Renormalization of Atomic-Scale Binding-Energy Relations

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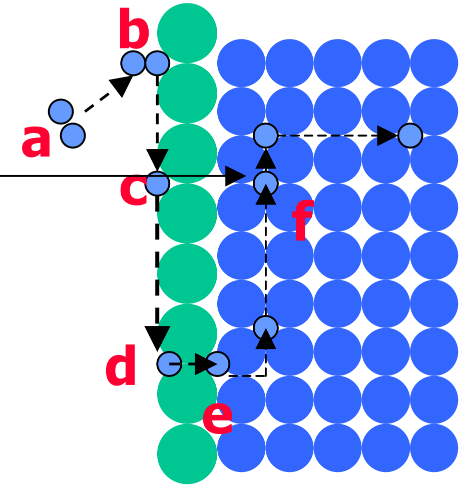
Stress-Corrosion Cracking

- Engineering model:
  - *Cohesive models of fracture*
  - *Coupling of cohesive models and surface chemistry*
  - *Adaptive FE stress analysis*
  - *FE analysis of impurity diffusion:*
    - *Stress-assisted diffusion*
    - *Opening-dependent mixed boundary conditions over cohesive zone*
- Goal:To predict time to failure of components under general load histories, environments.

Hydrogen embrittlement

- Hydrogen adsoption
- Hydrogen diffusion

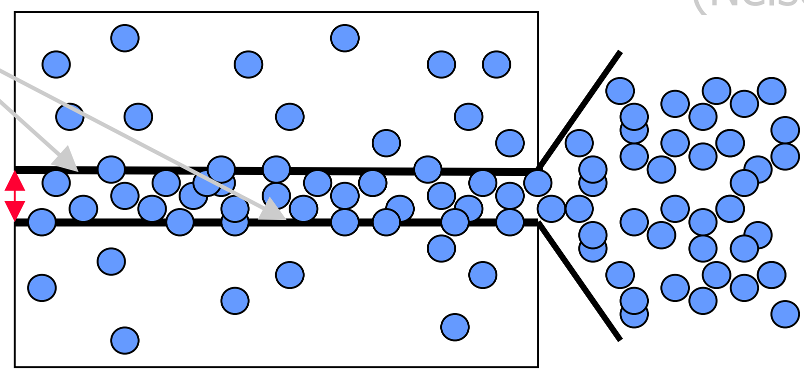


- Free energy density = f(T, $\Gamma^{\pm}$, δ)
- $df(\delta,\Gamma^{\pm}) = \sigma\, d\delta + \mu\, d\Gamma$

(Nelson 1972)

$\Gamma^{\pm}$= Surface concentrations

δ = Opening displacement



Environment defined by μ_{ext}

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

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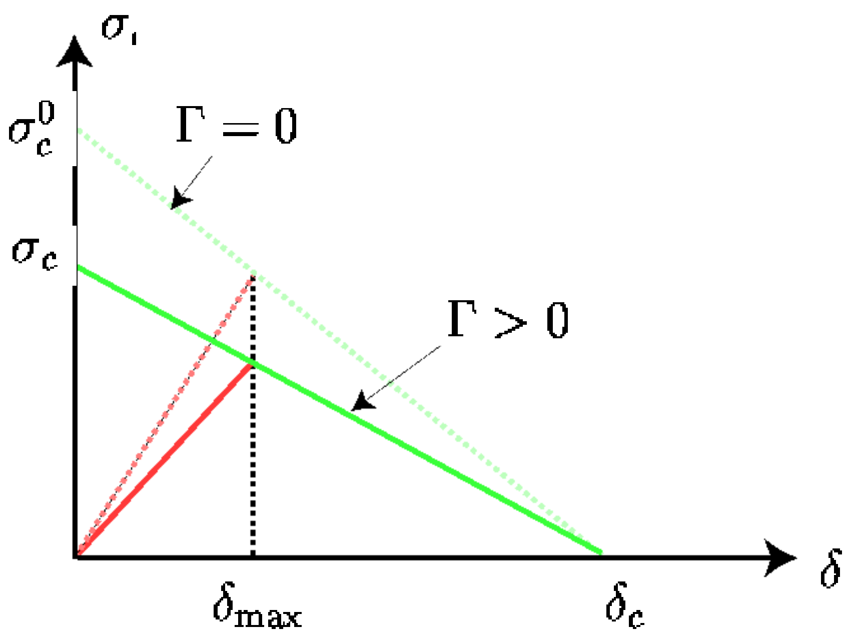
SCC – Cohesive model



- Segregant embrittlement: (Wang and Rice, 1989):

$$2\gamma_s(\Gamma) = 2\gamma_s^0 - (\Delta g_b^0 - \Delta g_s^0)\,\Gamma$$

- Effect on cohesive law:

$$\sigma_c(\Gamma) = \sigma_c^0 - \frac{(\Delta g_b^0 - \Delta g_s^0)}{\delta_c}(\Gamma^+ + \Gamma^-)$$

Impurity	$-\Delta g_s^0$	$-\Delta g_b^0$	$\Delta g_b^0 - \Delta g_s^0$
C	73 to 85	50 to 75	-2 to 35
P	76 to 80	32 to 41	35 to 48
Sb	83 to 130	8 to 25	58 to 122
S	165 to 190	50 to 58	107 to 140

(Steel, 300K, g in KJ/mol; after Wang and Rice, 1989)

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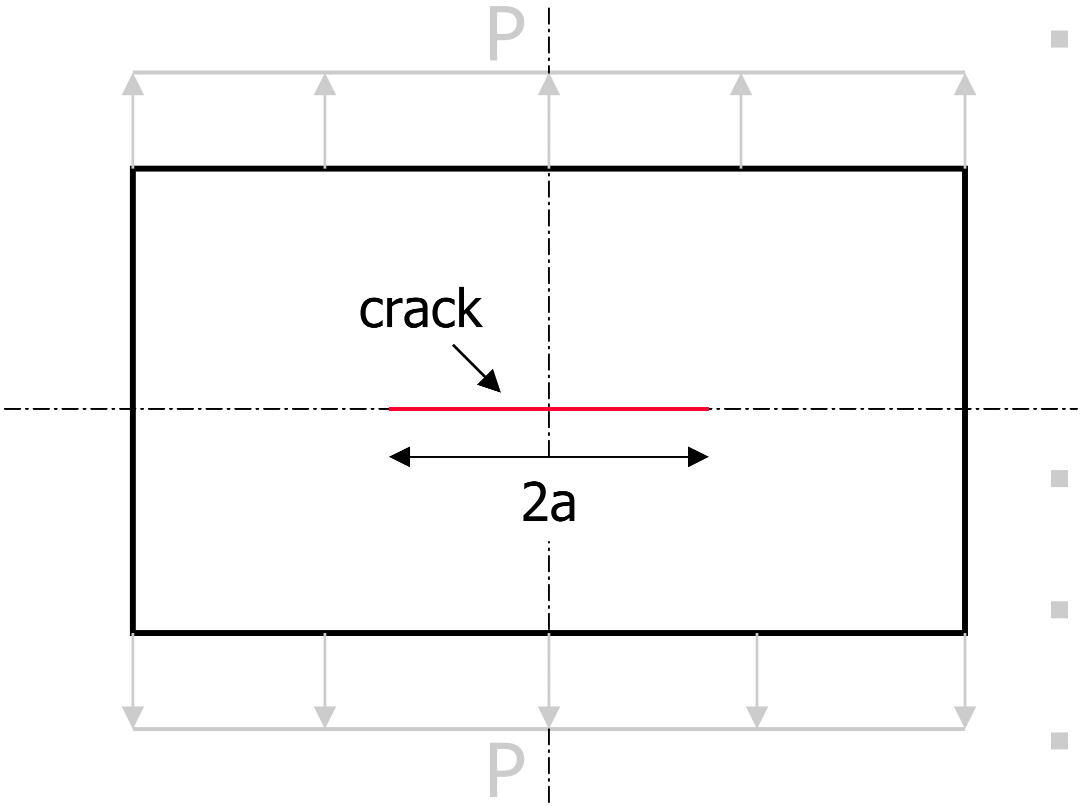
SCC – Experimental Validation



Center crack panel geometry.

- Material: Steel
  - $E = 207$ GPA
  - $\nu = 0.3$
  - $\sigma_0 = 325$ MPa
  - $G_c = 30.0$ kJ/m^2
  - $\sigma_C = 840$ Mpa
  - $D = 1.27e\text{-}8$ m^2/s
- Load.
  - $P = 260$ MPa (Constant).
- Initial crack size
  - $a = 10$ mm
- Impurity (hydrogen)
  - $V = 7.116e\text{-}6$ m^3 / mol
  - $\Delta V = 2e\text{-}6$ m^3 / mol
  - $C_0 = 2.084e21$ atoms/ m^3

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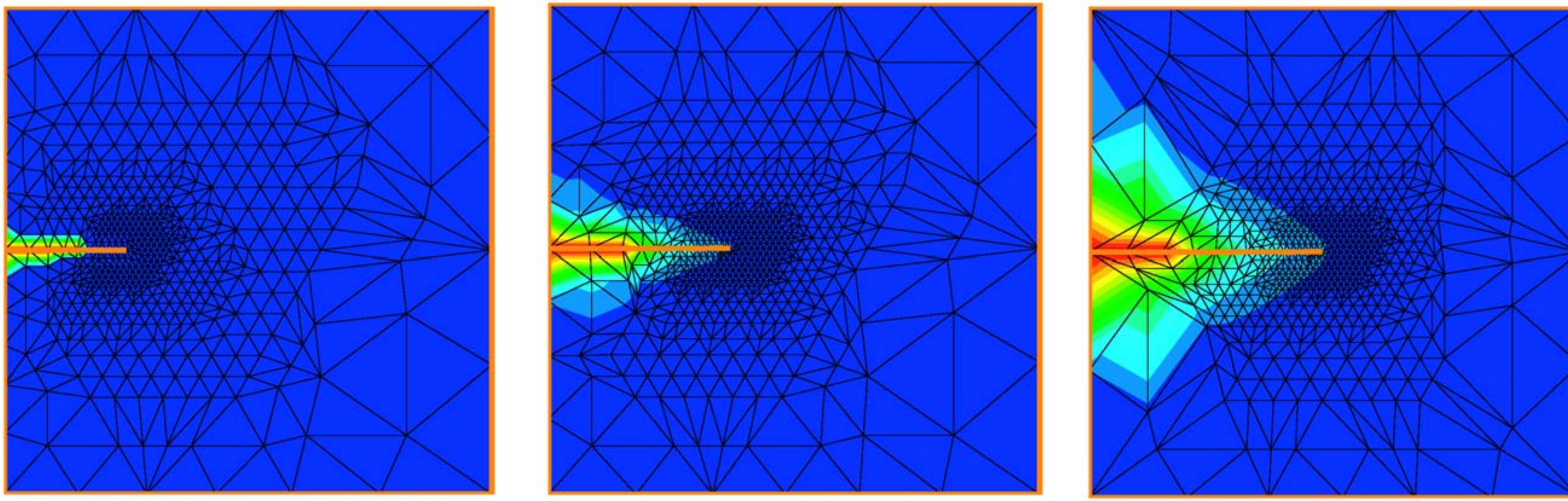
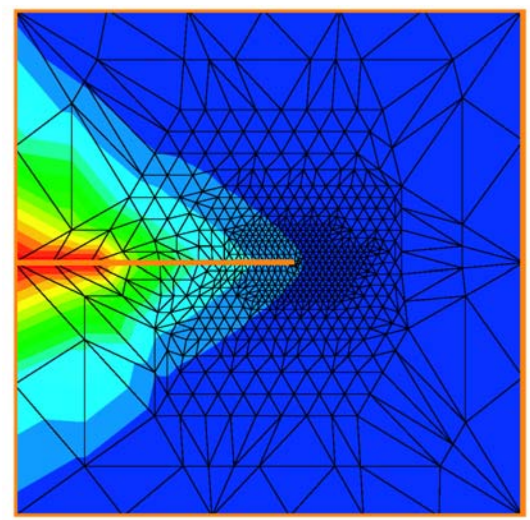
SCC – Experimental validation

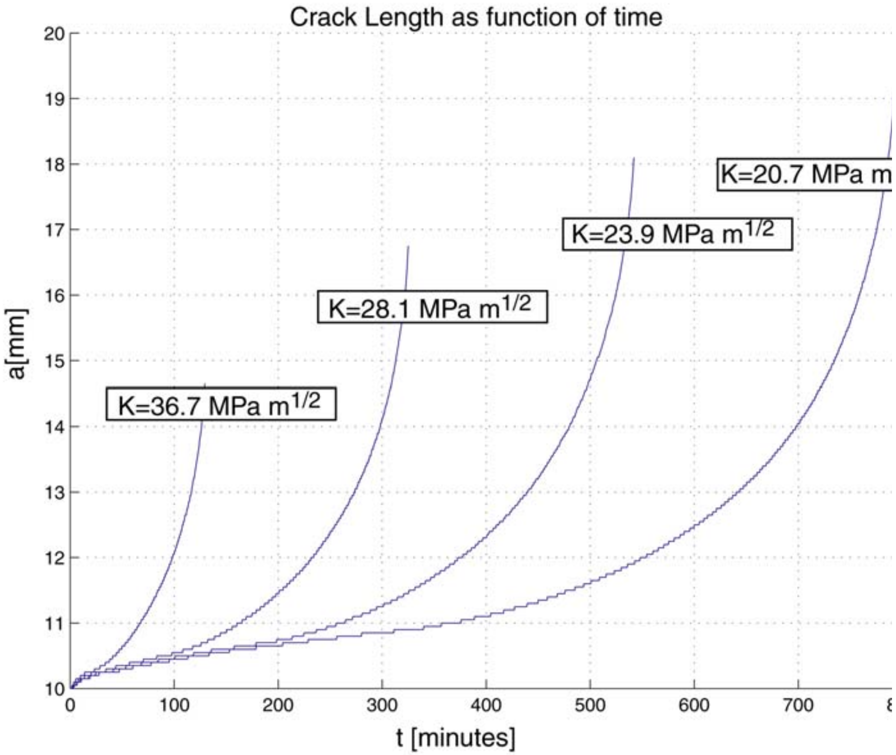


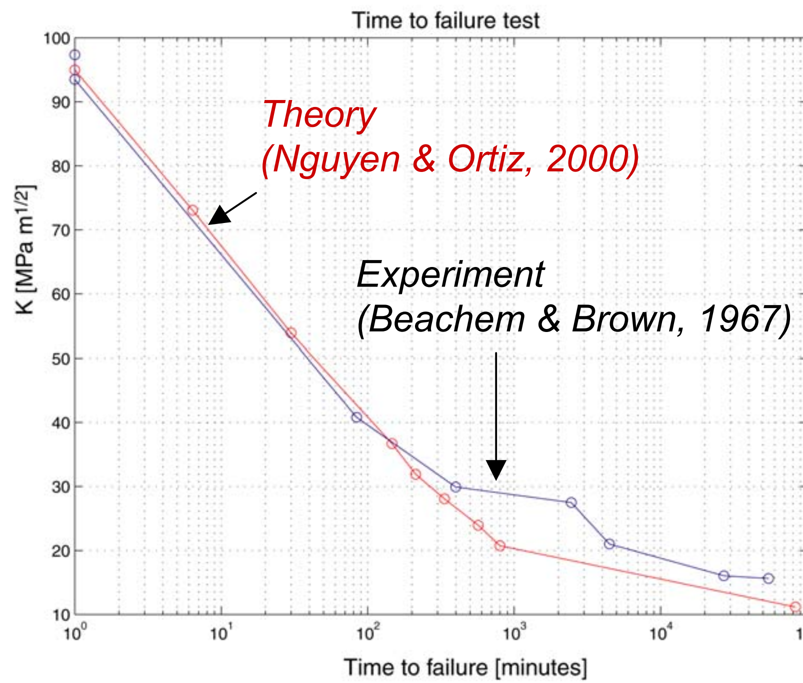
Contours of hydrogen concentration
(Nguyen and Ortiz, 2000)

(Movie)



SCC - Experimental validation





(Nguyen and Ortiz, 2000)

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Multiscale Modeling of Fracture

- Engineering models of material behavior are fraught with uncertainty, empiricism
- The only way to remove uncertainty is to model the underlying physical mechanisms directly
- Often unit mechanisms occur over multiple scales simultaneously and bear a hierachical relationship: Multiscale modeling
  - *Macro $\Rightarrow$ micro: Driving forces*
  - *Micro $\Rightarrow$ macro: Averaging*
- Lengthscale hierarchy stops at the atomistic level
- Application to fracture: Use atomic-scale binding energy relations calculated *ab initio*

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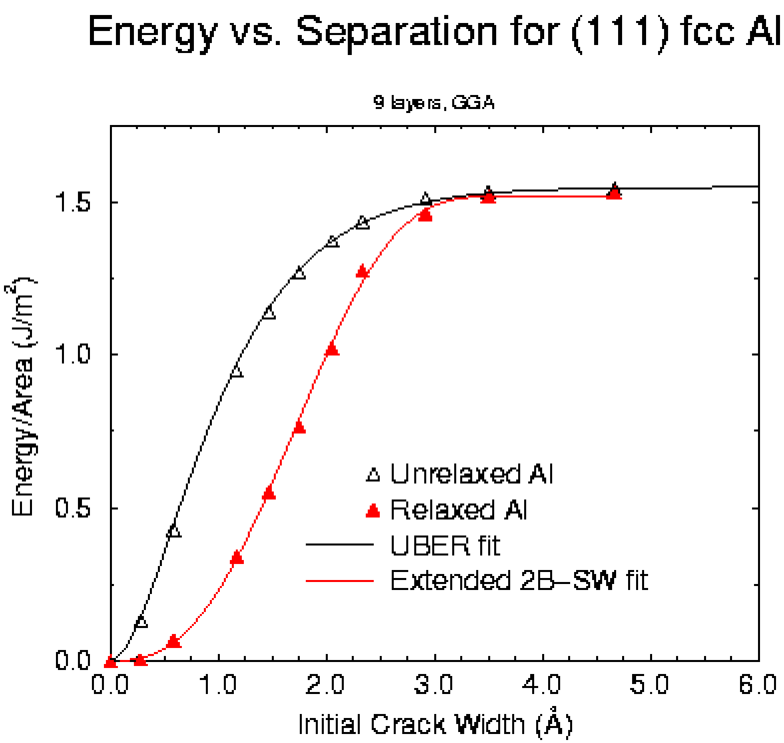
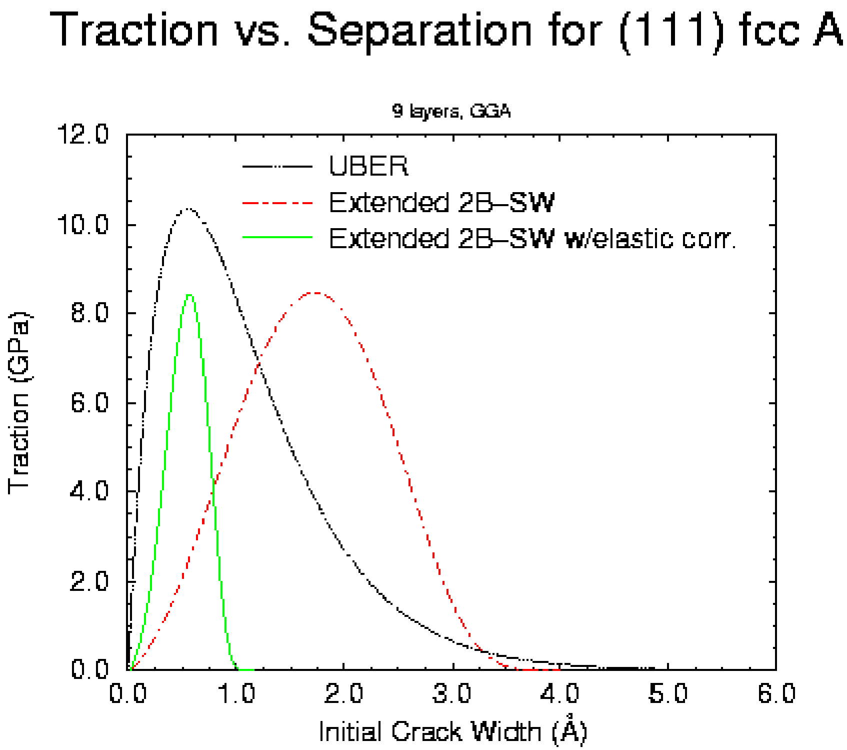
Multiscale Modeling of Fracture

Ab-initio studies of decohesion in Aluminum and Alumina

(EAA Jarvis, RL Hayes and EA Carter, *ChemPhysChem*, 2000)





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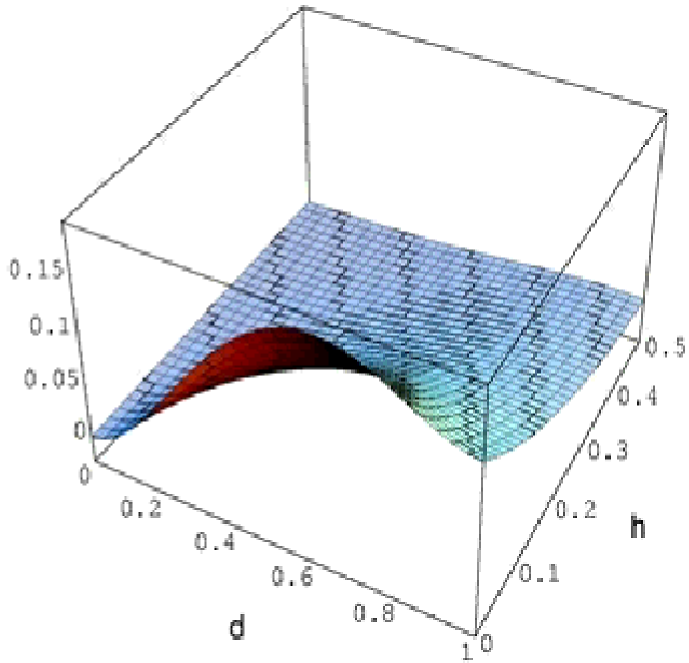
Multiscale Modeling of Fracture

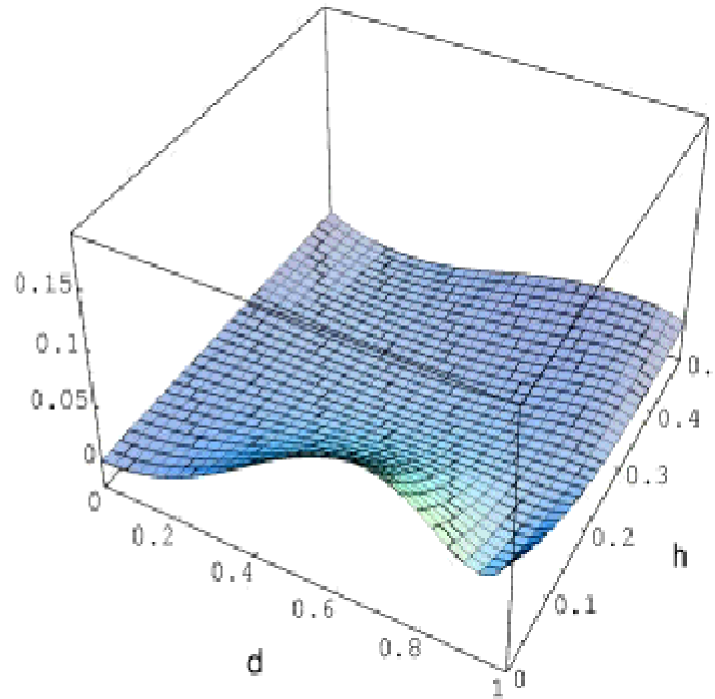
Ab-initio studies of Hydrogen embrittlement in Aluminum

(Park and Kaxiras, 2000)

- Without Hydrogen:



- With Hydrogen:



Calculated stacking-fault surfaces
as functions of interplanar sliding (d)
and interplanar separation (h)

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Multiscale Modeling: The Chasm

- Cohesive-zone size: $R \sim E' G_c / \sigma_c^2$
- Typical cohesive-zone size from atomic-scale binding energy relations: $\boxed{R \sim 1\,\mathrm{nm}}$
- This is beyond resolution afforded by macroscopic simulations: Need to coarse-grain atomistic laws
- Resolution gaps and techniques to address them:
  - *Turbulence: Subgrid models*
  - *Shock physics: Artificial viscosity models*
  - *Solids with microstructure: Theories of effective behavior*
    - *Weak convergence, energy relaxation*
    - *Statistical mechanics, renormalization group*

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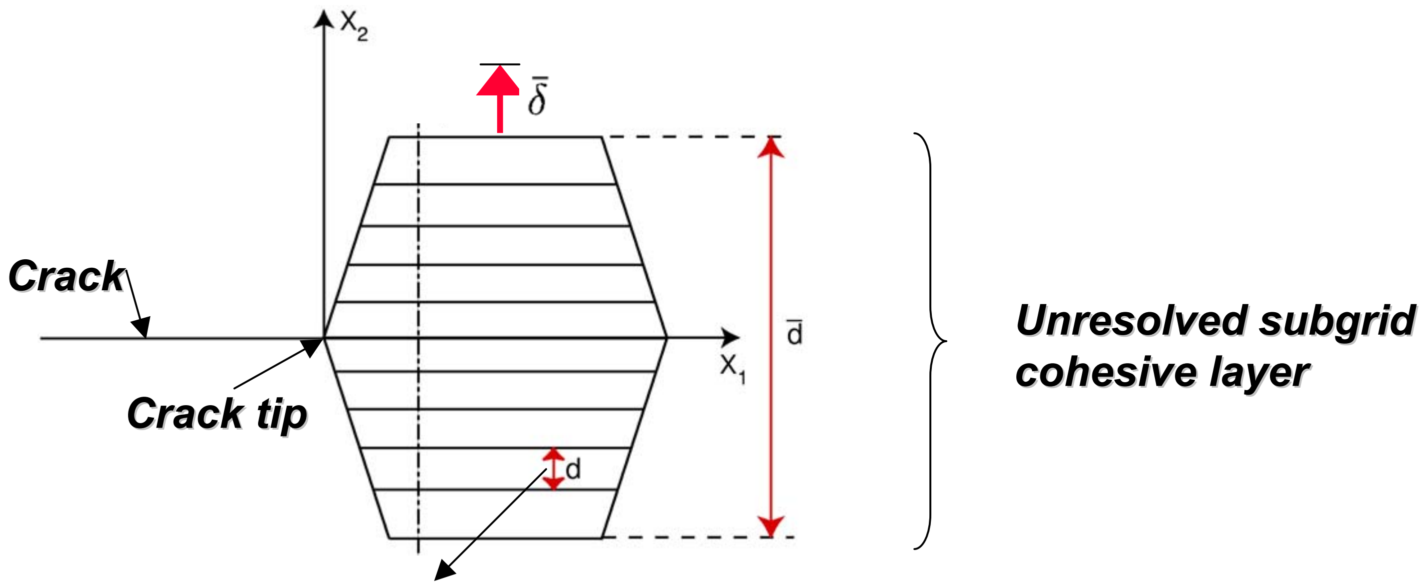
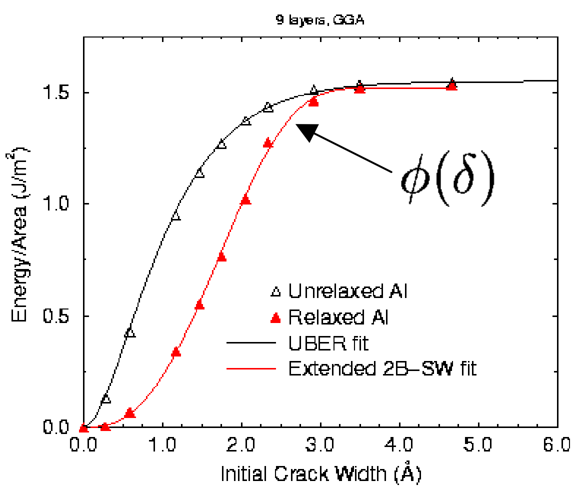
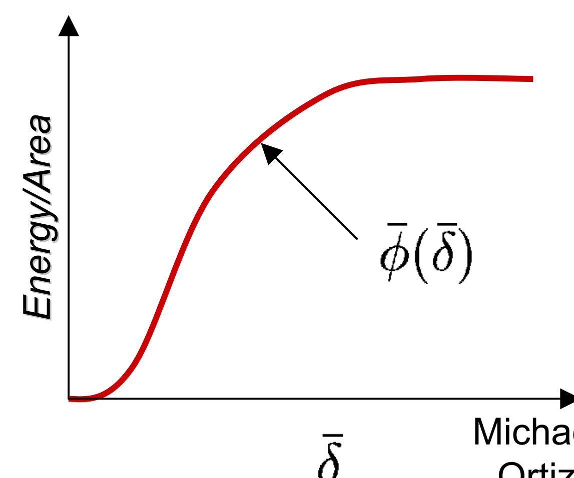
Renormalization of *ab initio* BER



Energy vs. Separation for (111) fcc Al



$$N = \bar{d}/d \gg 1$$



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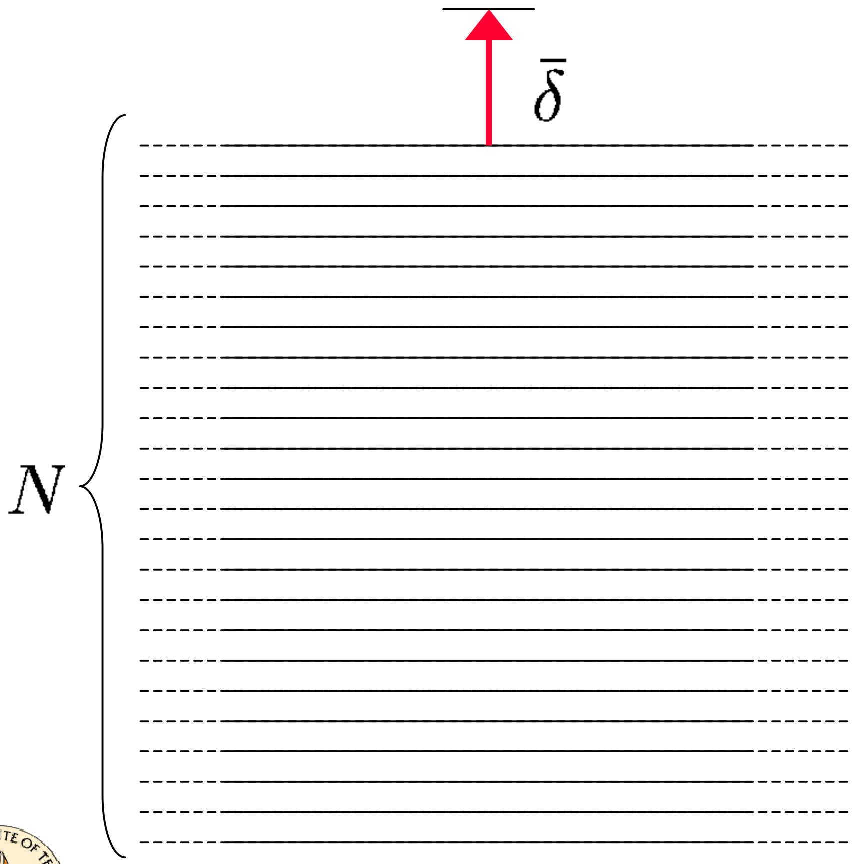
Renormalization & energy minimization

- Operating principle: Energy minimization,



$$E^{\text{tot}} = \sum_{i=1}^{N} \phi(\delta_i)$$

$$\bar{\phi}(\bar{\delta}) = \inf_{\{\delta_1,\dots,\delta_N\}} \sum_{i=1}^{N} \phi(\delta_i)$$

$$\bar{\delta} = \sum_{i=1}^{N} \delta_i$$

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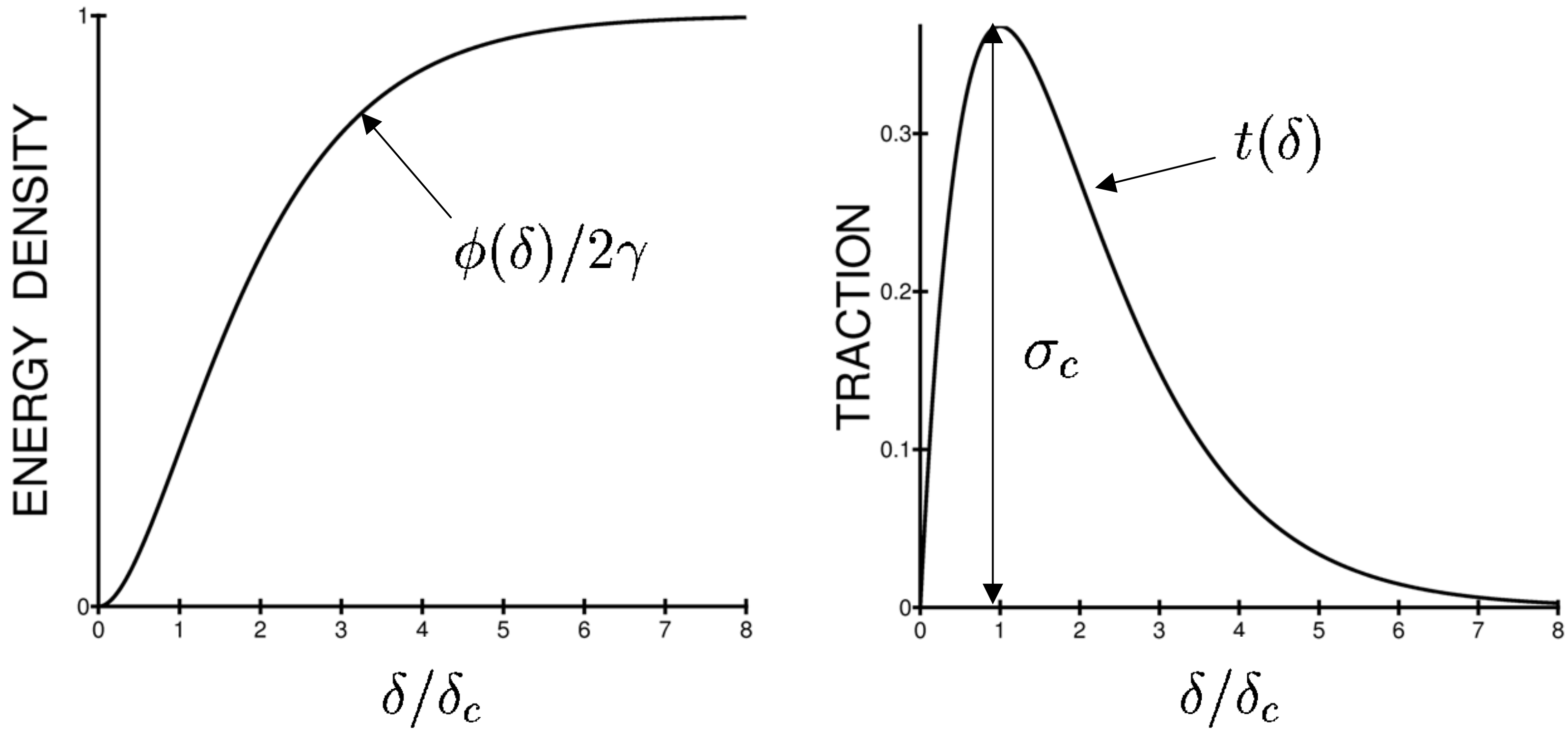
Renormalization - Assumptions



- Assumptions: Interatomic potential continuous, nondecreasing,
  - *i)* $\phi(0) = 0,$
  - *ii)* $\phi \to 2\gamma \;\; as \; \delta \to \infty,$
  - *iii)* $\phi \sim (C/2)\delta^2 + o(\delta^2), \quad C = (1/d)c_{ijkl}m_i m_j m_k m_l > 0$

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Renormalization – Asymptotic analysis

Theorem: *Let* $\phi(\delta) : [0,\infty) \to [0, 2\gamma]$ *be continuous, nondecreasing,* $\phi(0) = 0$, $\phi \to 2\gamma$ *as* $\delta \to \infty$, *and let*

$$\lim_{\delta \to 0^+} \frac{\phi(\delta)}{\delta^2} = \frac{C}{2}, \quad C > 0$$

Then:

$$\bar{\phi}(\bar{\delta}) \sim \min\{\frac{\bar{C}}{2}\bar{\delta}^2, 2\gamma\} = \begin{cases} (\bar{C}/2)\bar{\delta}^2, & \text{if } \bar{\delta} < \bar{\delta}_c \\ 2\gamma, & \text{otherwise} \end{cases}$$

asympotically as $N \to \infty$.

Effective parameters:

$$\bar{\delta}_c = 2\sqrt{\frac{\gamma N}{C}}, \quad \bar{\sigma}_c = 2\sqrt{\frac{C\gamma}{N}}, \quad \bar{C} = \frac{C}{N}$$

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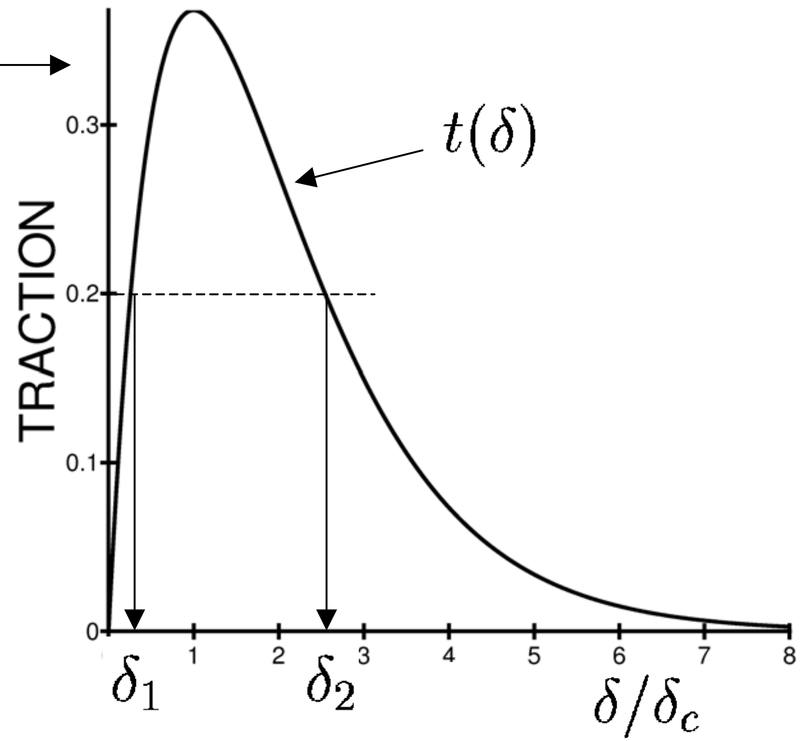
Renormalization – Asymptotic analysis

- Equivalent reformulation of the problem:

$$
\begin{aligned}
\bar{\phi}(\bar{\delta}) &= \inf_{\{(\delta_1,\delta_2),(N_1,N_2)\}} \{N_1\phi(\delta_1) + N_2\phi(\delta_2)\} \\
t(\delta_1) &= t(\delta_2) \\
\bar{\delta} &= N_1\delta_1 + N_2\delta_2 \\
N &= N_1 + N_2 \\
0 &\leq \delta_1 < \delta_c \\
\delta_2 &> \delta_c
\end{aligned}
$$



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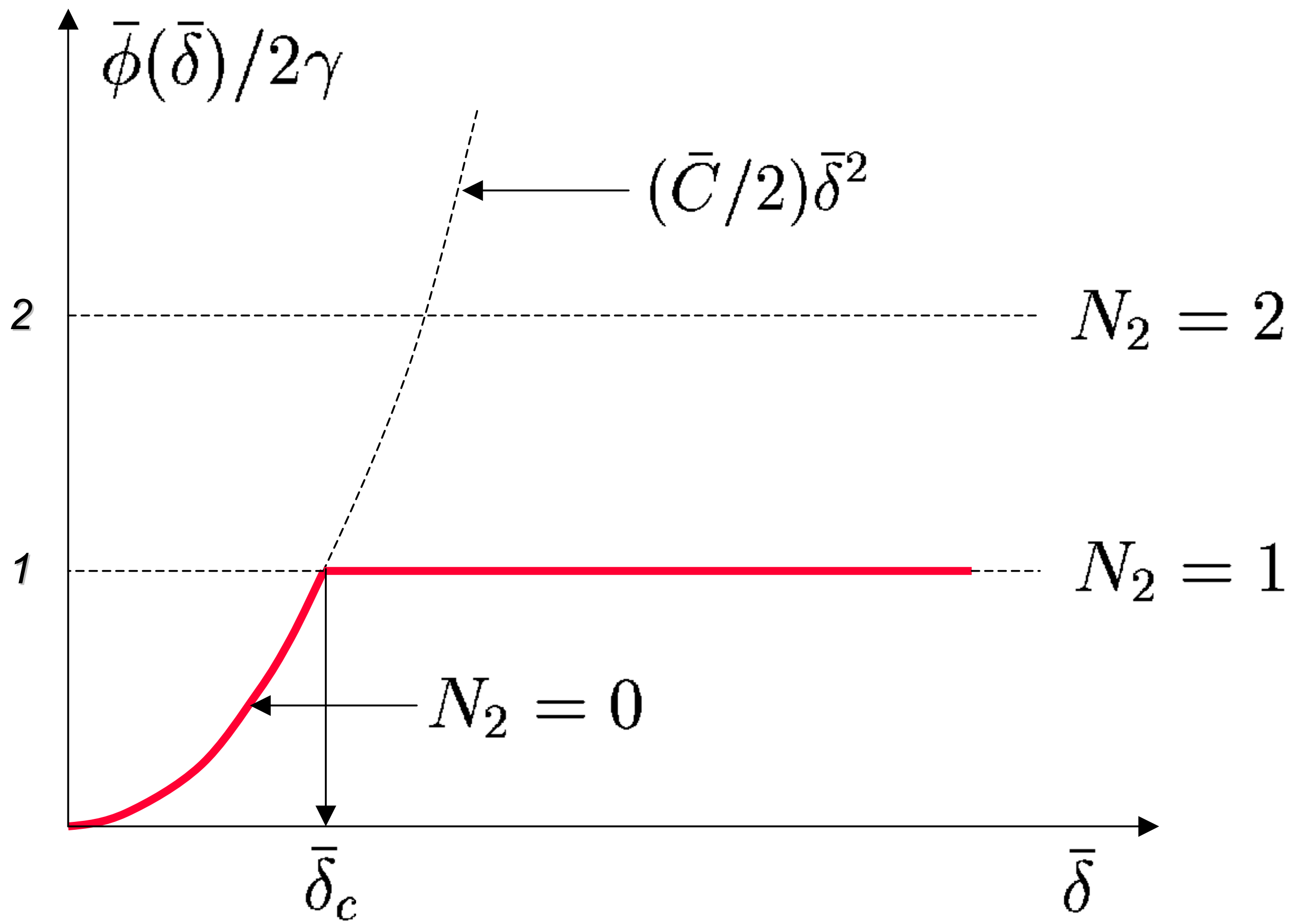
Renormalization – Asymptotic analysis

- Asymptotically, as $N \to \infty$,



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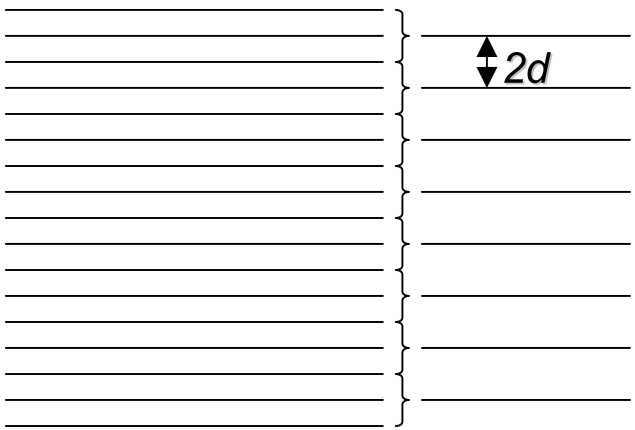
Renormalization of *ab initio* BER

- Cohesive-layer potential attains a *universal asymptotic form* (parabolic + constant), independently of the form of the atomistic BER
- The renormalized peak stress scales as: $1/\sqrt{N}$
- The renormalized critical opening displacement scales as: $\sqrt{N}$
- Surface energy is preserved under renormalization
- The only information from the atomistic BER which `survives' renormalization is:
  - *Elastic moduli*
  - *Surface energy*
- The renormalized cohesive zone size scales as: $R \sim \bar{d}$

The renormalization group

- Renormalization group for cohesive layer:



Decimation

$$
\begin{aligned}
\tilde{\phi}(\delta) &= \inf_{\{\delta_1,\delta_2\}} \{\phi(\delta_1) + \phi(\delta_2)\} \\
\delta &= \delta_1 + \delta_2 \\
(R\phi)(\delta) &= \tilde{\phi}(\sqrt{2}\delta)
\end{aligned}
$$

- Scaling: Set $(R\phi)(\delta) = \tilde{\phi}(\lambda\delta)$. Require elastic moduli to be preserved by the RG transformation:

$$R\phi = \phi, \ \forall\phi \text{ quadratic iff } \lambda = \sqrt{2}$$

RG – Properties of the transformation

- *R* preserves monotonicity: $\delta_1 < \delta_2 \;\Rightarrow\; R\phi(\delta_1) < R\phi(\delta_2)$
- *R* preserves fracture energy: $R\phi(\infty) = \phi(\infty) = 2\gamma$
- *R* preserves elastic moduli: $R\phi''(0) = \phi''(0) = C$
- *R* preserves ordering: $\phi < \psi \Rightarrow R\phi < R\psi$
- The function: $\bar{\phi}(\bar{\delta}) \sim \min\{\frac{\bar{C}}{2}\bar{\delta}^2, 2\gamma\}$ is a fixed point of *R*

RG – Convergence to fixed point

Theorem: *Let* $\phi(\delta) : [0,\infty) \to [0, 2\gamma]$ *be continuous, nondecreasing,* $\phi(0) = 0$, $\phi \to 2\gamma$ *as* $\delta \to \infty$, *and*

$$\lim_{\delta \to 0^+} \frac{\phi(\delta)}{\delta^2} = \frac{C}{2}, \quad C > 0$$

Let:

$$\bar{\phi}(\bar{\delta}) \sim \min\{\frac{\bar{C}}{2}\bar{\delta}^2, 2\gamma\} = \begin{cases} (\bar{C}/2)\bar{\delta}^2, & \text{if } \bar{\delta} < \bar{\delta}_c \\ 2\gamma, & \text{otherwise} \end{cases}$$

$\phi_0 = \phi$, *and*

$$\phi_n = R\phi_{n-1} = R^n \phi_0, \quad n = 1, \dots, \infty$$

Then $\phi_n \to \bar{\phi}$ *uniformly in* $[0, \infty)$.

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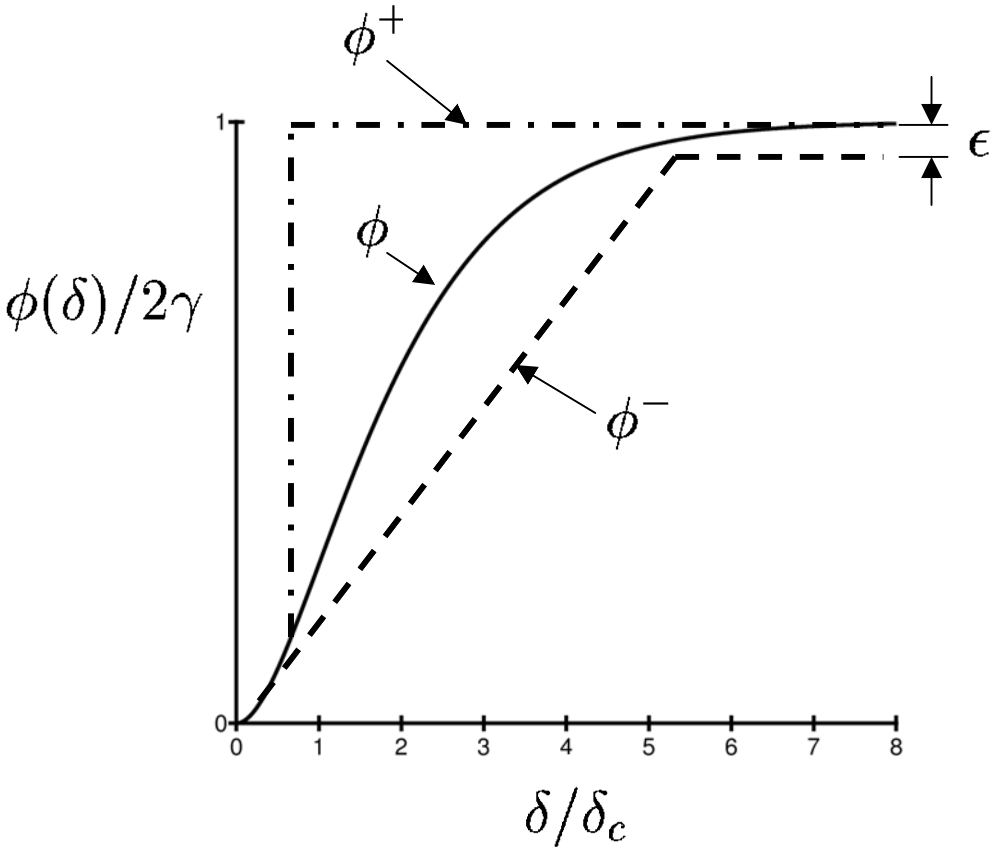
RG - Proof of convergence



$$R^n\phi^{\pm} \to \bar{\phi} \text{ uniformly in } [0,\infty) \Rightarrow R^n\phi \to \bar{\phi} \text{ uniformly in } [0,\infty)$$
$$\text{as } n \to \infty, \quad \epsilon \to 0^+$$

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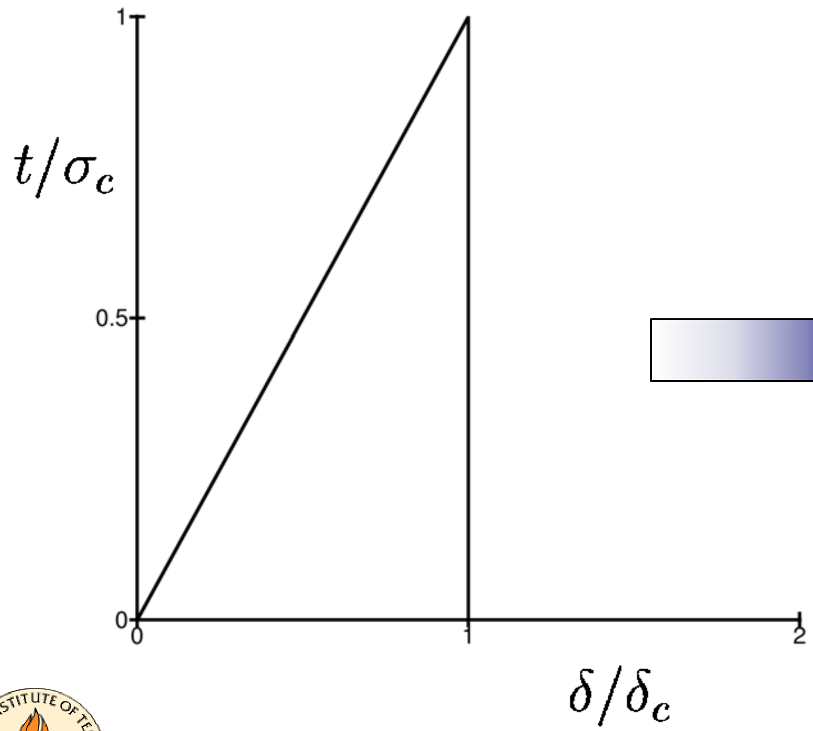
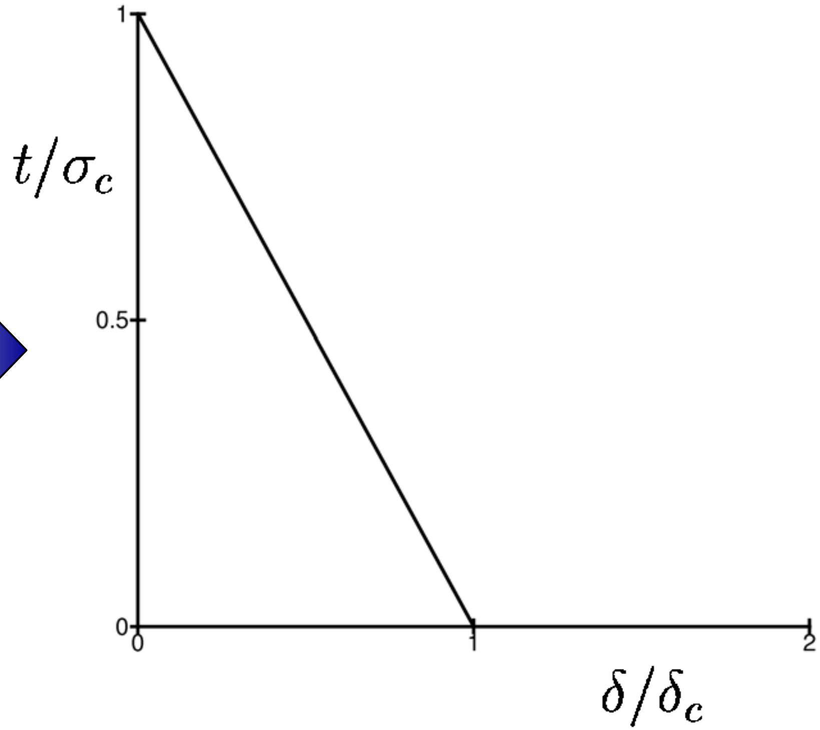
Elastic correction - Cohesive law

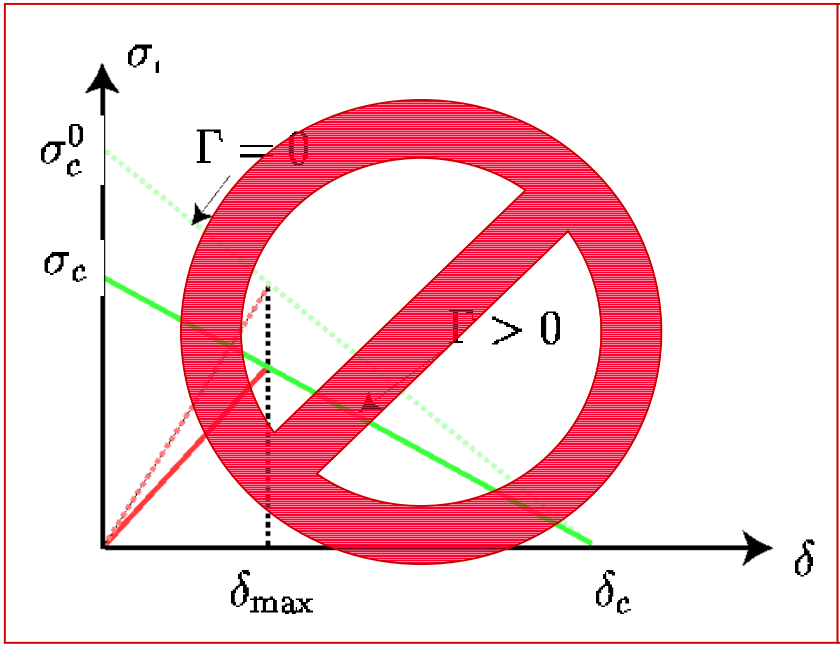
- Need to perform correction to avoid double counting of elasticity of matrix (Rice, 1992; Beltz and Rice, 1992)

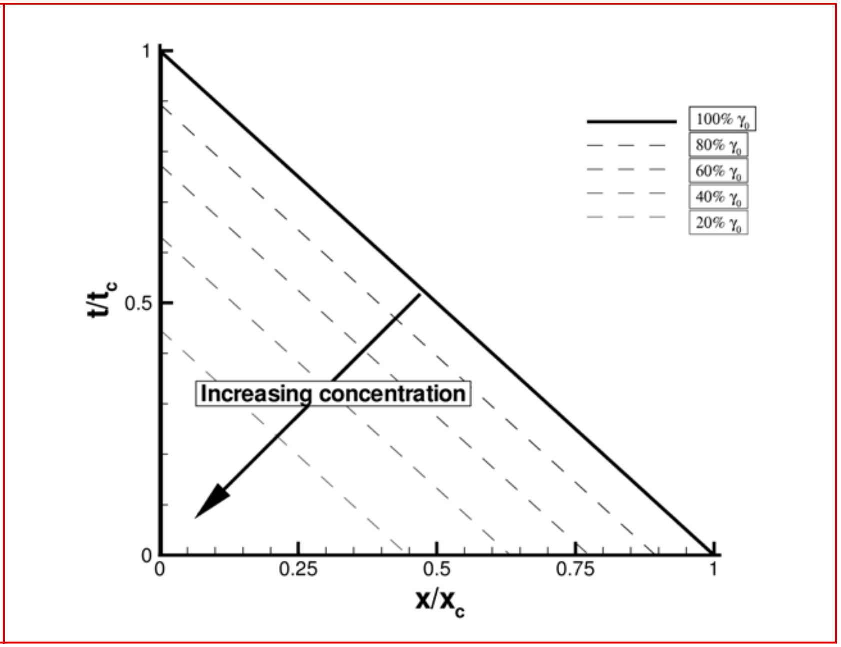




Chemistry-dependent cohesive law

- Assumption: Elastic moduli independent of impurity concentration





$$\bar{\delta}_c = 2\sqrt{\frac{\gamma N}{C}}, \quad \bar{\sigma}_c = 2\sqrt{\frac{C\gamma}{N}}$$

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Concluding remarks

- Multiscale analysis can guide engineering modeling and help eliminate uncertainty
- The lengthscale gap between *ab initio* BERs and engineering models may effectively be bridged by (nonstandard) renormalization
- Renormalization leads asymptotically to a universal form of the macroscopic cohesive law
- Renormalized cohesive laws may be regarded as subgrid models which compensate for the lack of resolution of engineering models
- Connection/interaction to plasticity, microcracking, lattice deffects, and other fracture mechanisms remains to be explored…

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Unsolved problems…

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