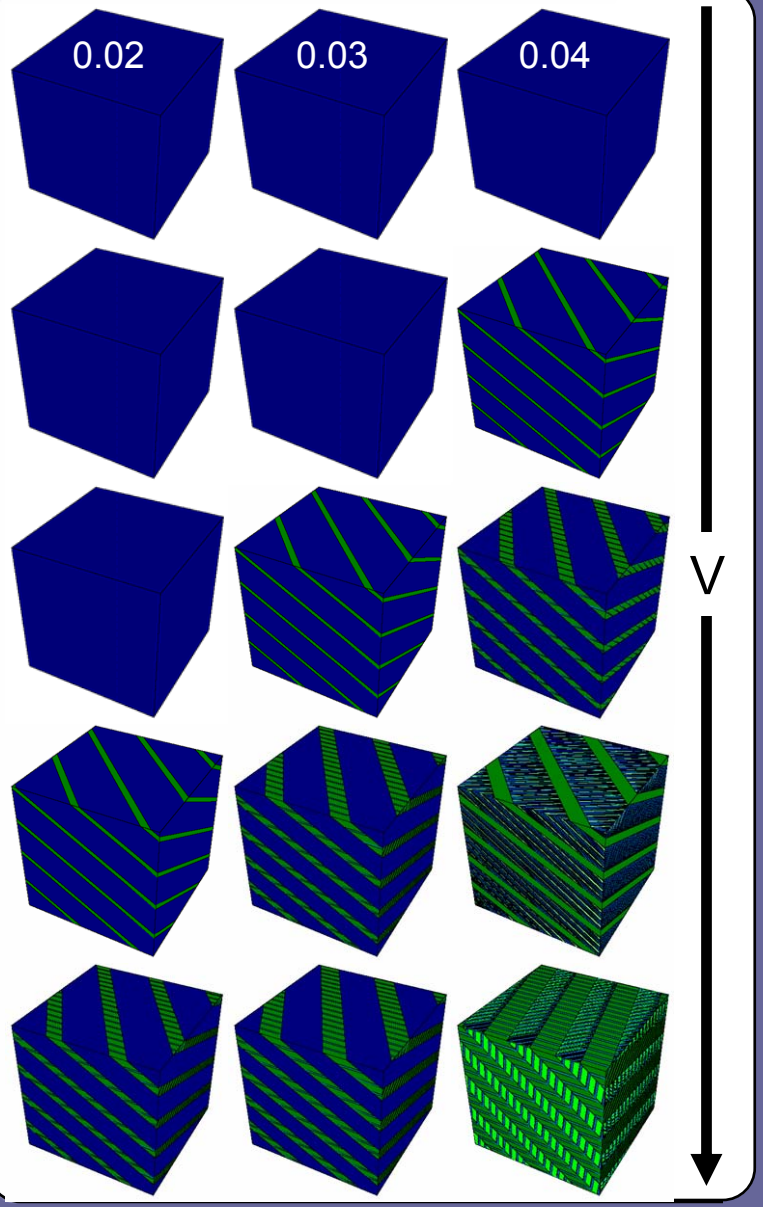
Approximate by expanding around minimum energy deformation at each volume.

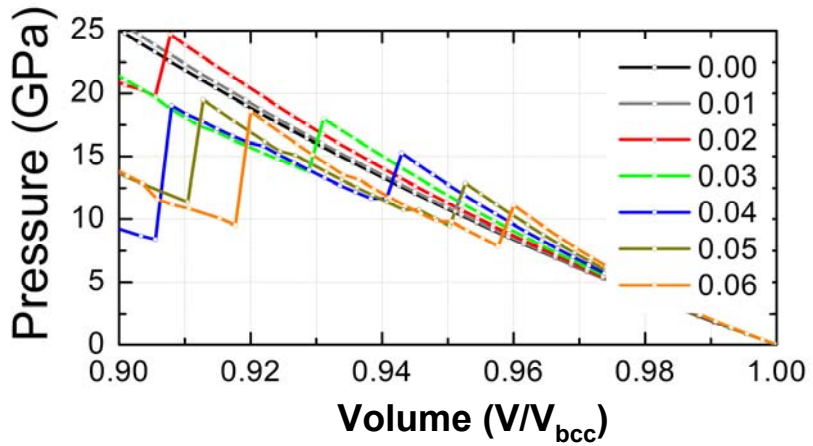
$$E(\varepsilon, V) = E_0(V) + (\varepsilon - \varepsilon_0(V))^T \lambda_V (\varepsilon - \varepsilon_0(V))$$

λ_V =Elastic Constants at volume V

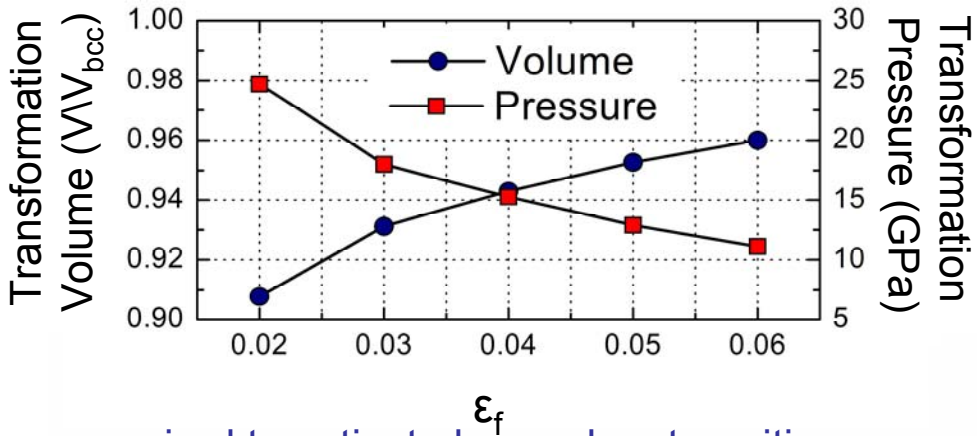
ε_0= Equilibrium Strain at volume V

Role of Shear





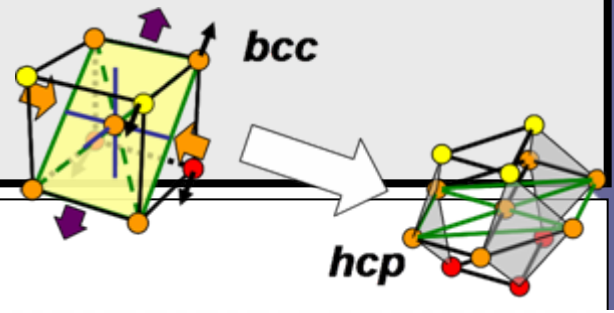
P-V discontinuities indicate laminate formation



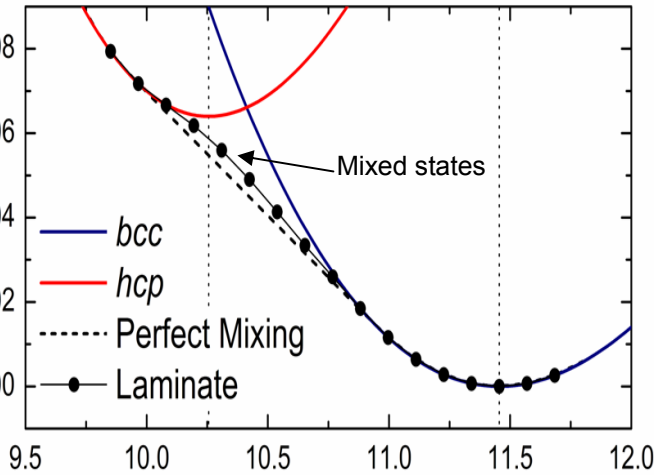
- shear required to activate bcc → hcp transition
- increasing shear lowers the TP and increases the TV
- Range in measured TPs likely due to varying amounts of shear in experiments

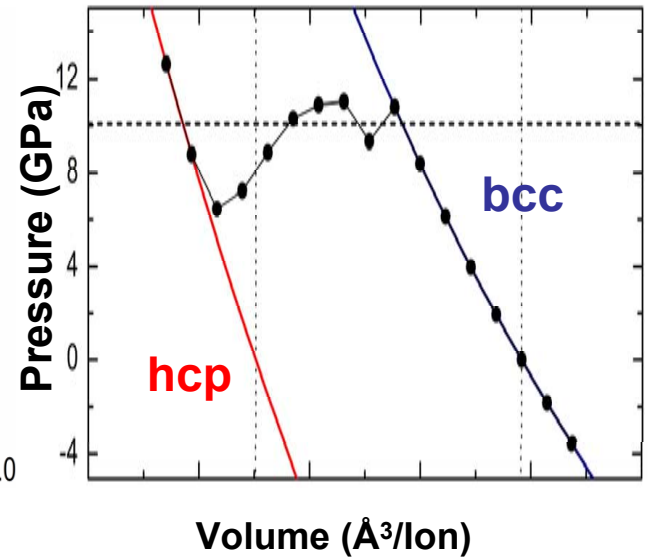
bcc → *hcp* minimum energy transition path

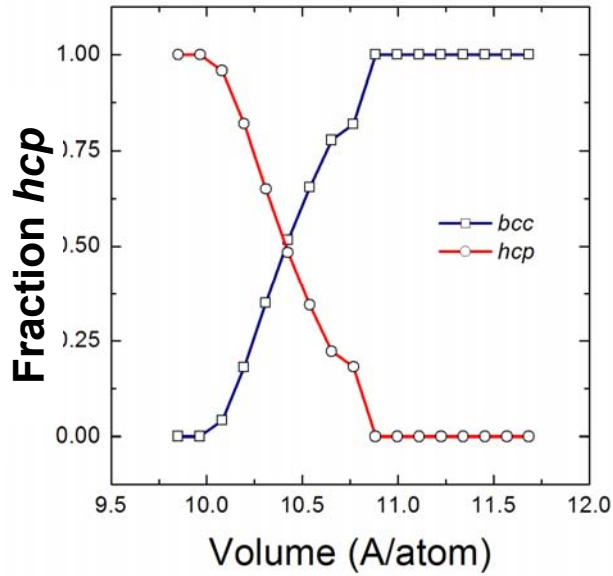
(K. Caspersen, et al. PRL, 2004)



- compression normal to (100)
- elongation along (110)
- shuffle (110) layers

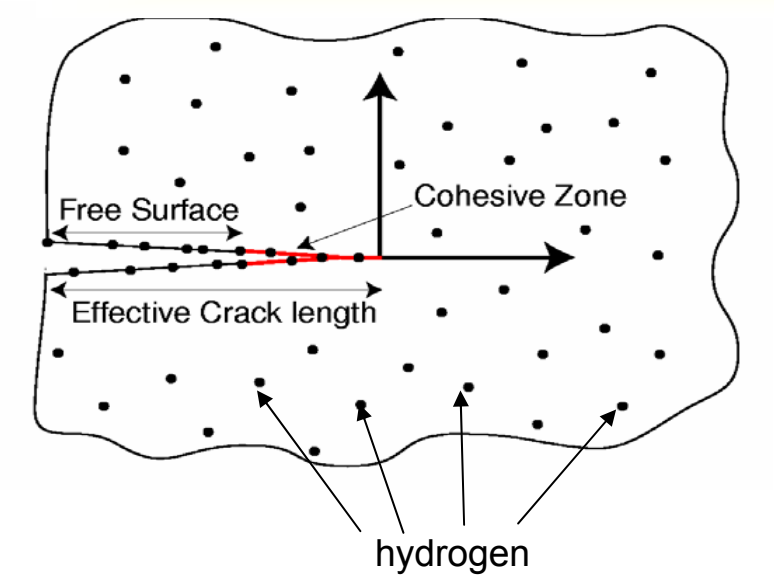


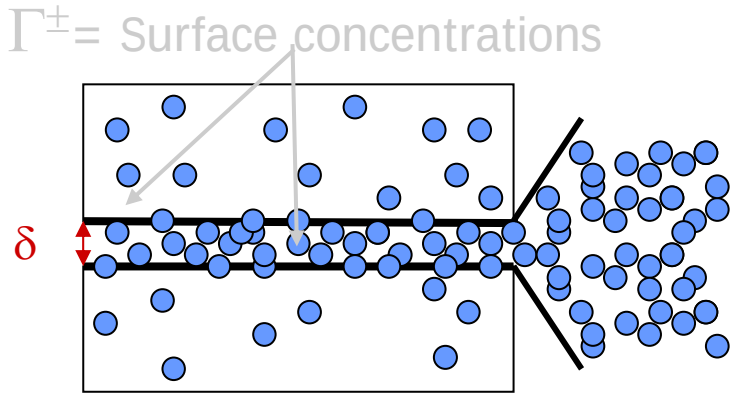




- Inclusion of laminates allows energy to decrease, exhibiting mixed states
- Higher energy than Gibbs construction (line of common tangent) due to real constraints on laminate formation (kinematic compatibility)
- Transition pressure consistent with measured values
- The sample transforms to hcp at ~10 GPa, while upon decompression, the transition to pure bcc occurs at ~5 GPa => ~5 GPa measured pressure hysteresis may be due to kinematic constraints of microstructure

Hydrogen Embrittlement in Steel: Multiscale Decohesion Model



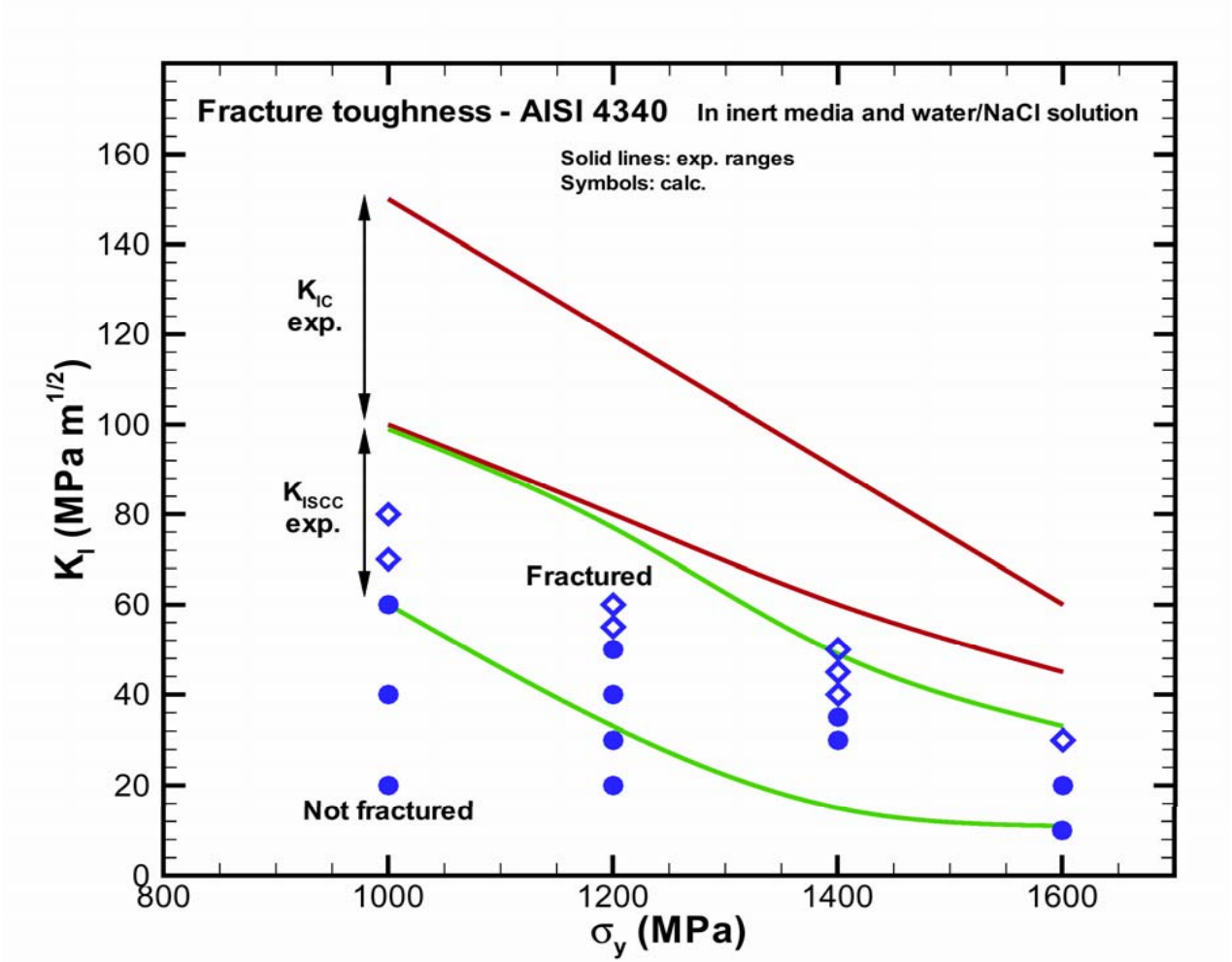


Schematic of interface/impurity system
(Rice & Wang, 1989)

Stress-assisted impurity diffusion coupled to continuum elasticity, plasticity, & cohesive zone fracture mechanics with quantum-based cohesive laws

Serebrinsky, Carter, Ortiz, J. Mech. Phys. Solids, 2004

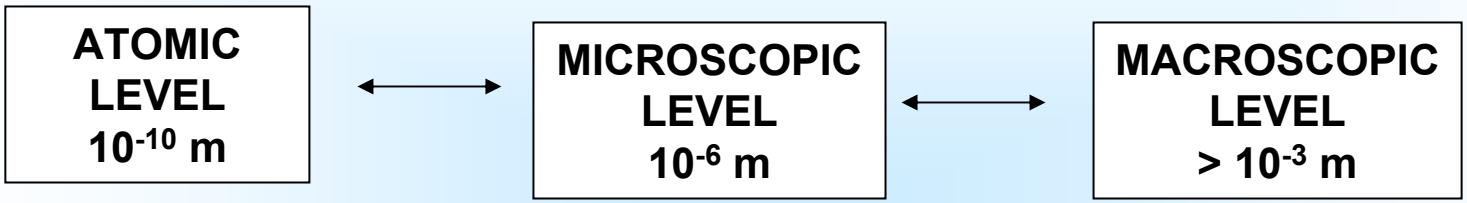
For various forms of steel, the model predicts stress corrosion cracking thresholds within known experimental bounds…



Hydrogen-induced decohesion mechanism consistent with experimental data.

CHALLENGES FOR ALL OF US

- How to get to long time scales (fs -> min)
- Seamless spatial integration across scales



- Statistics in *ab initio* Molecular Dynamics and its brethren
- Accuracy inversely proportional to size in Quantum Mechanics
- Cheap, yet accurate force fields
- Portability/Distributability of codes across networks/foreign platforms written in Fortran 77/90, C, C++ . . .

BRIDGING TIME SCALES

- Variable/Multiple MD time step methods (Schlick, Tuckerman, etc.) – **doesn't get to truly long times**
- Rare event dynamics (Bennett, Chandler, etc.) – **must know TS:**
  - Umbrella sampling (Valleau,Tully, etc.)
  - Blue moon ensemble (Carter, Ciccotti, Hynes, Kapral)
- Accelerated Dynamics (Voter) – **no need of TS/final state:**
  - hyperdynamics (**TST**), parallel replica dynamics (**$E_a \sim kT$**)
  - temperature accelerated dynamics (**requires long trajectories before payoff, obeys TST**)
- Path Dynamics (Elber) – **need initial/final states**
- Ensemble Dynamics, Patch Dynamics (Deuflhard, Kevrekidis) – **only probabilities (Deuflhard) & extrapolations**

Unfortunately, no general method for getting to long times yet, with accurate forces, without prior knowledge or assumptions, for specific trajectories (to look at single molecule behavior, for example)…

Open Issues in Multiscale Simulation

- Connections between scales
  - heat conduction, mass transfer
  - sequential input or on-the-fly
  - feedback
- Optimal algorithms
- Uncertainty Management
- Model Validation

  atomic behavior => macroscopic properties
- Unifying mathematical theory
- Bridging time scales beyond transition state theory…
- From materials to biology…