Prediction and Multiscale Modeling of Corrosion and Wear

M. Ortiz
California Institute of Technology
In collaboration with E.A. Carter
(Princeton University)

Opening plenary lecture given at the
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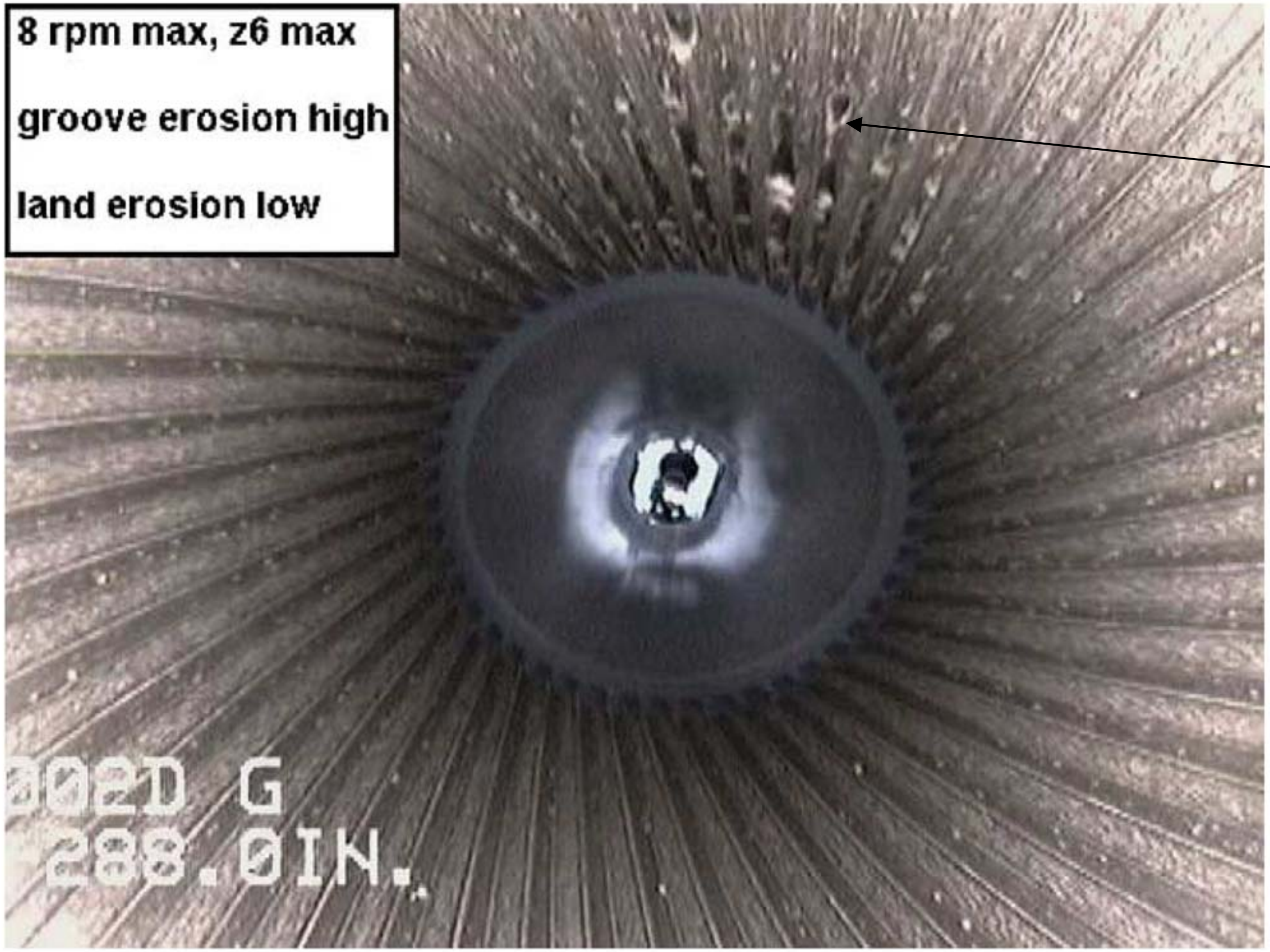
Gun-bore erosion in artillery systems

Gun-bore erosion in artillery systems



pitting

Typical 360◦ magnifying borescope micrograph of LCCr/ 8 rpm/zone six charge-related second-quarter-life land and groove erosion near the bore origin (Sopoka, Rickarda and Dunn, *Wear* **258**:2005, 659–670)

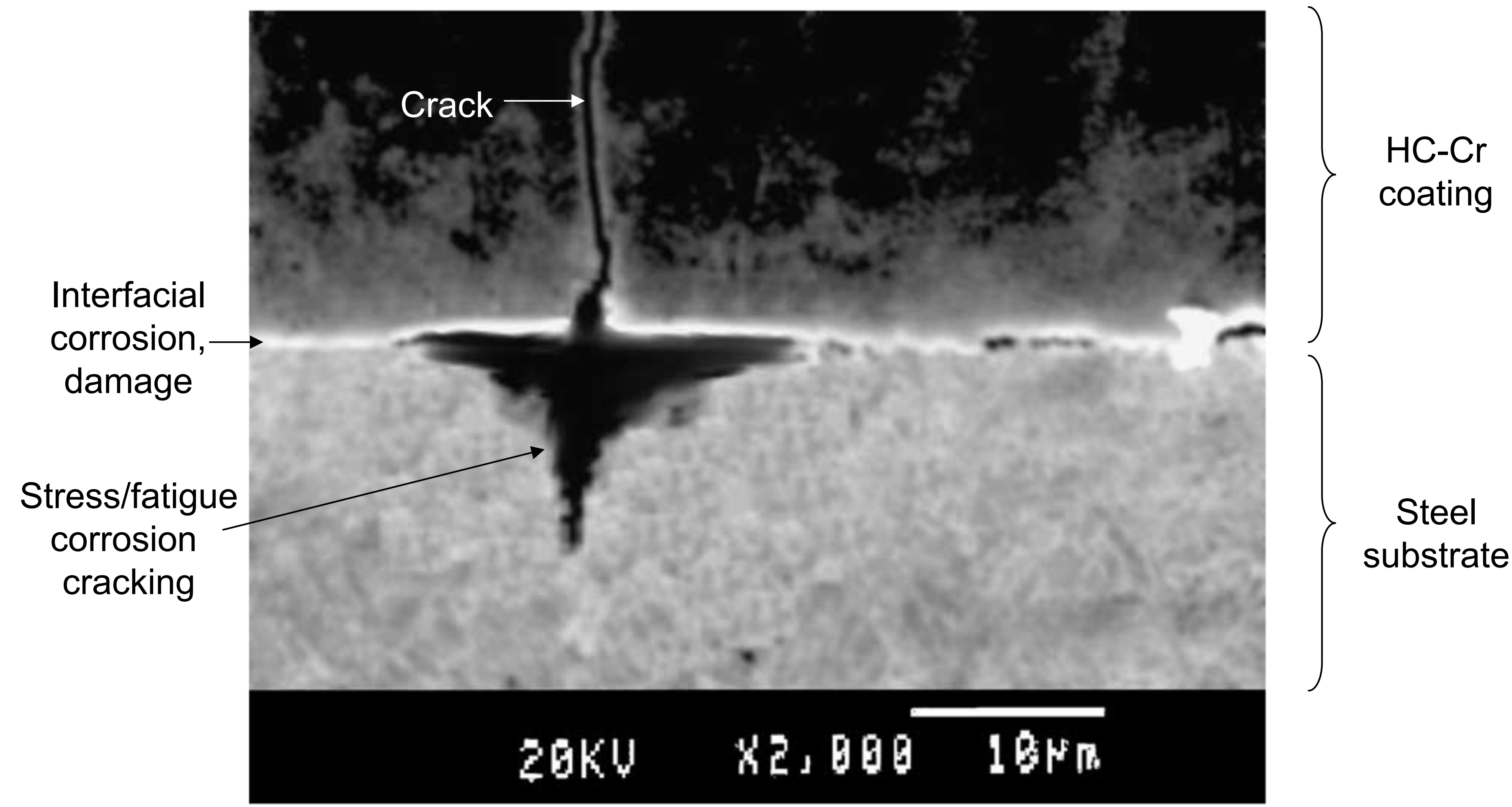
Gun-bore erosion in artillery systems

Land erosion

Groove erosion

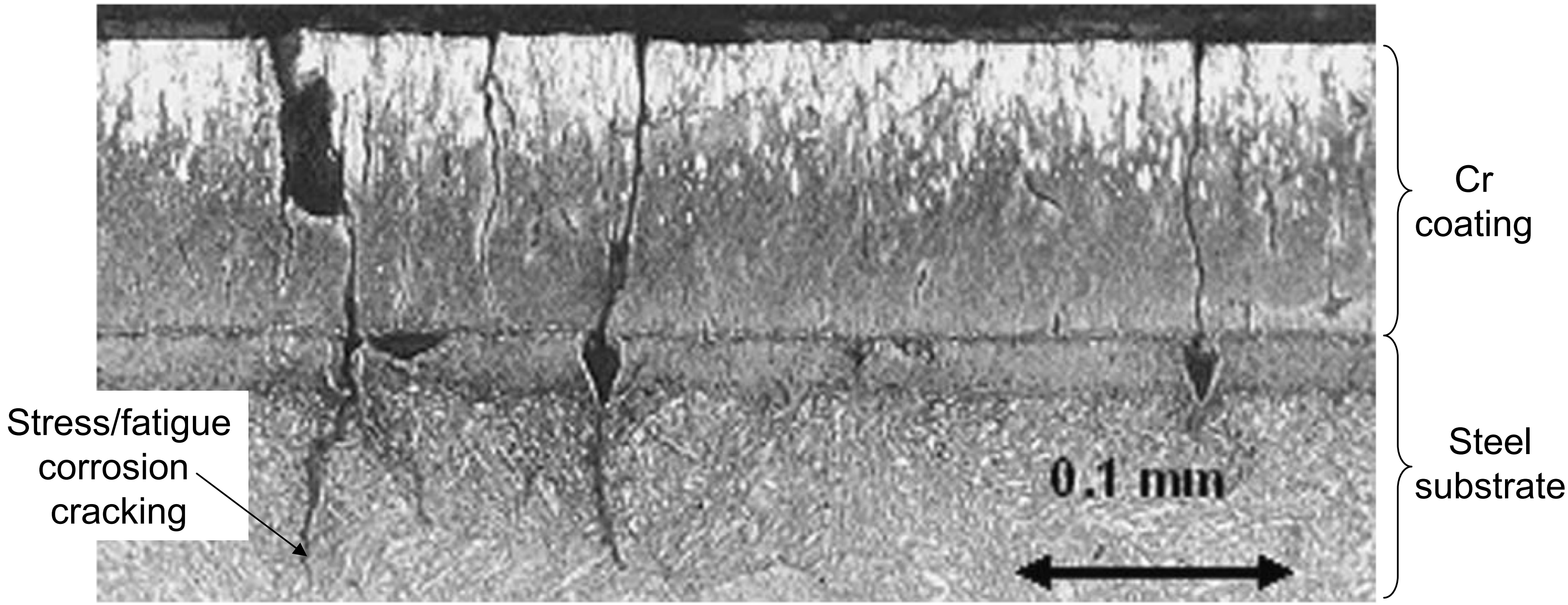
Typical magnifying borescope micrograph of HC-Cr/1 rph/zone six charge related midlife erosion at the 12:00 bore origin.
(Sopoka, Rickarda and Dunn, *Wear* **258**:2005, 659–670)

Gun-bore erosion in artillery systems



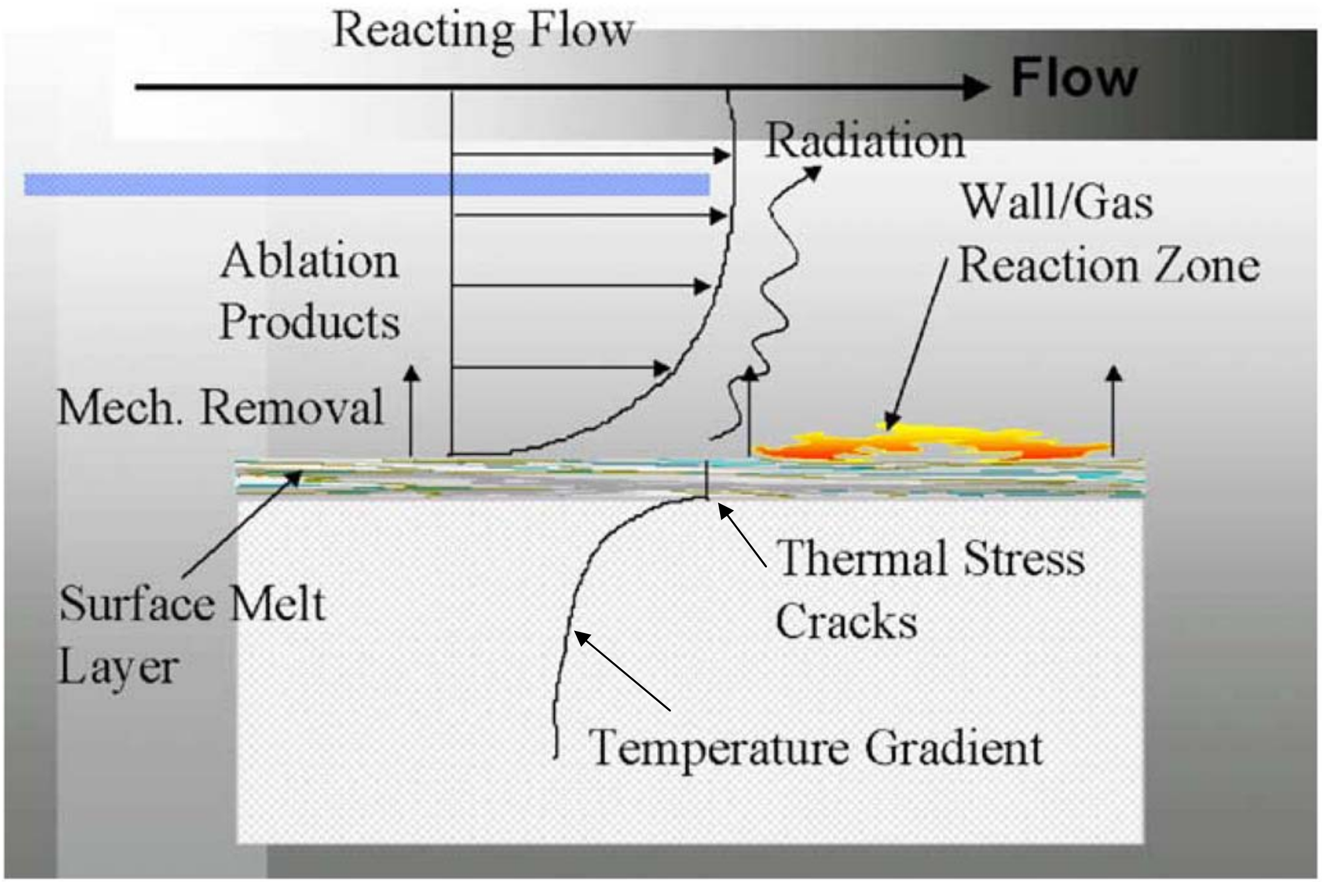
Typical SEM cross-sectional micrograph of HC-Cr/zone six charge related of land and groove substrate erosion through a micro-crack at the 12:00 bore origin (Sopoka, Rickarda and Dunn, *Wear* **258**:2005, 659–670)

Gun-bore erosion in artillery systems



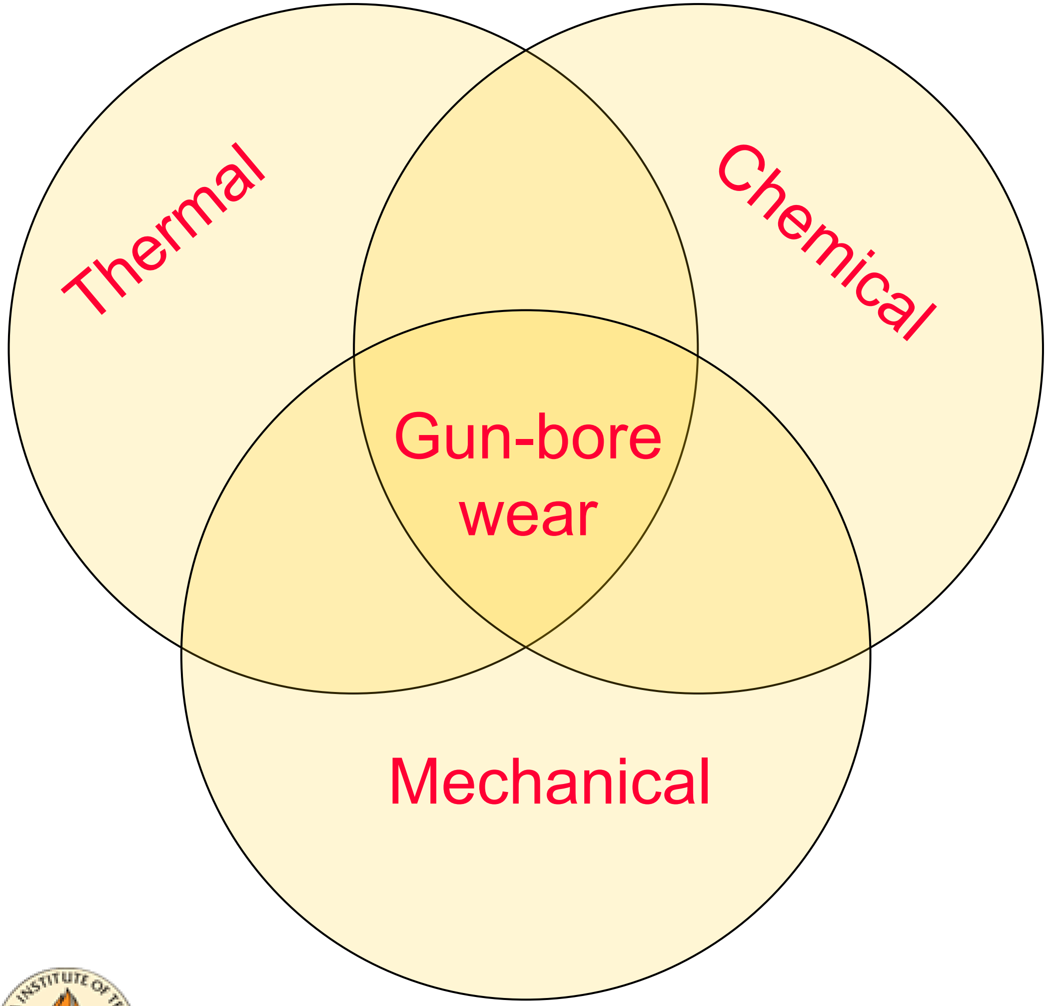
Metallographic section of the electroplated Cr-on-steel 120 mm tube following 118 cannon firings (Underwood, Vigilante, Mulligan and Todaro, *ASME Trans.* **128**:2006, 168–172)

Gun-bore erosion in artillery systems



General schematic of the thermal–chemical–mechanical erosion mechanisms (Sopoka, Rickarda and Dunn, *Wear* **258**:2005, 659–670)

Gun-bore erosion in artillery systems



- Gun-bore wear involves the simultaneous operation of three factors:
  - *Thermal: heating, thermal gradient, thermal stress cracks, radiation, surface melting.*
  - *Chemical: reacting flow, gas-wall reactions, corrosion.*
  - *Mechanical: cracking, ablation, spallation.*
- resulting in:
  - *Micro and macro-pitting.*
  - *Condemnation.*

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The larger picture: Model-based certification

- Ultimate objective: **Certification** of complex systems by a rigorous quantification of design **margins** and performance **uncertainties**
- Performance of complex systems is difficult to quantify based on testing alone
- Model-based certification: Develop physics-based, high-fidelity models enabling rigorous quantification of performance uncertainties with a small number of tests
- System behavior often occurs on multiple length and time scales, requiring multiscale modeling
- Ultimate goal: Knob-free (first-principles) predictive simulation.

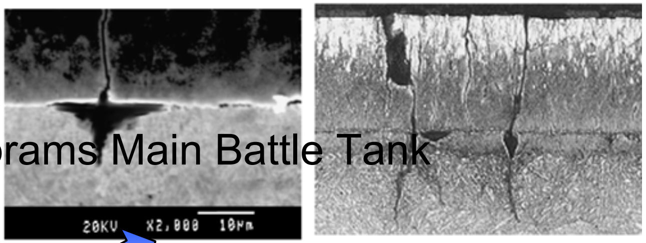
Wear – Multiscale modeling

Sopoka *et al.*, *Wear,* **258**, 659 (2005)
Gaudett a& Scully, *Metall. Mat. Trans.*, **25**, 775 (1994)
Wang et al., *Phys. Rev. B*, **68**, 224101 (2003)
Yamaguchi *et al.*, *Science*, **309**, 393 (2005)
Jiang and Carter, *Phys. Rev. B*, **70**, 064102 (2004)

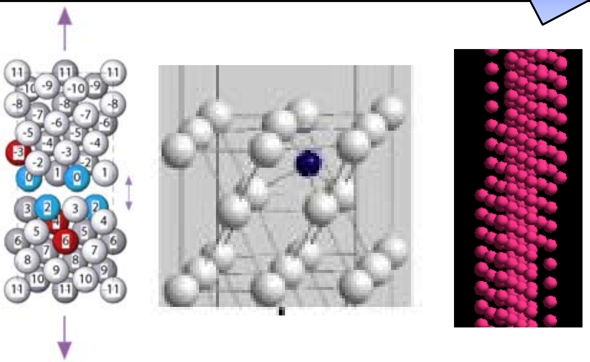
M1 Abrams

Macroscale:
- wear rates
- life assessment
- certification

Mesoscale:
- plasticity
- diffusion
- fracture



M1 Abrams Main Battle Tank



Nanoscale:
- impurity absorption, mobility
- grain-boundary decohesion
- lattice defects, dislocations
- chemical reactions

time: ns, μs, ms

length: nm, μm, mm

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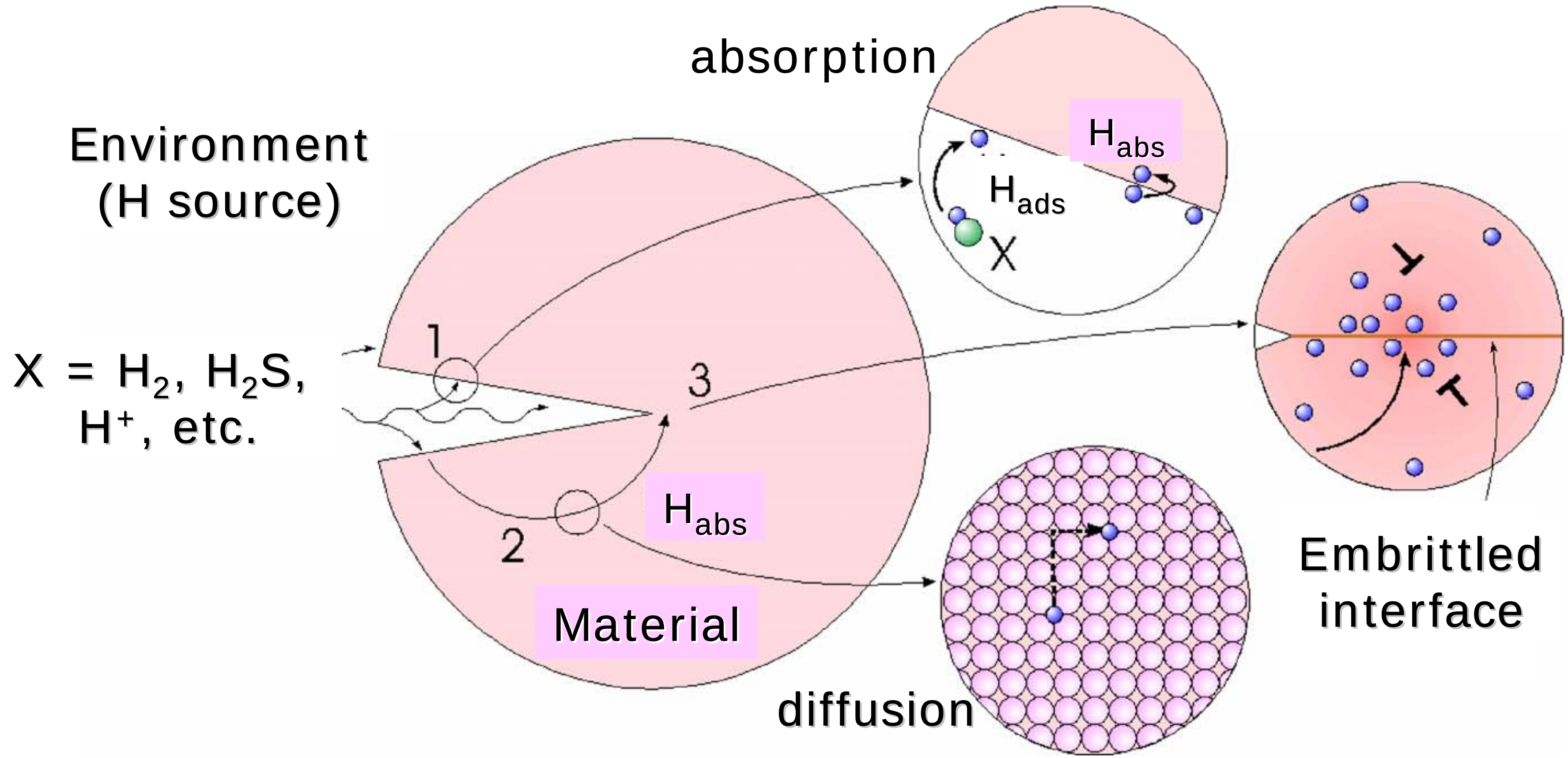
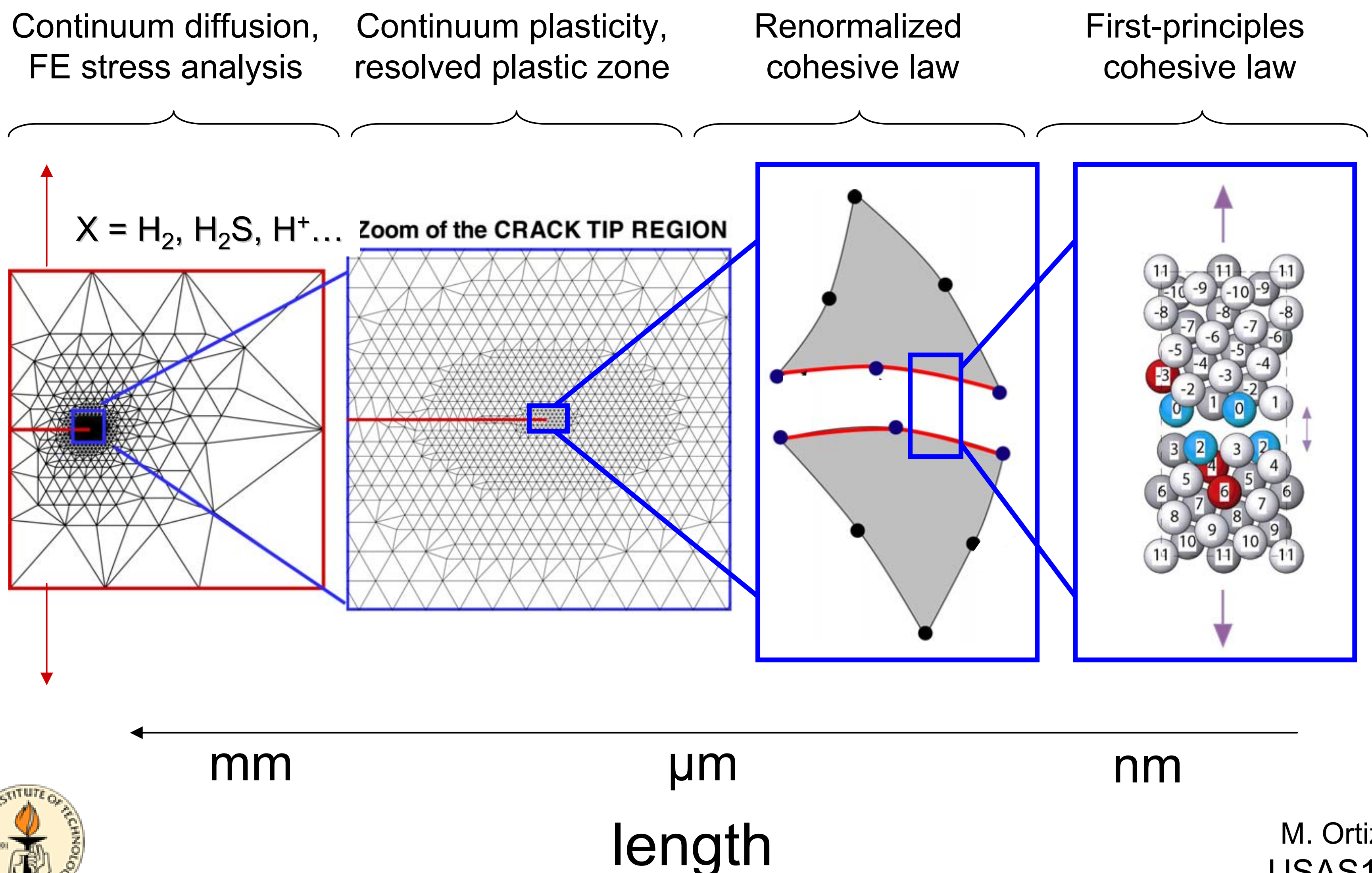
Model problem – Hydrogen embrittlement



- Possible mechanisms for step 3:
  - ***Hydrogen-enhanced decohesion (HED)***
  - *Hydrogen-enhanced localized plasticity (HELP)*
  - *Hydrogen-related phase changes (HRPC)*

HE – Multiscale model



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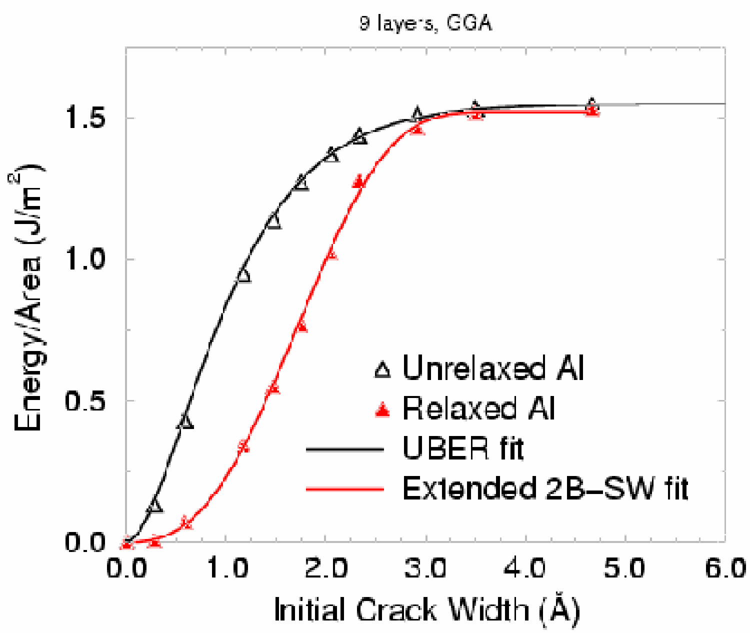
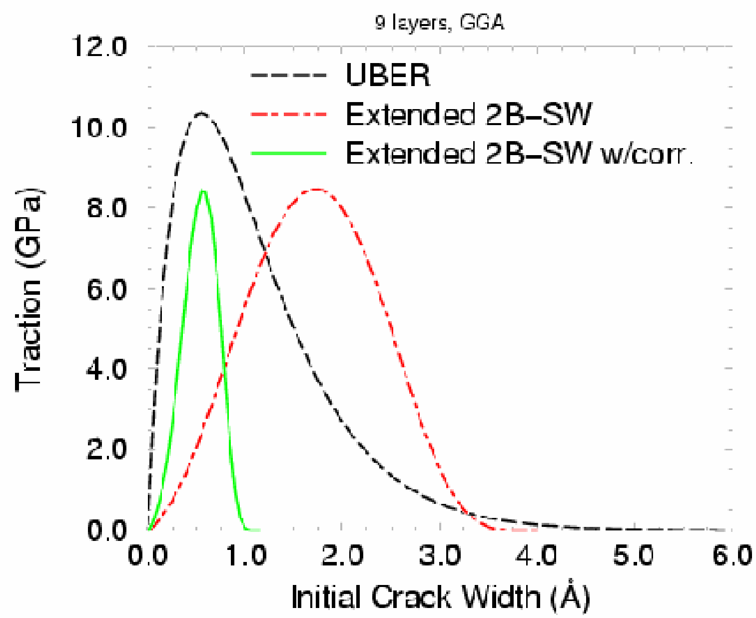
Cohesive laws – First principles

$$t = \frac{\partial \phi}{\partial \delta}$$

(111) fcc Al



(111) fcc Al

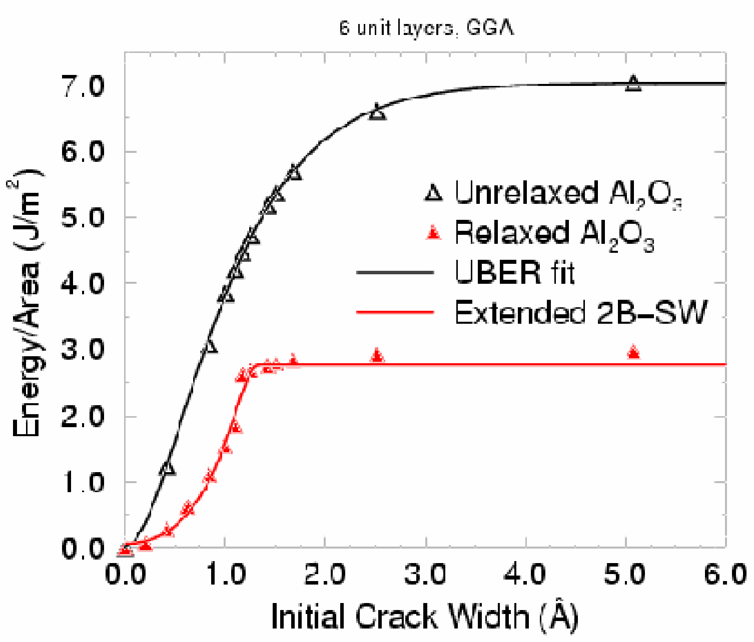


Jarvis, Hayes and Carter, *Chem. Phys. Chem.*, **1** (2001) 55.

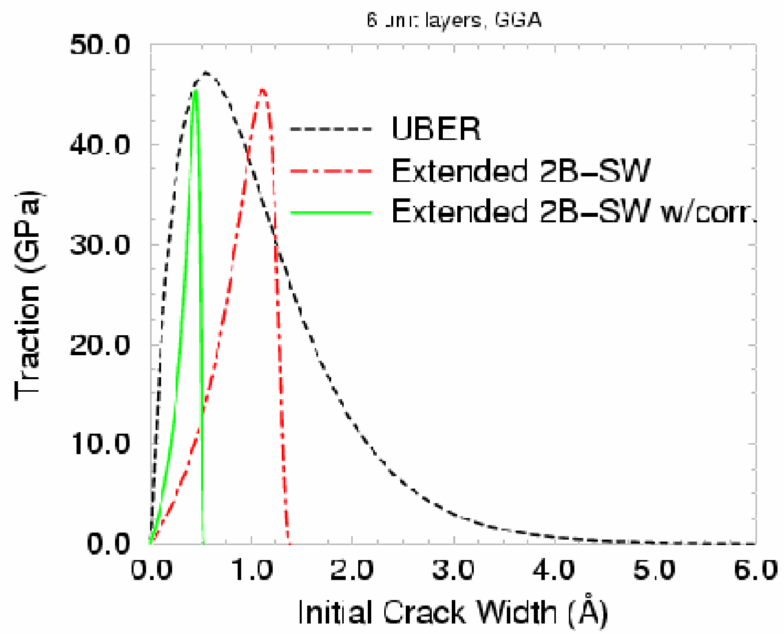
Cohesive laws – – First principles

$$t = \frac{\partial \phi}{\partial \delta}$$

(0001) Al_2O_3



(0001) Al_2O_3

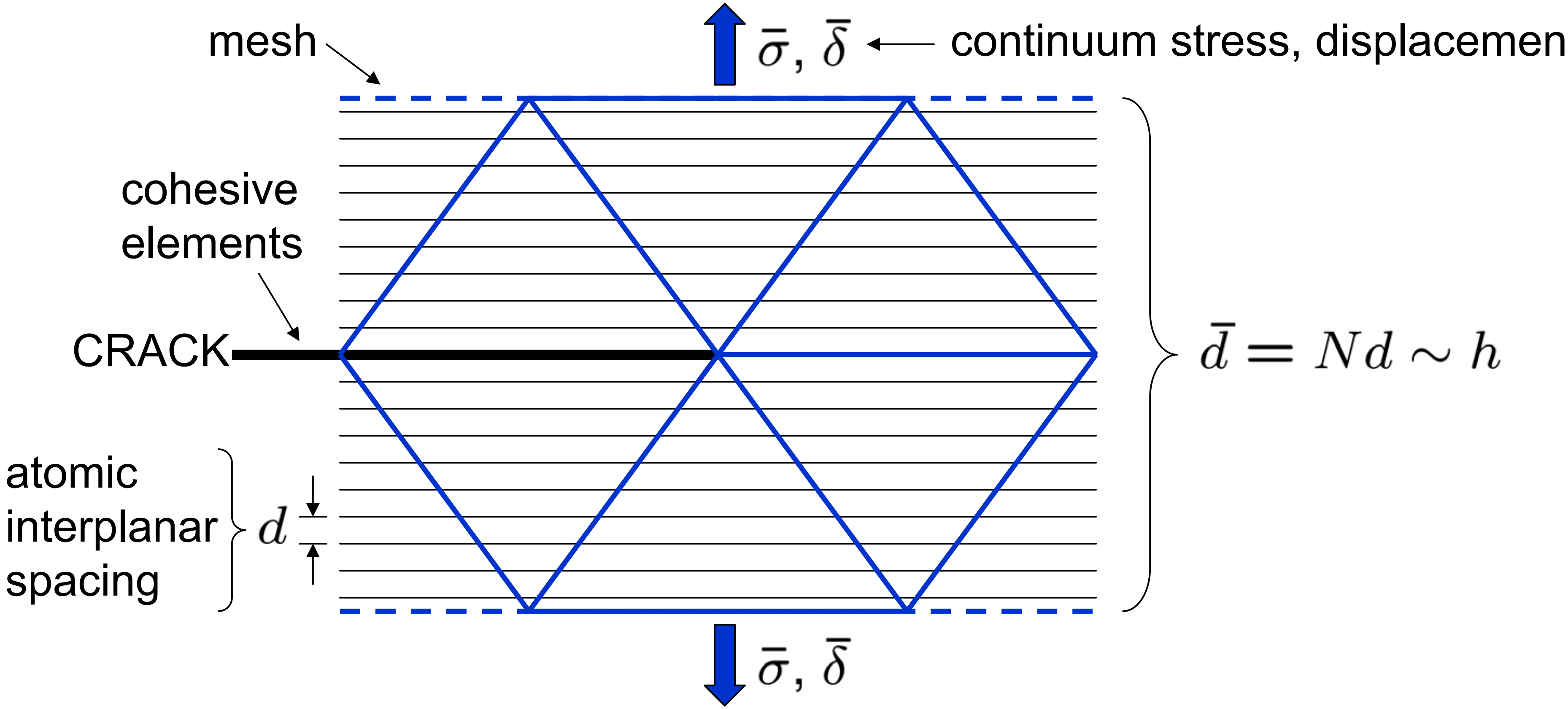


Jarvis, Hayes and Carter, *Chem. Phys. Chem.*, **1** (2001) 55.

Cohesive laws – First principles

- Ab initio cohesive laws:
  - *Peak stress ~ theoretical strength*
  - *Critical opening displacement ~ atomic lattice spacing*
  - *Critical energy release rate ~ Relaxed surface energy*
  - *Cohesive length ~ atomic lattice spacing*
  - *Mesh resolution requirement ~ atomic lattice spacing*
- Continuum stresses limited by yield stress, mesh size
- Cannot embed first-principles cohesive laws directly in continuum calculations
- Must upscale (coarse-grain, renormalize) the first-principles cohesive law to continuum scale

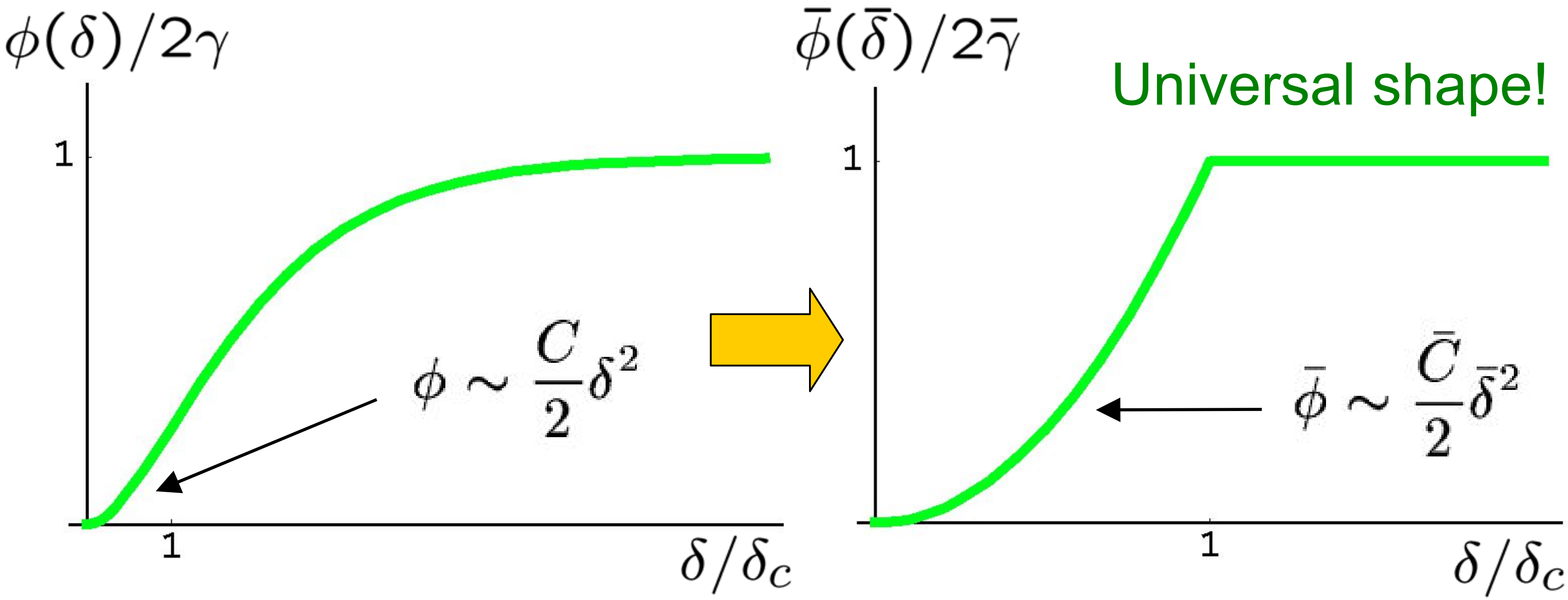
Cohesive laws – Upscaling



- Effective (upscaled) cohesive law:
  - *N interatomic planes, first-principles cohesive law*
  - *Rice-Beltz elastic correction*

Cohesive law – Upscaling

Ab-initio cohesive law — Renormalized cohesive law

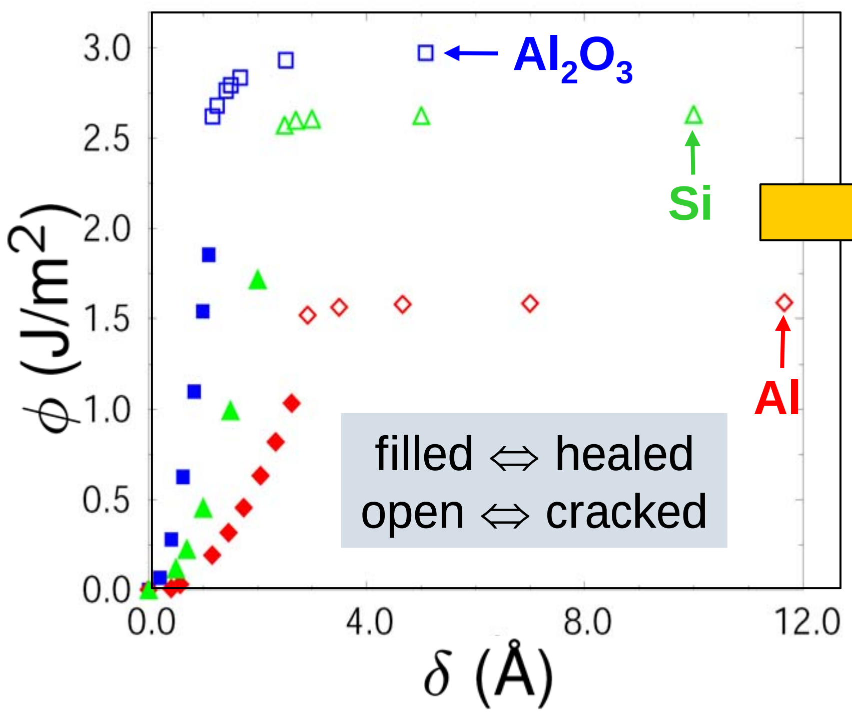


$$\bar{\sigma}_c = \sigma_c/\sqrt{N}, \quad \bar{\delta}_c = \delta_c\sqrt{N}, \quad \bar{C} = C/N$$

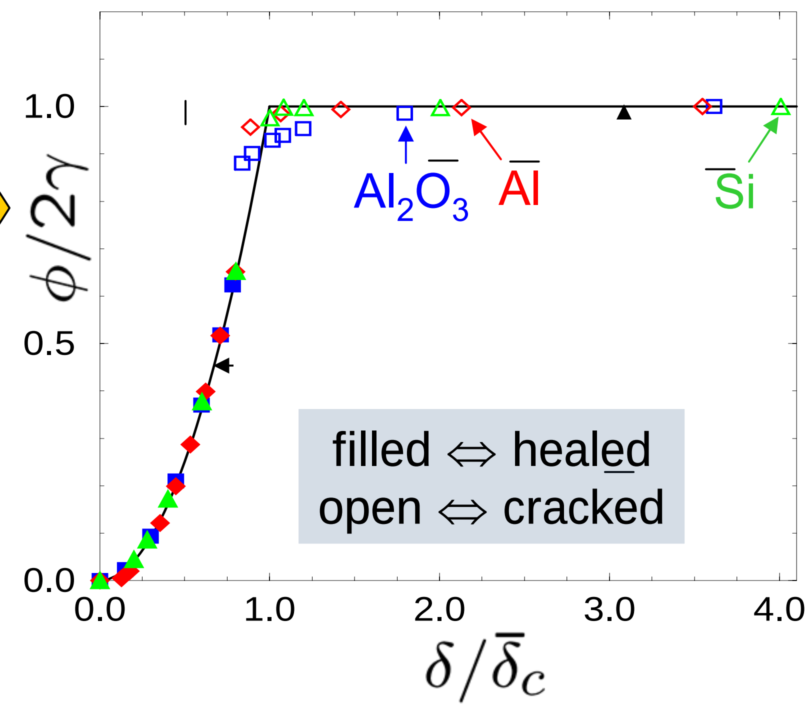
Nguyen and Ortiz, *J. Mech. Phys.Solids*, **50** (2002) 1727.
Hayes, Ortiz and Carter, *Phys. Rev. B*, **69** (2004) 172104
Braides, Lew and Ortiz, *Arch. Rational Mech. Anal.*, **180** (2006) 151.

Cohesive law – Upscaling

Ab-initio cohesive law



Renormalized cohesive law



Metal, semiconductor, and ionic ceramic all fall on same universal curve

Hayes, Ortiz and Carter, *Phys. Rev. B*, **69** (2004) 172104

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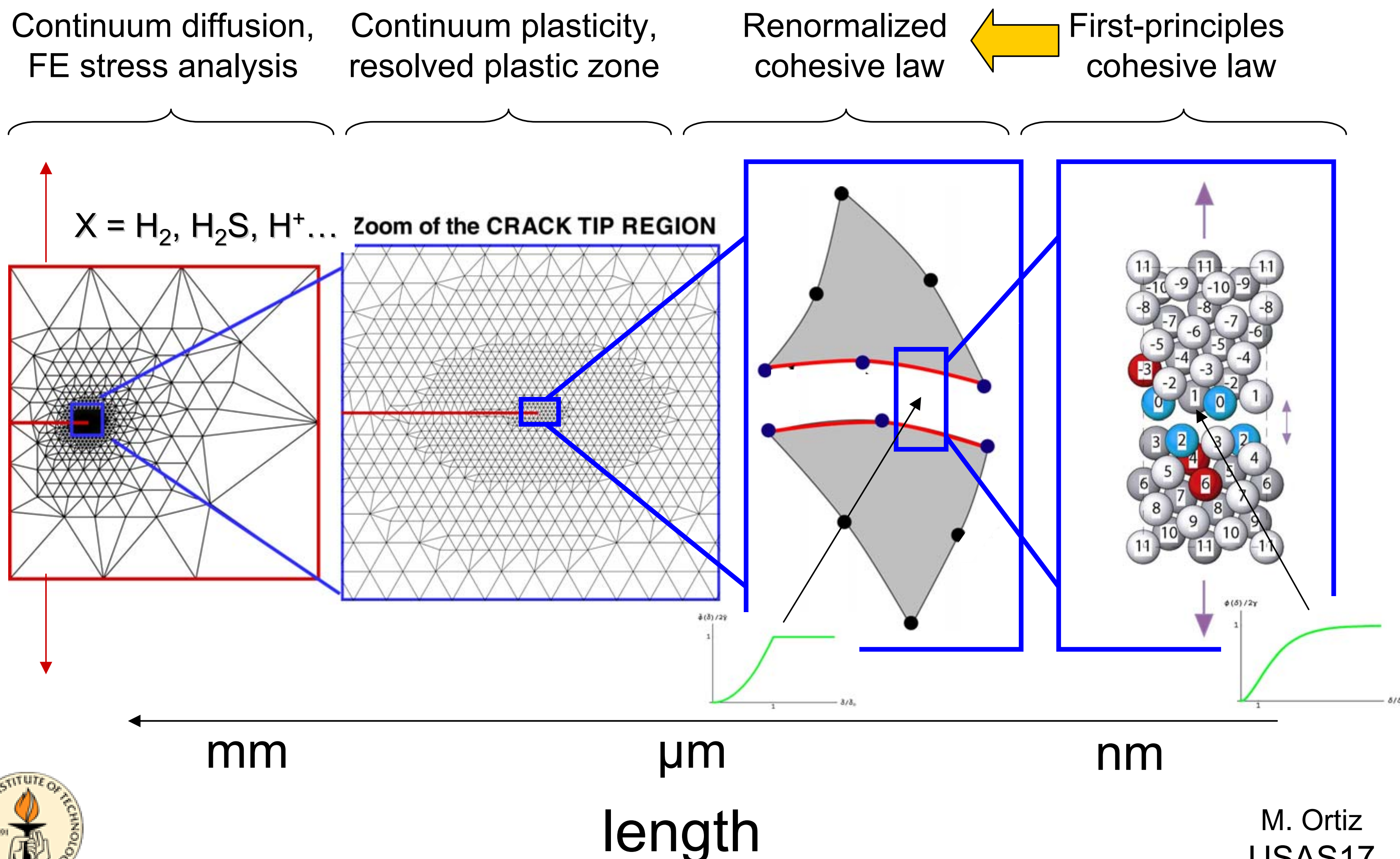
Cohesive laws – Upscaling

- Continuum cohesive law attains asympotically a *universal asymptotic form* independent of the form of the atomistic cohesive law
- The renormalized peak stress scales as: $\sigma_c/\sqrt{N}$
- The renormalized COD scales as: $\delta_c\sqrt{N}$
- Surface energy is preserved under renormalization
- The only information from the atomistic cohesive law that passes to the continuum is: i) Initial slope; ii) Surface energy
- The renormalized cohesive zone size is automatically resolved by mesh size

HE – Multiscale model



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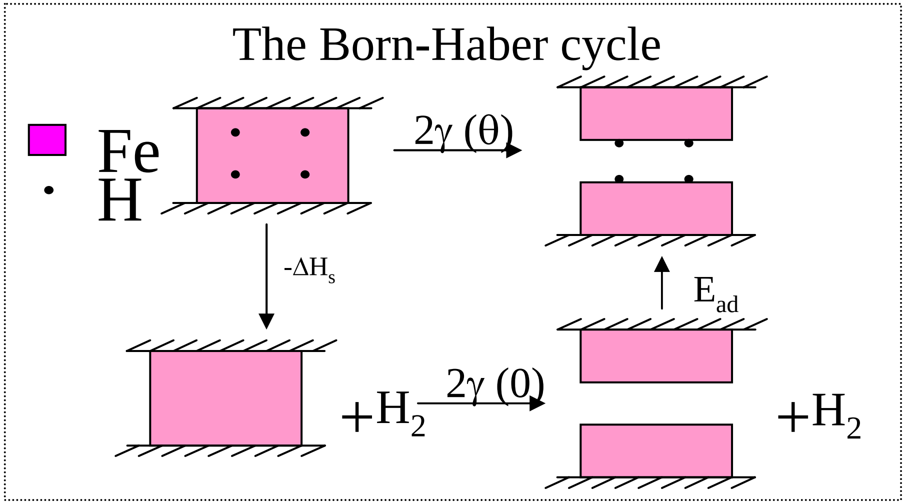
Segregation-enhanced decohesion

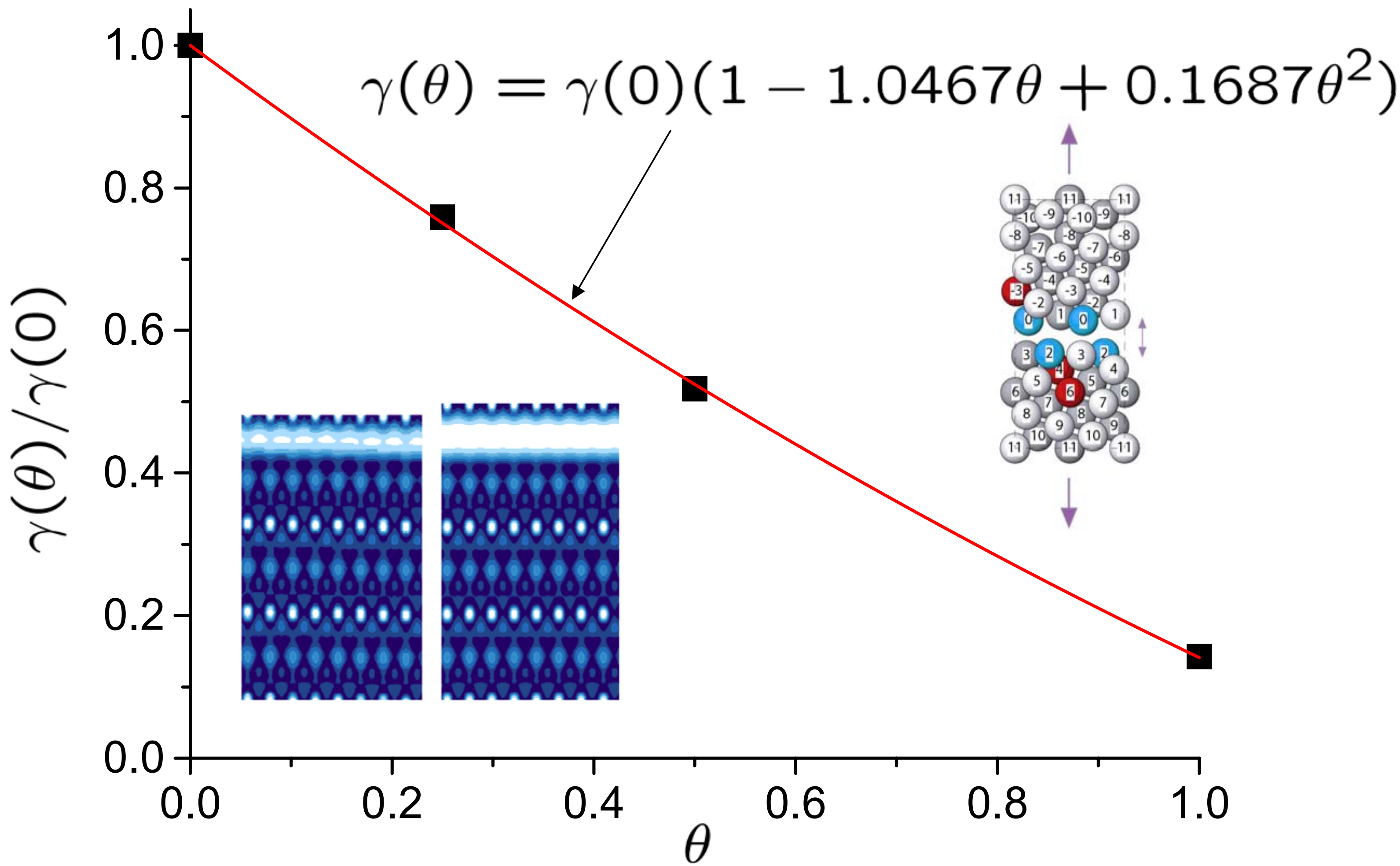


$$2\gamma(\theta) = -\Delta H_s + 2\gamma(0) + E_{ad}$$

(Jarvis, Hayes and Carter, *Chem. Phys. Chem.*, **1**, *55,* 2001)

Θ_H (ML)	$-\Delta H_s$ (J/m^2)	$2\gamma(0)$ (J/m^2)	E_{ad} (J/m^2)	$2\gamma(\theta)$ (J/m^2)
0	0	4.856	0	4.856
0.25	-0.427	4.856	-0.748	3.681
0.50	-0.854	4.856	-1.516	2.486
1.00	-1.708	4.856	-2.550	0.598

Hydrogen-enhanced decohesion of Fe(110)



First-principles calculations of coverage dependence of suface energy in Fe(110) (Jarvis, Hayes and Carter, *Chem. Phys. Chem.*, **1**, *55,* 2001)

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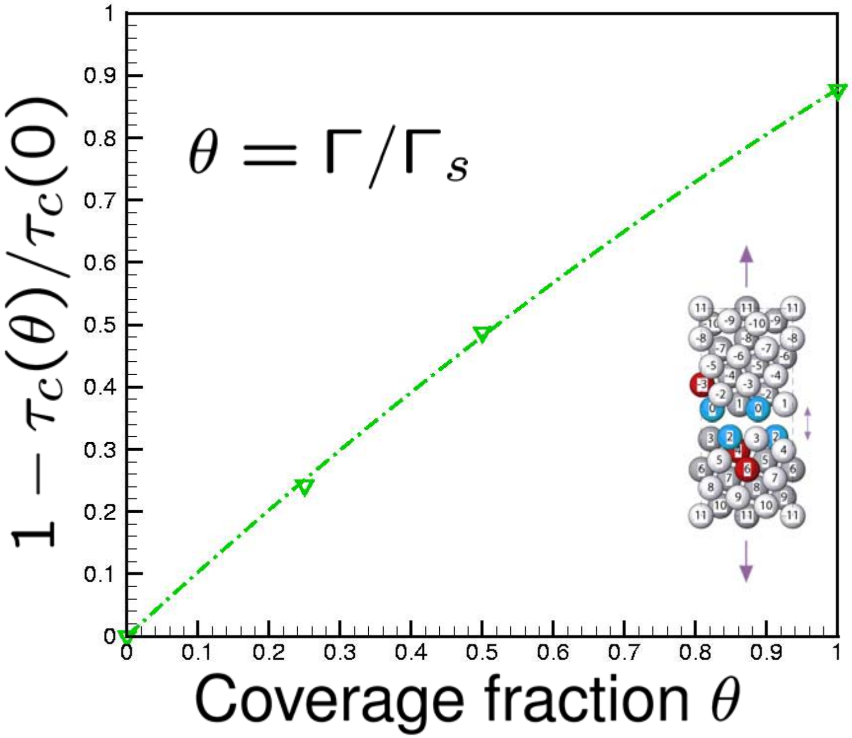
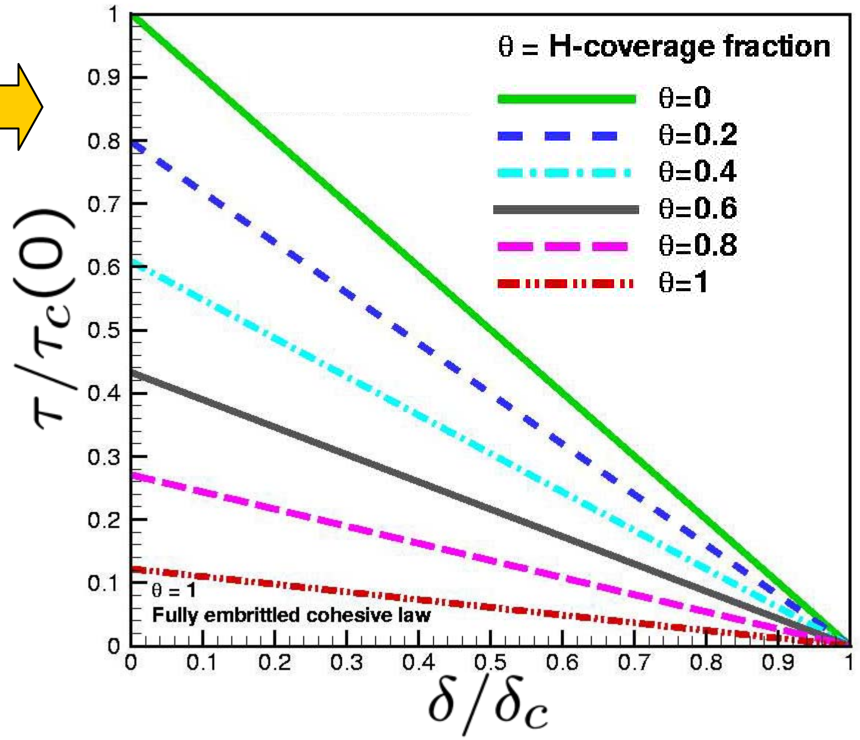
Cohesive law – Effect of H coverage



Coverage *vs*. cohesive strength
(Jiang and Carter, Phys. Rev. B, **67** (2003) 214103; Surf. Sci., **547** (2003) 85)



Coverage *vs*. cohesive law
(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

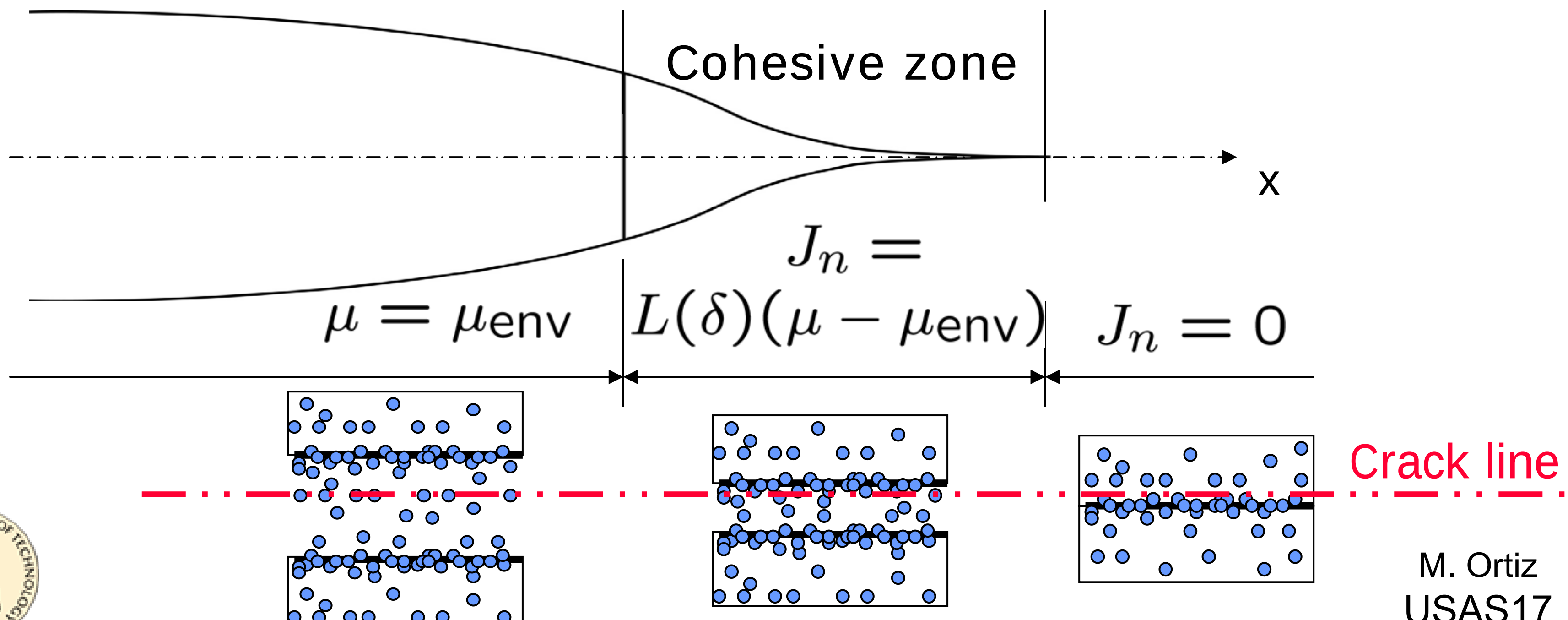
$$\tau(\delta,\theta) = \tau_c(\theta)(1-\delta/\delta_c)$$

$$\tau_c(\theta) = \tau_c(0)(1-1.0467\theta+0.1687\theta^2)$$

HE – Hydrogen diffusion

- Diffusion equation: $C_{,t} - \mathrm{div}(MC\,\mathrm{grad}\mu) = 0$
- Chemical potential: $\mu = \mu_0(T) + RT\log(C/C_0) - pV$
- Surface coverage: $\Gamma = \Gamma^s/[1 + C^{-1}\exp(\triangle g/RT)]$

  (Langmuir-McLean)
- Boundary conditions:



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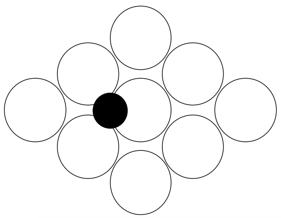
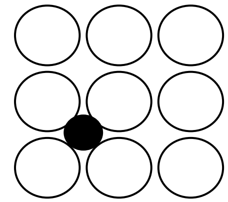
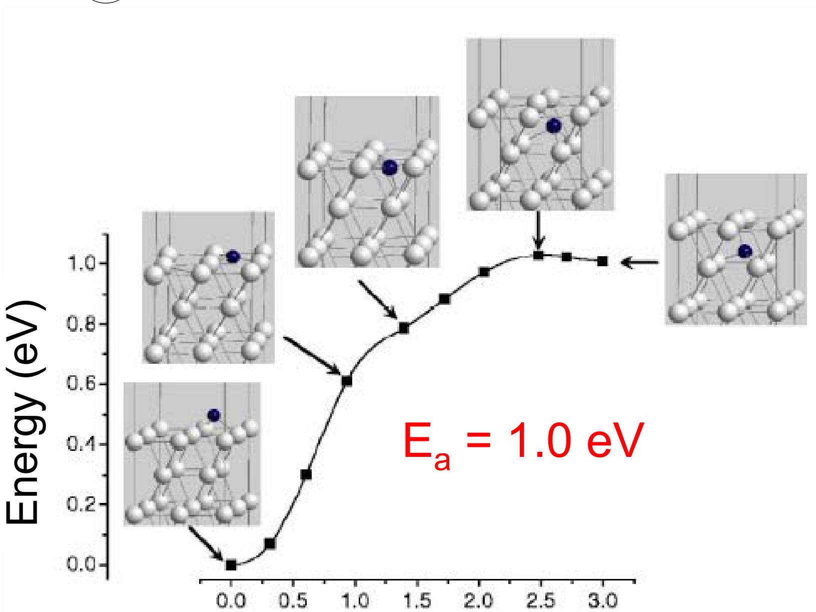
Hydrogen absorption into Fe

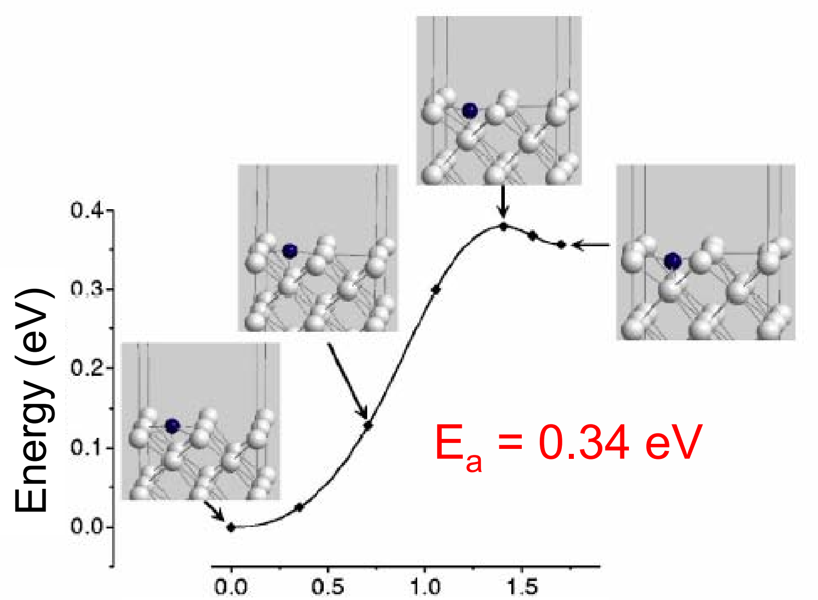


H/Fe(110)



H/Fe(100)



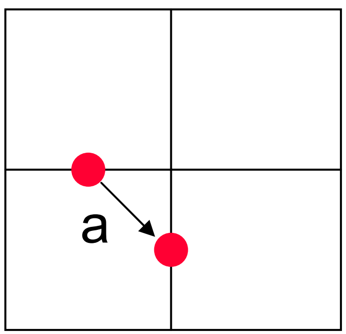


Hydrogen absorption paths and energies into Fe(100) and Fe(110)
(Jiang and Carter, Phys. Rev. B, **67**, 214103 (2003); Surf. Sci., **547**, 85 (2003); Phys. Rev. B, **70**, 064102 (2004))

Hydrogen diffusion in strained Fe

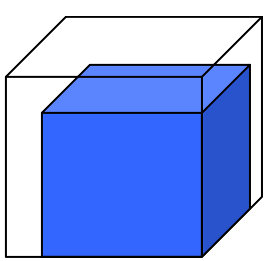
$$D(T) = D_0 \exp(-(\Delta E + \Delta ZPE)/k_B T)$$

Hops between T-sites::



Volumetric deformation:

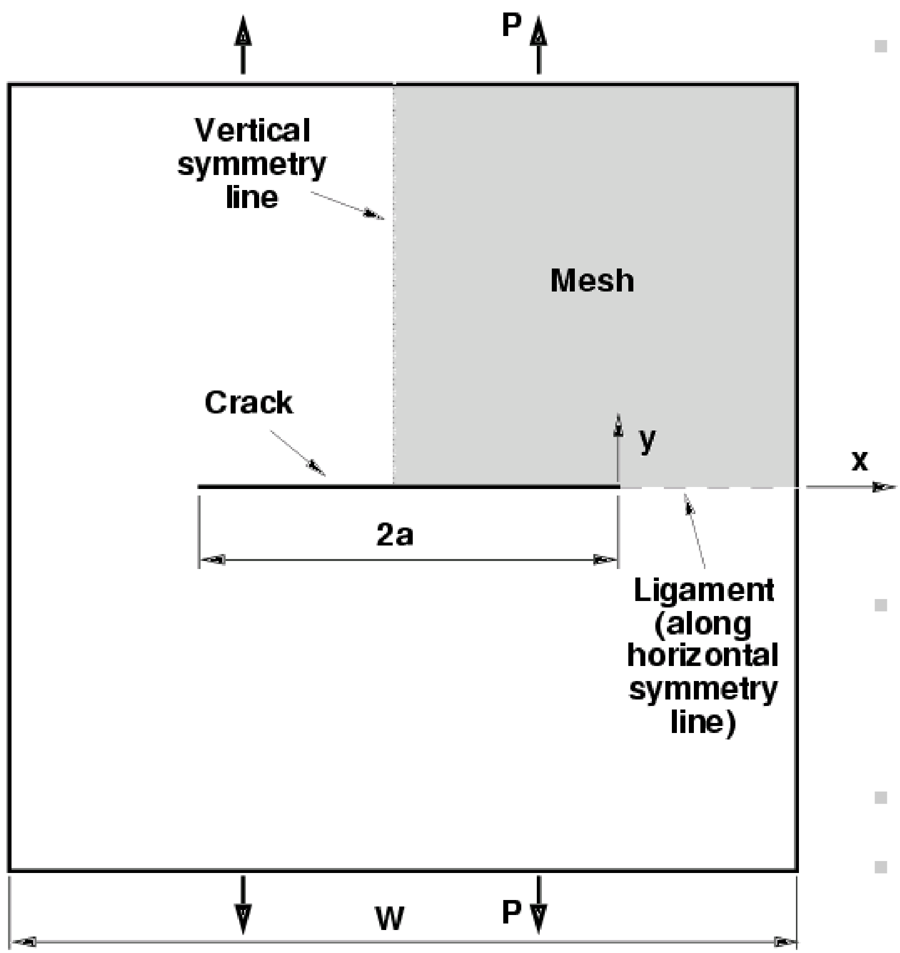
$$\boldsymbol{F} = \begin{bmatrix} 1+\epsilon & 0 & 0 \\ 0 & 1+\epsilon & 0 \\ 0 & 0 & 1+\epsilon \end{bmatrix}$$



ε (%)	D_0 (10^{-7} m^2/s)	ΔE (eV)	ΔE+ΔZPE (eV)
-2	1.872	0.095	0.044
-1	1.814	0.094	0.046
0	1.818	0.092	0.044
1	1.730	0.092	0.048
2	1.680	0.091	0.050

(Ramasubramaniam and Carter, in progress)

HE - Case Study



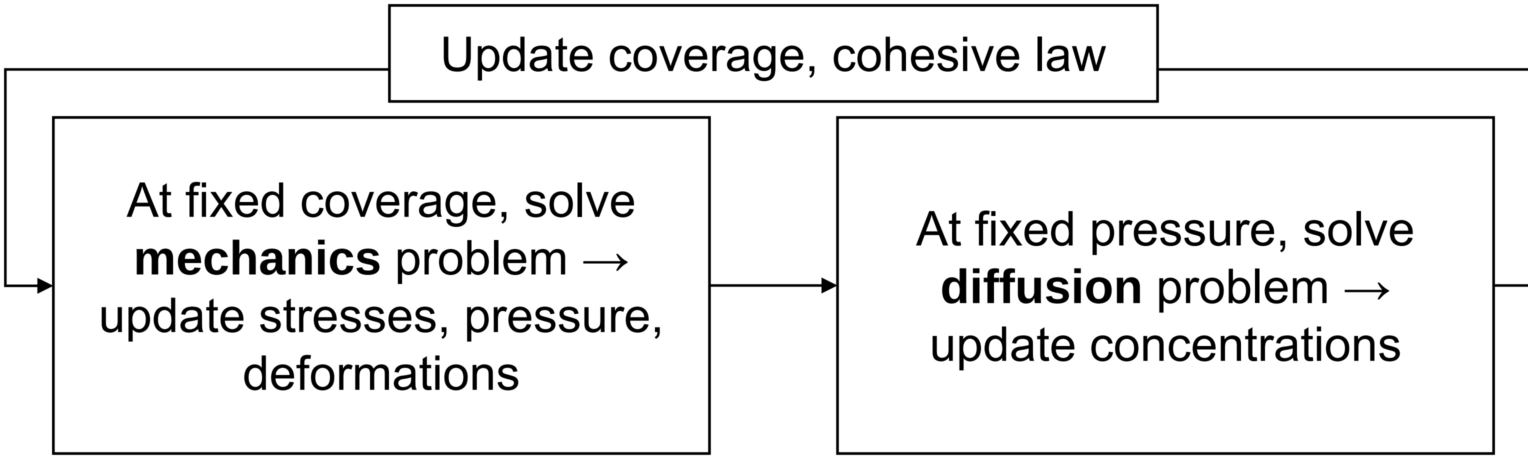
Center crack panel geometry.

(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

- Material: AISI 4340 (Q&T) high-strength steel in seawater
  - E = 210 GPa
  - ν = 0.3
  - σ_{y0}= 1000 - 1600 Mpa
  - N = 0.042 - 0.087
  - K_c = 45 - 150 MPa $m^{1/2}$
  - τ_C = 4000 - 6400 Mpa
  - V = 7.116e-6 m^3 / mol
- Impurity (hydrogen)
  - $D(T_{amb})$ = 1.0 x 10^{-10} m^2/s
  - ΔV= 2.0 x 10^{-6} m^3/mol
- Load: Applied P (corresp. K)
- Environment
  - T = 300-450 K
  - $C_{eq,0}$ = 0.1-10 ppm wt = 5.5 x (10^{-6} -10^{-4})

Finite-Element Analysis

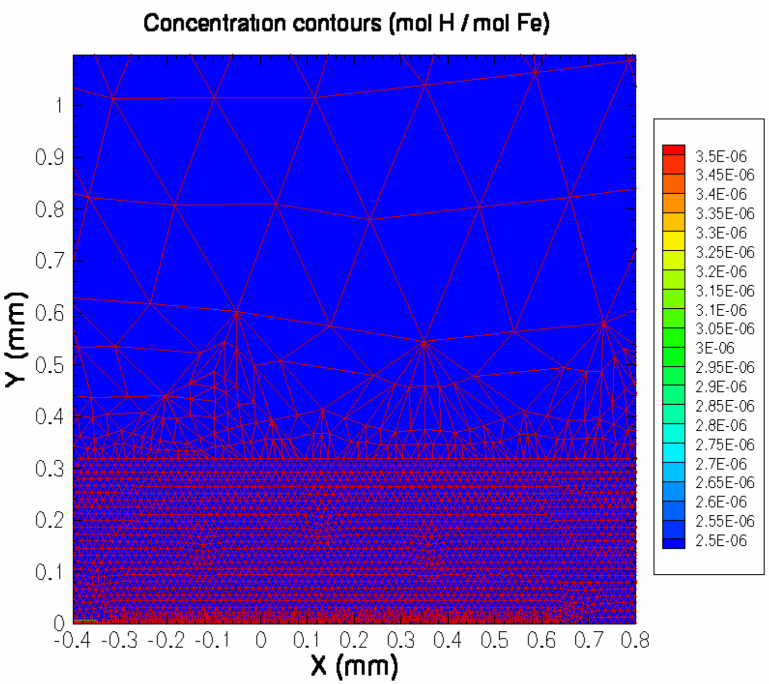
- Solution method: staggered procedure,

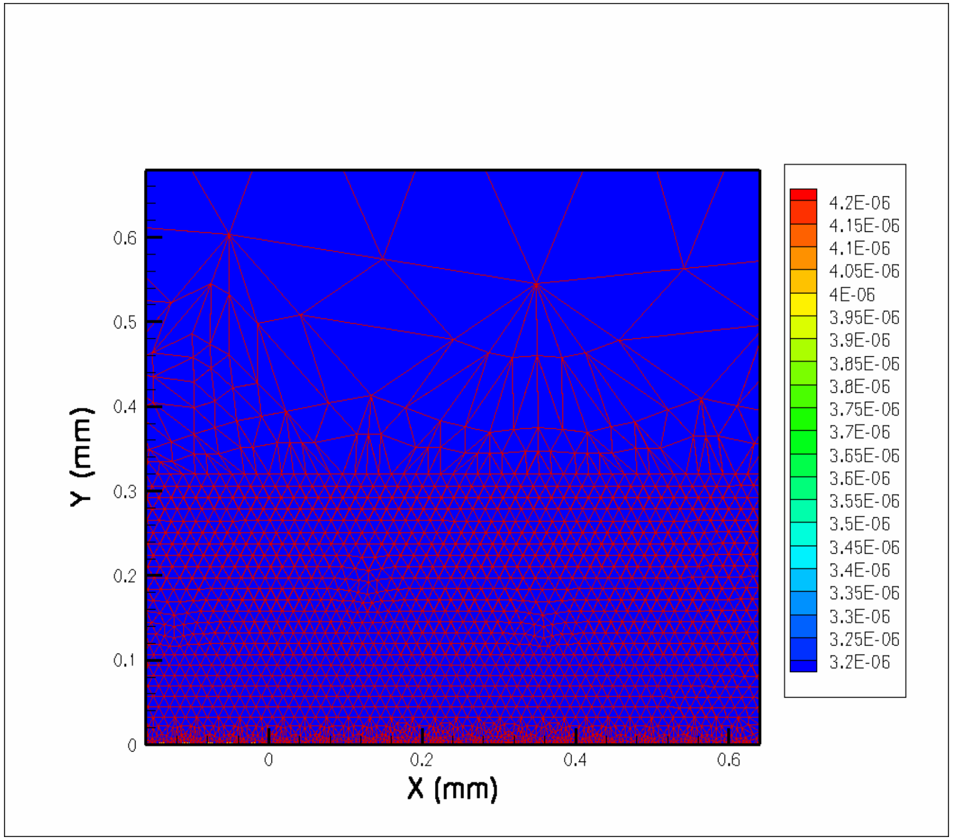


- BC Crack flanks:
  - Equilibrium impurity coverage on crack flanks: $C=C_{eq}(p)$
  - At the cohesive zone: $J_n=0$.
- BC at external boundaries: $C=0$.
- IC: $C=C_{eq}(p)$ on crack flanks; $C=0$ elsewhere.

(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

HE – Hydrogen concentration





(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

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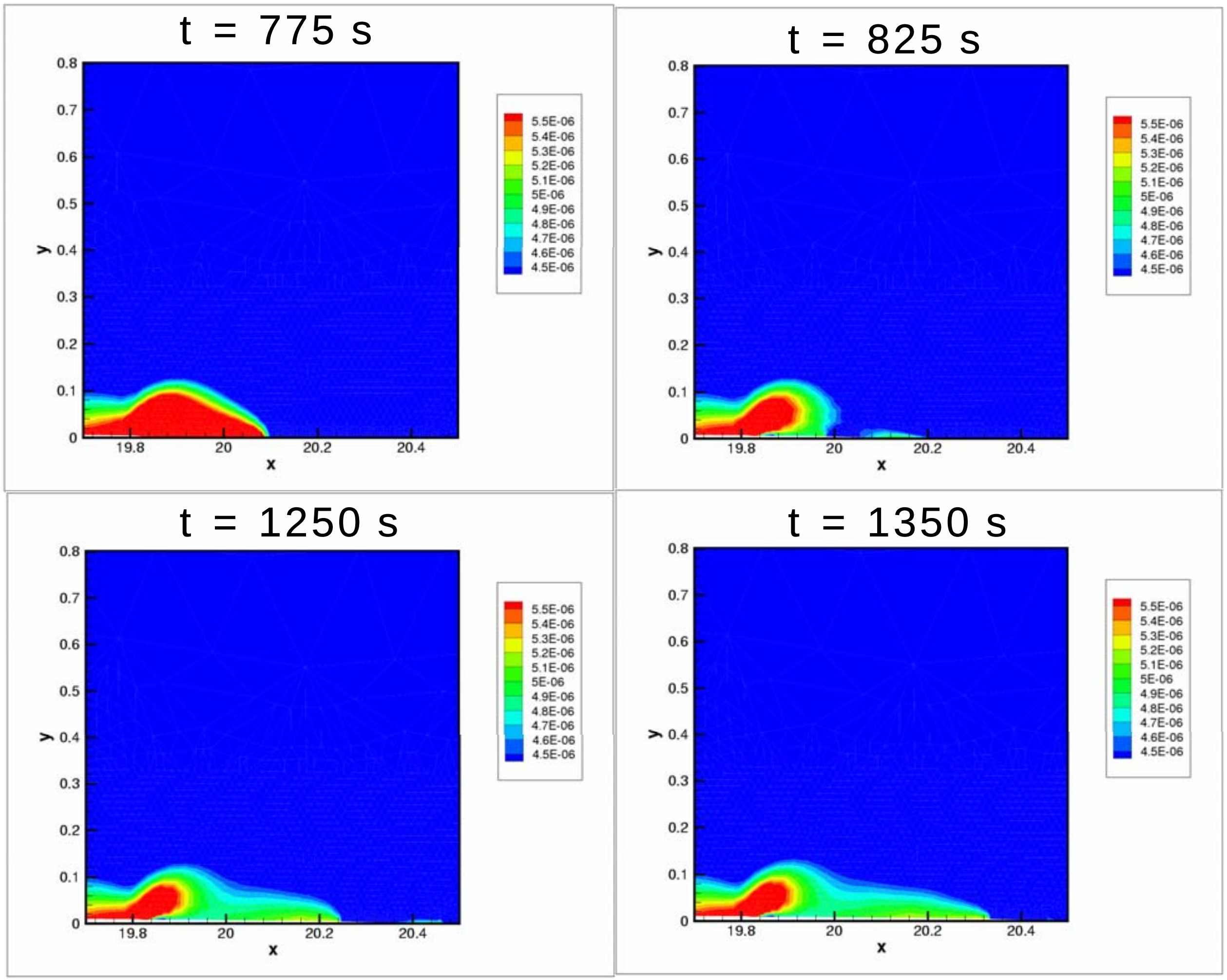
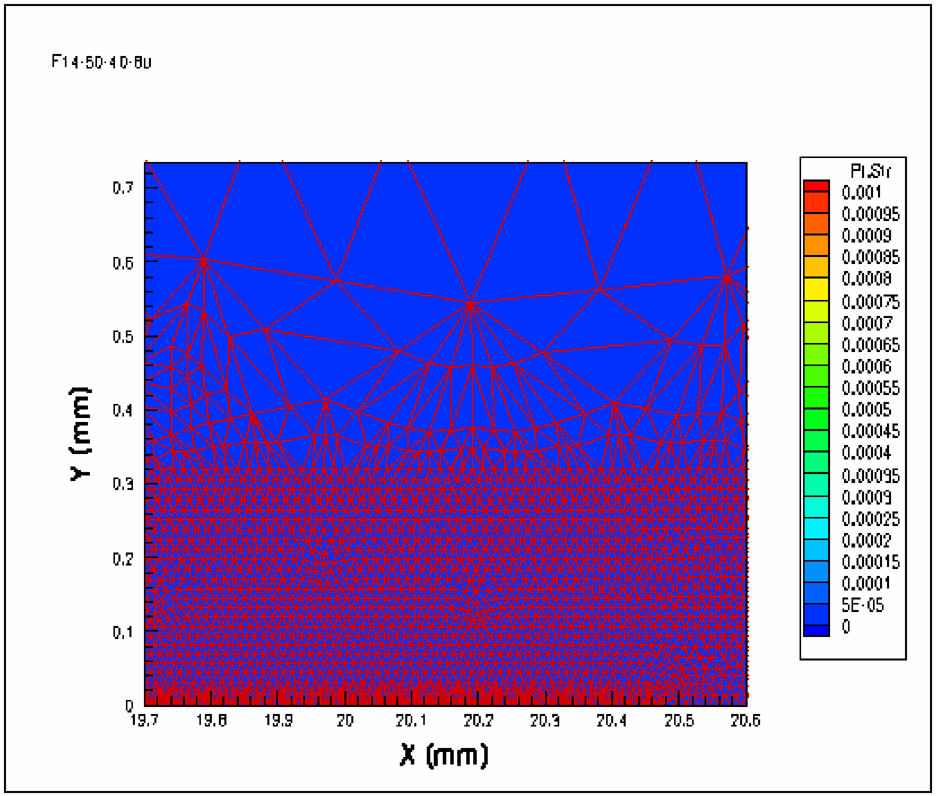
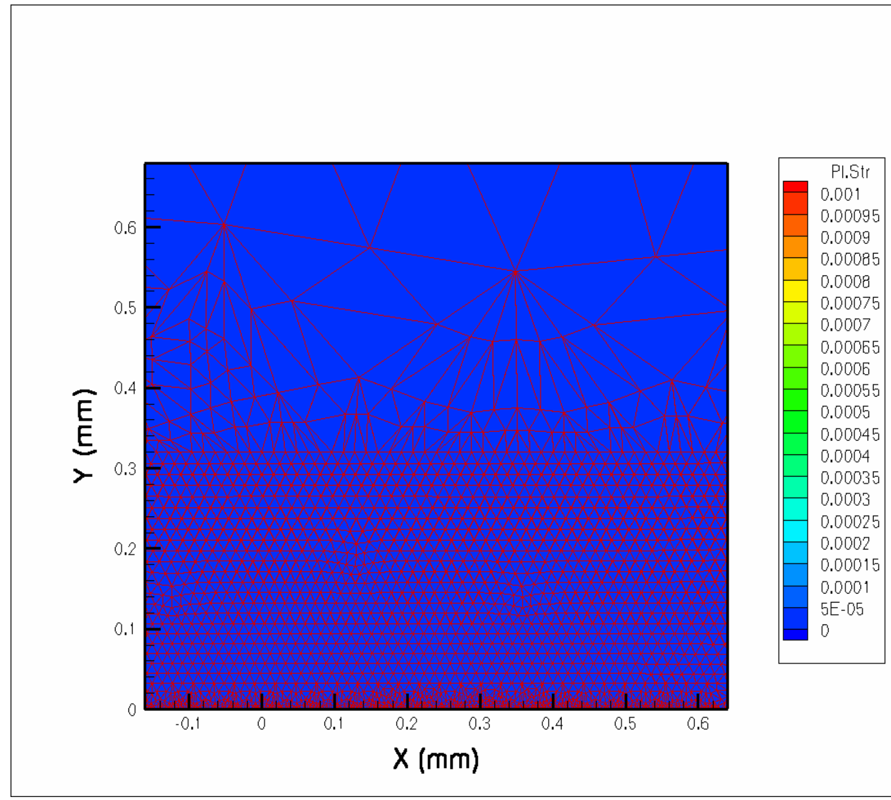


(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

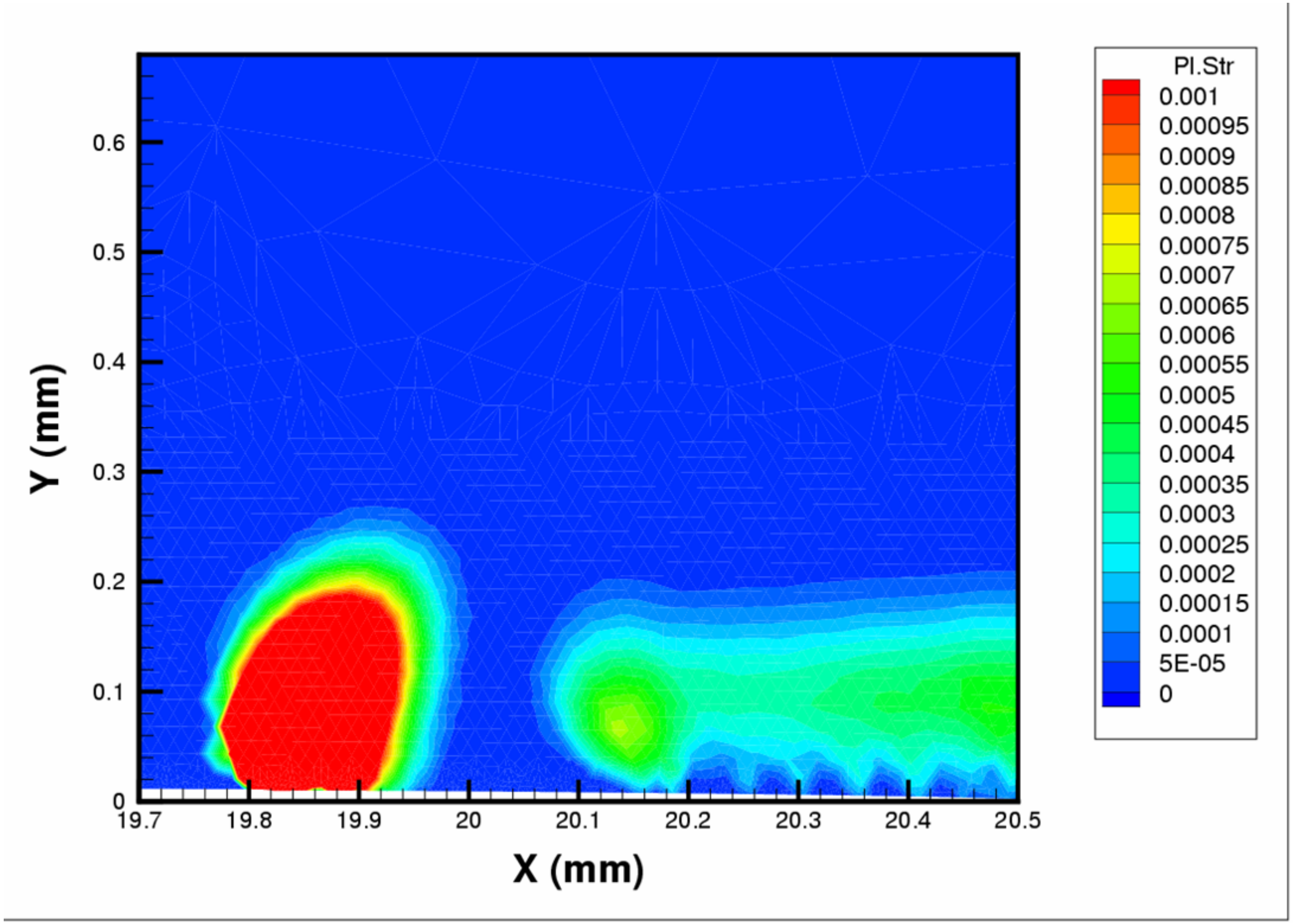
HE – Plastic strain





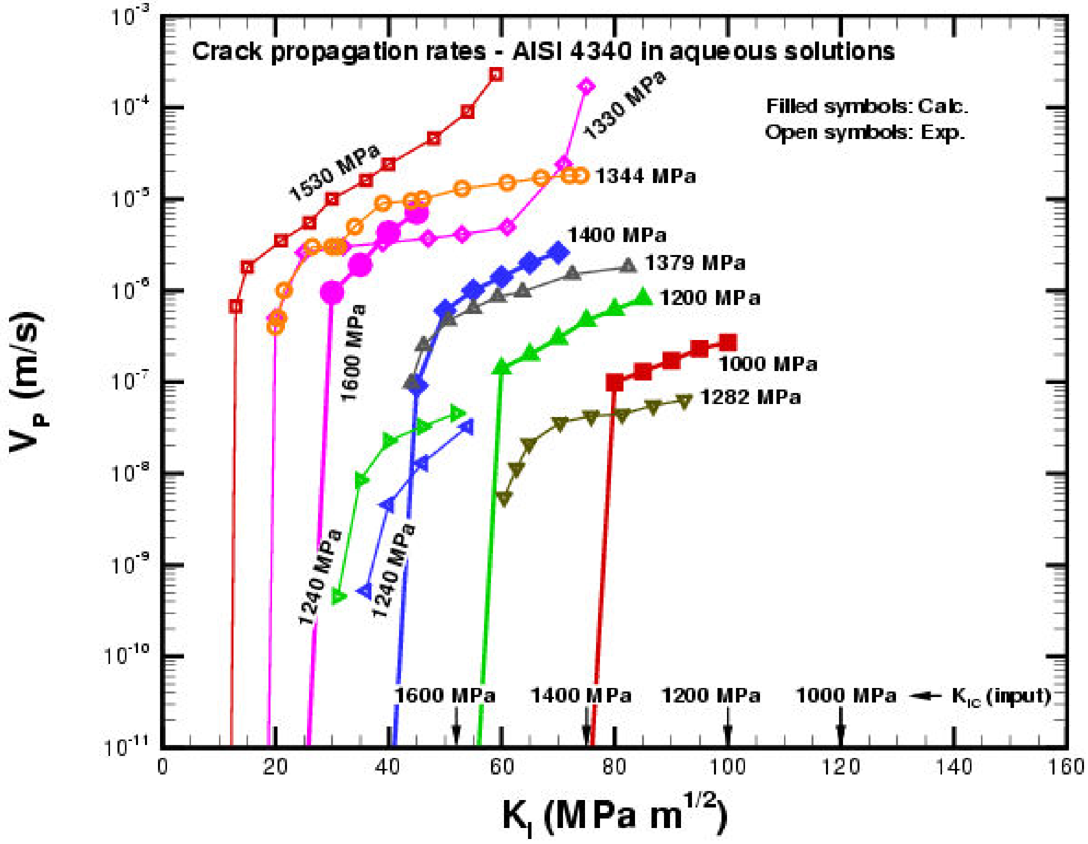
(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

HE – Plastic strain



(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

HE – Propagation velocity



- Calculated curves reproduce existence of threshold K_{ISCC} and plateau $V_{P,II}$.
- Trends agree with experiments, considering the large scatter.

(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

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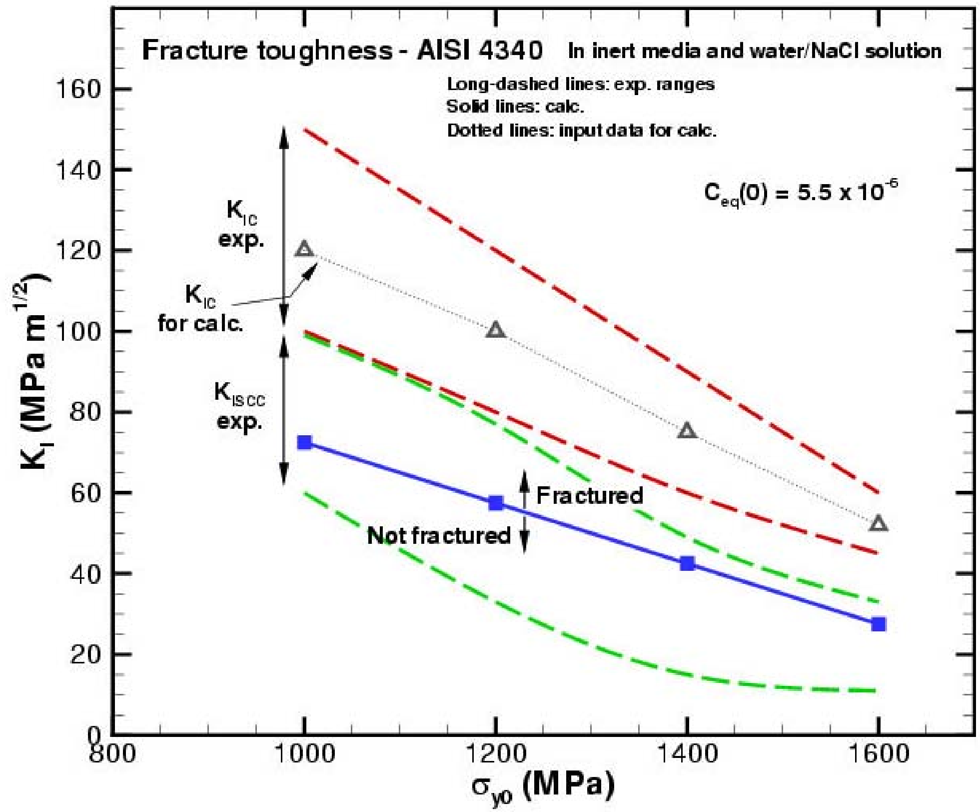
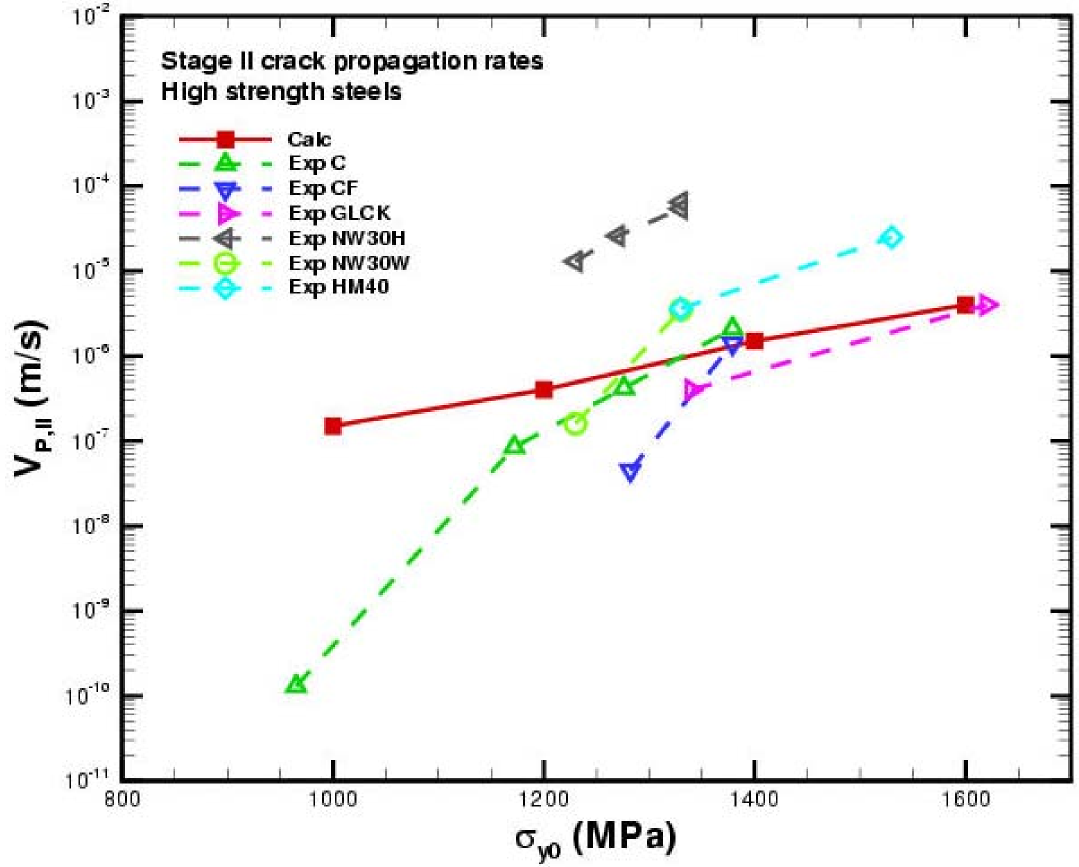
HE - Threshold K_{ISCC} vs. σ_y



(Serebrinsky, Carter and Ortiz,
J. Mech. Phys. Solids, **52** (2004) 2403)

- Calculated curve reproduces experimental trend.
- For high σ_y calculations approach upper experimental bound.
- Crack morphology changes from transgranular at low σ_y to intergranular at high σ_y.
- At high σ_y, a stronger effect of H on grain boundaries (not accounted for) would improve agreement. Likewise for t_i vs. K_I.

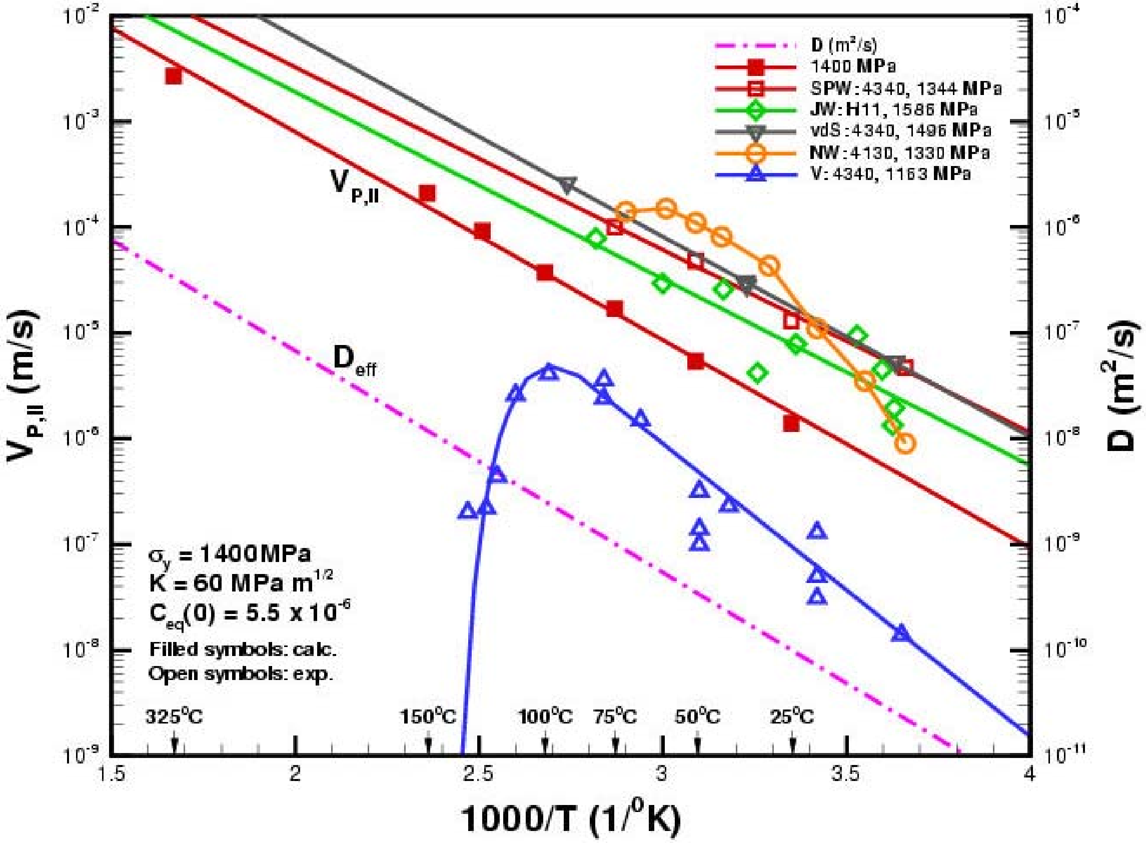
HE - Plateau $V_{P,II}$ vs. σ_y



(Serebrinsky, Carter and Ortiz,
J. Mech. Phys. Solids, **52** (2004) 2403)

- Results for several high strength steels in various media included.
- Calculated curve reproduces experimental trend.
- For high σ_y, a stronger effect of H on grain boundaries (not accounted for) would improve agreement in slope.
- For low σ_y there is a paucity of data.

HE - $V_{P,II}$ vs. temperature



- Several high strength steels included.
- Calculated curve reproduces increasing (Arrhenius) part.
- Calculated activation energy for $V_{P,II}$, Q_V, is similar to that taken for D_{eff}, Q_D ◷ 40kJ/mol.
- Fall in $V_{P,II}$ (generally observed) at high T not reproduced.

(Serebrinsky, Carter and Ortiz, *J. Mech. Phys. Solids*, **52** (2004) 2403)

Concluding remarks

- Multiscale model (chem + mech) predicts well HE in structural steels at low temperatures (< 100ºC)
- Model does not predict well:
  - *High-temperature behavior*
  - *Aluminum alloys*
- Unknown unknowns! HELP? HRPC? Others?
- Model still empirical and incomplete at the mesoscale
- Unmodelled length scales:
  - *Interaction between dislocations and H:*
    - *Solution hardening*
    - *Pipe diffusion*
  - *Polycrystalline structure: Grains and grain boundaries*
- When is enough enough?
- Experimental validation, uncertainty quantification!