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Decohesion Relationships for Hydrogen Induced Grain Boundary Embrittlement in Nickel extracted from Molecular Dynamics Simulations

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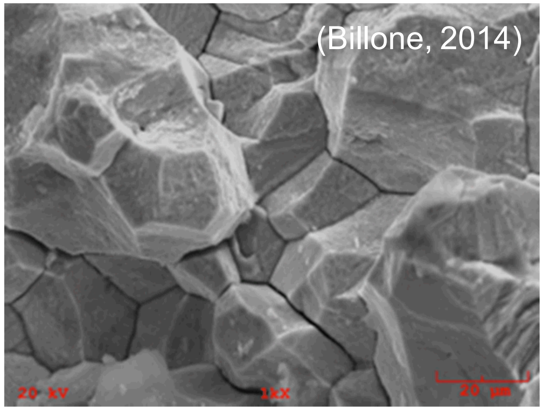
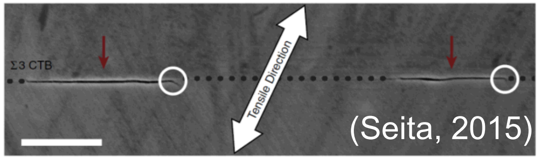
Why Hydrogen Matters

- H segregation to grain boundaries (sinks)
- Formation of metallic hydrides
- H - dislocation interactions (slip interference)

Intergranular Fracture

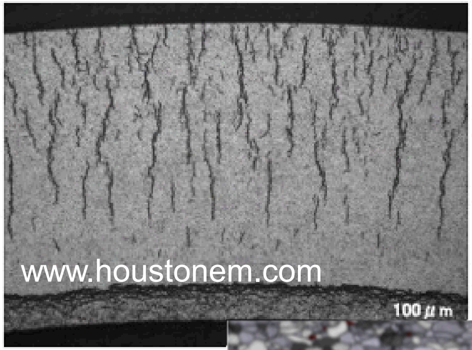


(Billone, 2014)

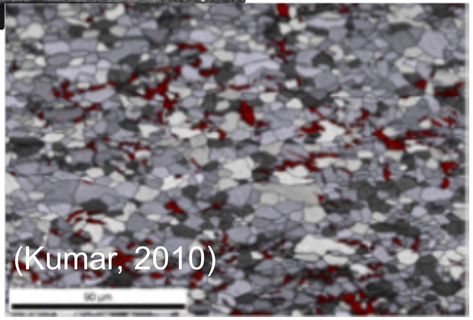


(Seita, 2015)

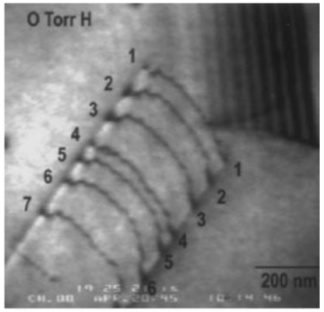
Clad Hydride Cracking

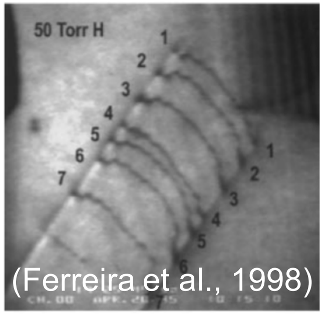


www.houstonem.com


(Kumar, 2010)

H Enhanced Plasticity





(Ferreira et al., 1998)

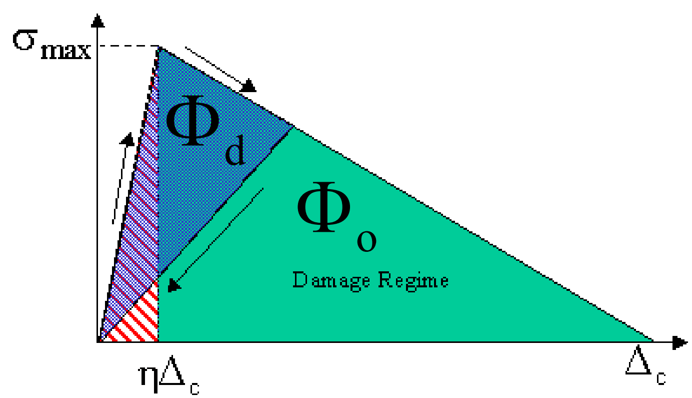
One of DOE's current R&D objectives is to extend lives of reactors and improve storage capabilities → Must understand H embrittlement

Models to describe Interface Decohesion

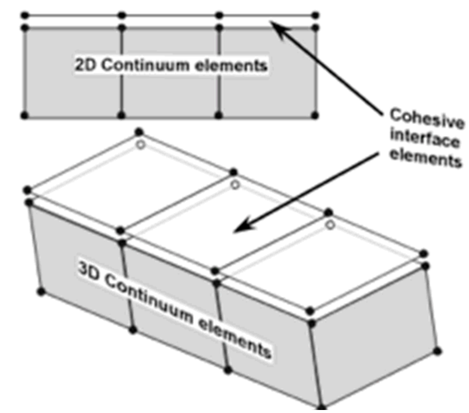
- Traction-separation decohesion potentials have been proposed to allow for predictive simulation of crack propagation path

$$\mathbf{T} = -\frac{\partial \Phi}{\partial \boldsymbol{\Delta}}$$

Needleman (1987)



Zhou and Zhai (1999)



Scheider (2008)

- Limitations to be addressed by atomistics
  - ➢ Do not account for dissipative mechanisms, such as dislocation nucleation and structural rearrangement at the interface during separation
  - ➢ Lack detailed information necessary to distinguish between interfaces with differing degrees of coherency, roughness or impurities

Fracture Simulation Approach

- Steady-state fracture approach (Yamakov, 2006)

Step 1
Build grain boundary structure

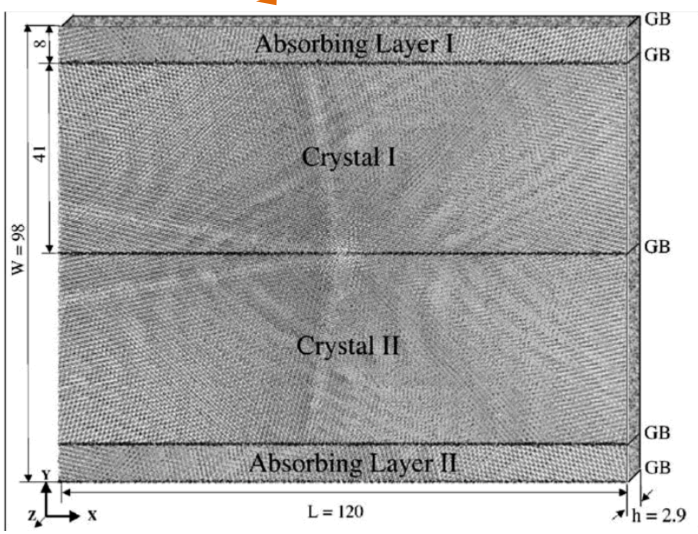
Step 2
Equilibrate system under pretension (driving force)

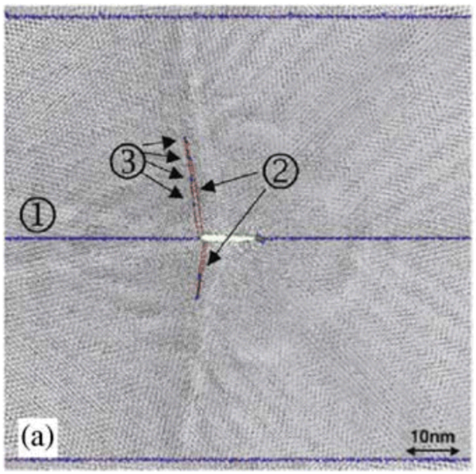
Step 3
Introduce atomically sharp crack

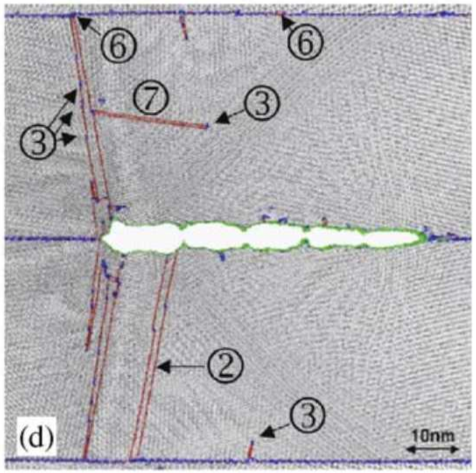
Step 4
Allow crack to grow under tensile prestress

Step 5
Averaging to extract decohesion form

Σ99 [110]







Avoids having to artificially assign a boundary velocity!

Fracture Simulation Approach

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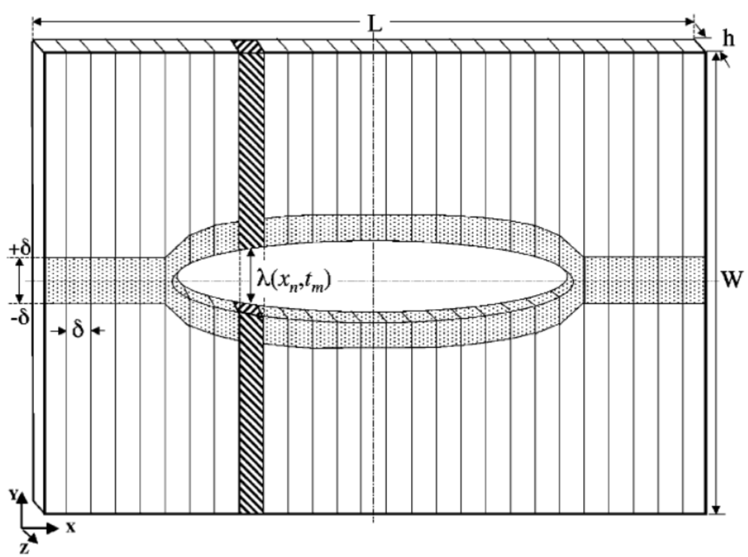
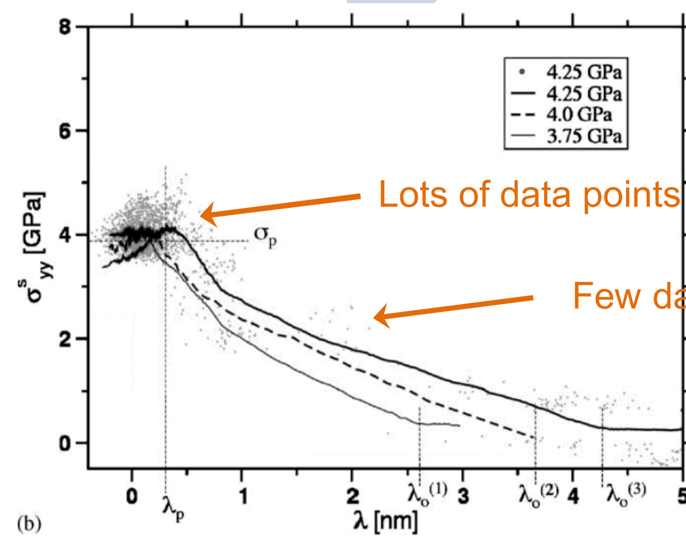


Σ99 [110]



Takes a statistical mechanics rather than a deterministic approach to T-Δ

Adding Hydrogen to the Grain Boundary

Step 1
Build **hydrogenated** grain boundary structure

Step 2
Equilibrate system under pretension (driving force)

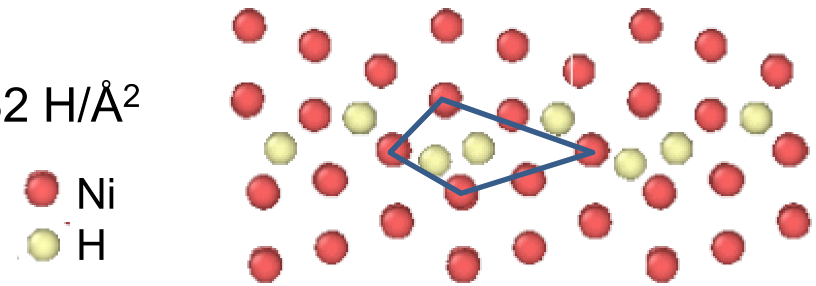
Step 3
Introduce atomically sharp crack

Step 4
Allow crack to grow under tensile prestress

Step 5
Validate results and Extract decohesion law

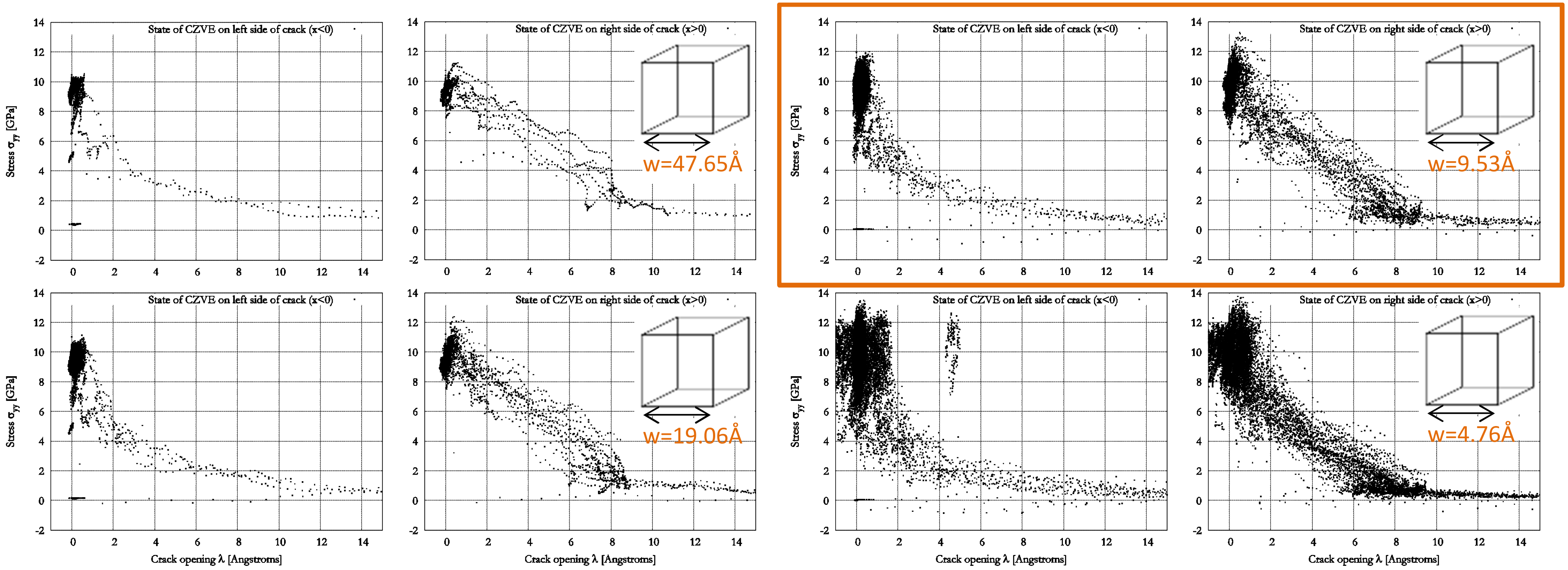
Step 0
Add %H to grain boundary

- Use Monte Carlo simulations by Chris O'Brien (Sandia) to identify the sites and equilibrium coverage of H in a $\Sigma 3$ (112)[110] STGB
  - $\mu = -2.35$ eV
  - Coverage: 0.132 H/Å^2



Role of CZVE Size

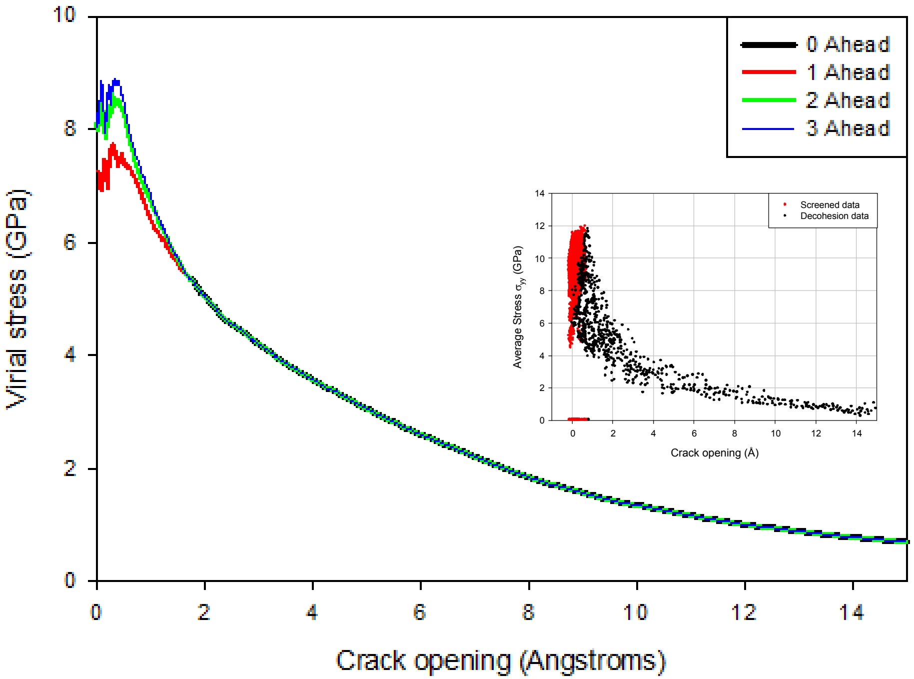
- Role of Cohesive Zone Volume Element size
  - 25%H Σ3 (112)[110] symmetric tilt grain boundaries
  - Hydrostatic prestress of 10 GPa tension prior to crack insertion

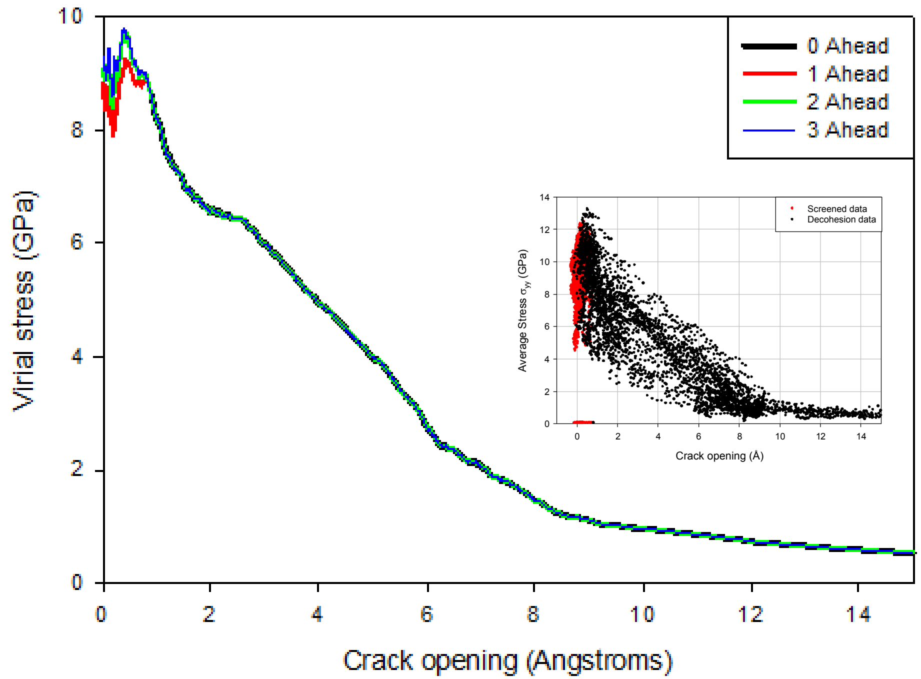


CZVEs too large do not provide sufficient data for statistical averaging, CZVEs too small capture dislocation nucleation processes far ahead of the crack tip

Deconvolution of Elasticity / Decohesion

- How many CZVEs ahead of the crack tip to include?
  - ➢ 25%H Σ3 (112)[110] symmetric tilt grain boundaries
  - ➢ Hydrostatic prestress of 10 GPa tension prior to crack insertion

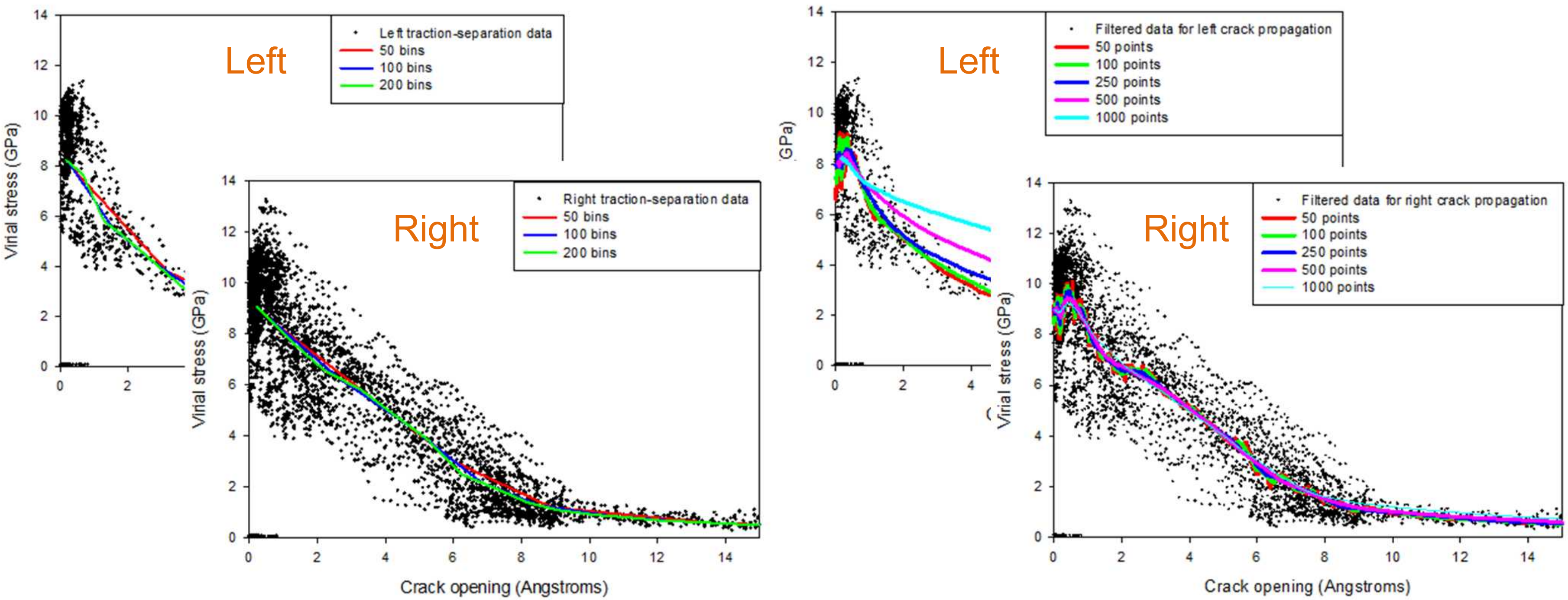




Using data from too many CZVEs ahead of the crack tip influences the peak in the traction-separation relationship

Numerical Averaging Technique

- How should the data be averaged?
  - ➢ 25%H Σ3 (112)[110] symmetric tilt grain boundaries
  - ➢ Hydrostatic prestress of 10 GPa tension prior to crack insertion

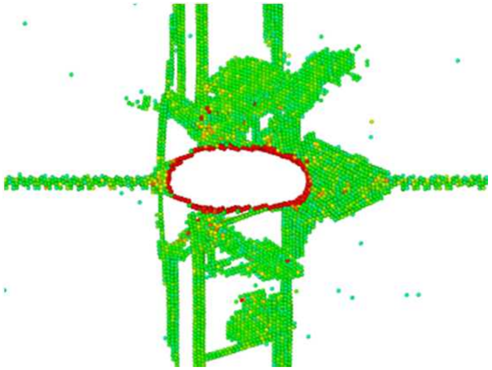


A running average technique is selected with M = 250 points to best capture the decohesion peak and fit the long range CTOD data

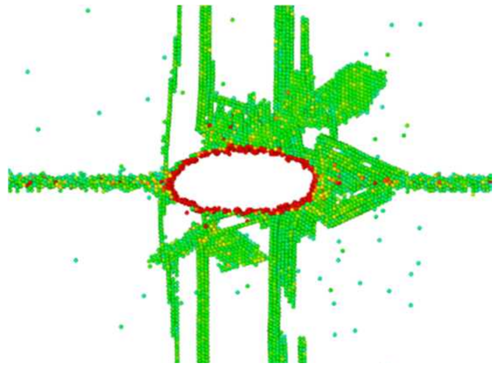
Study of Hydrogen Embrittlement

- Dislocation activity as a function of H coverage
  - ➢ Σ3 (112)[110] symmetric tilt grain boundaries
  - ➢ Prestress of 10 GPa prior to crack insertion

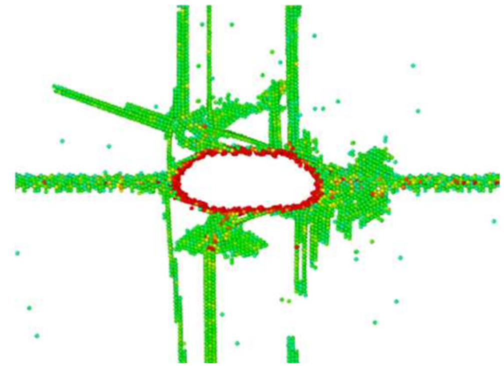
Don’t see much affect of H on plasticity



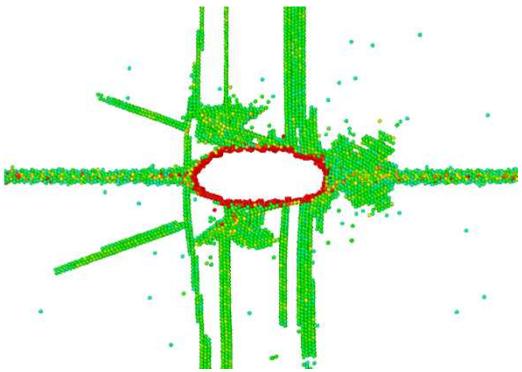
0%H



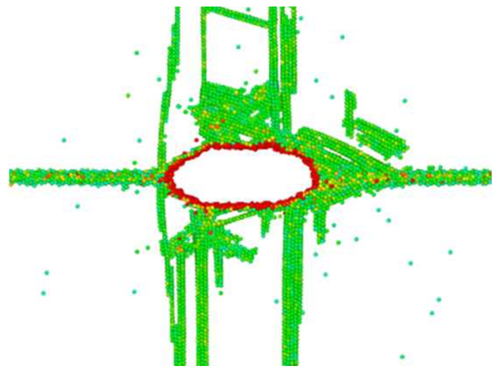
25%H



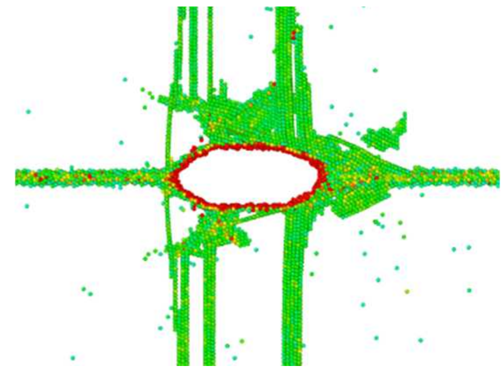
50%H



66.4%H



75%H



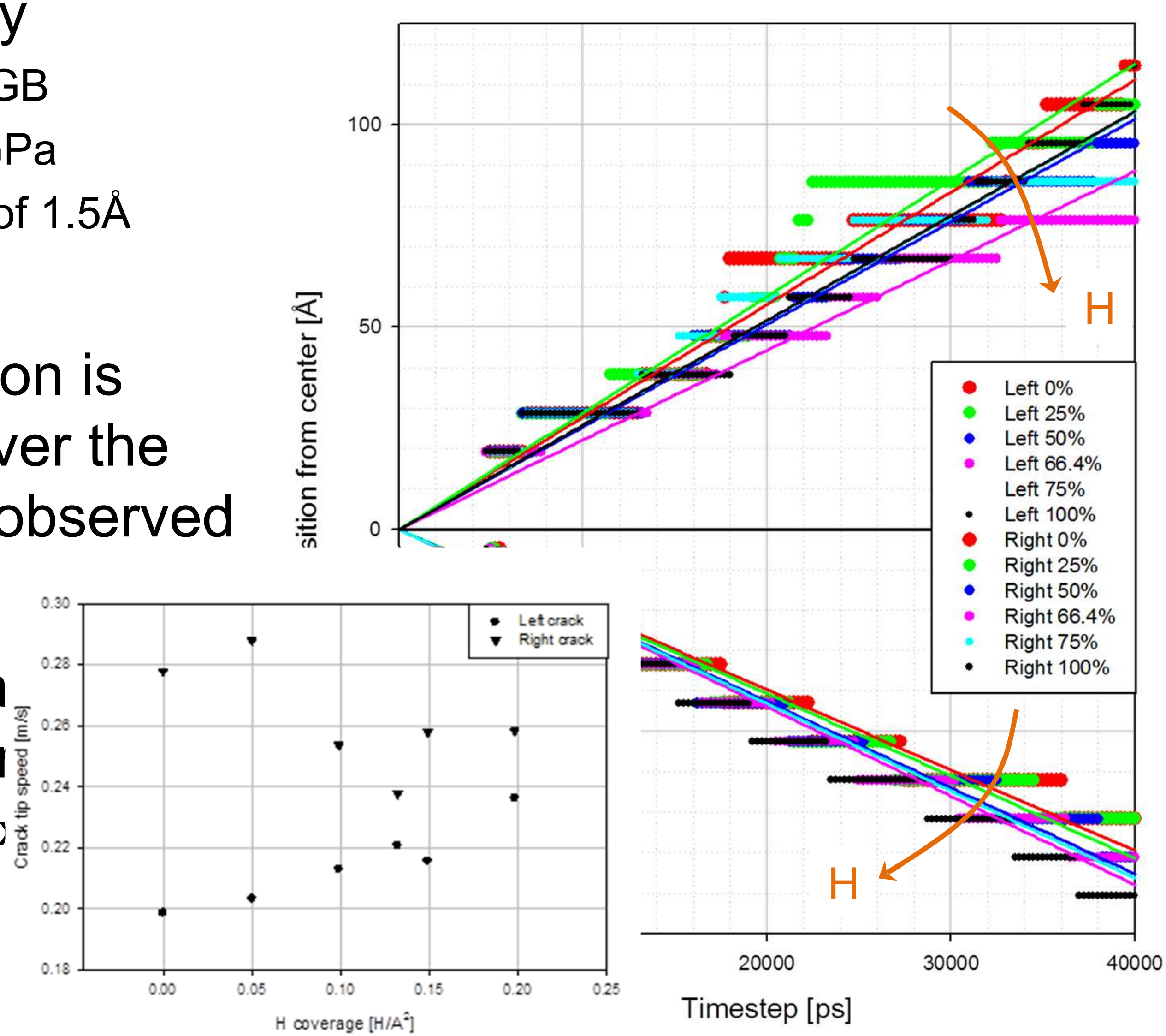
100%H

Study of Hydrogen Embrittlement

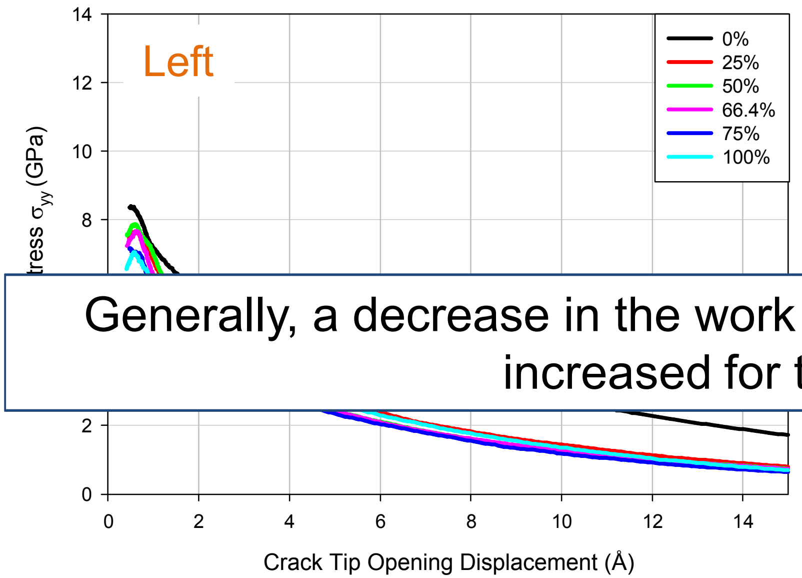
- Crack tip velocity
  - ➢ $\Sigma 3$ (112)[110] STGB
  - ➢ Prestress of 10 GPa
  - ➢ CTOD threshold of 1.5Å

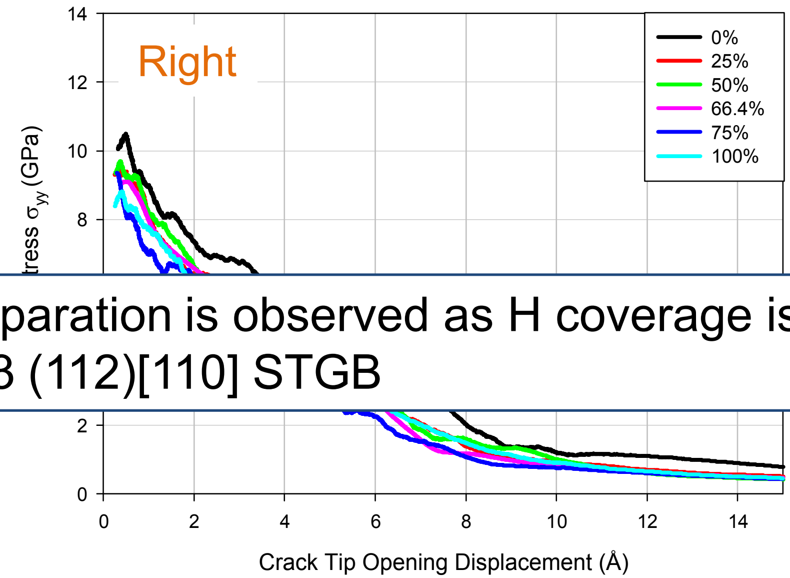
- Crack propagation is "steady state" over the simulation time observed

- Role of H on cra velocity is asymı
  - ➢ Slows down for +
  - ➢ Speeds up for –x

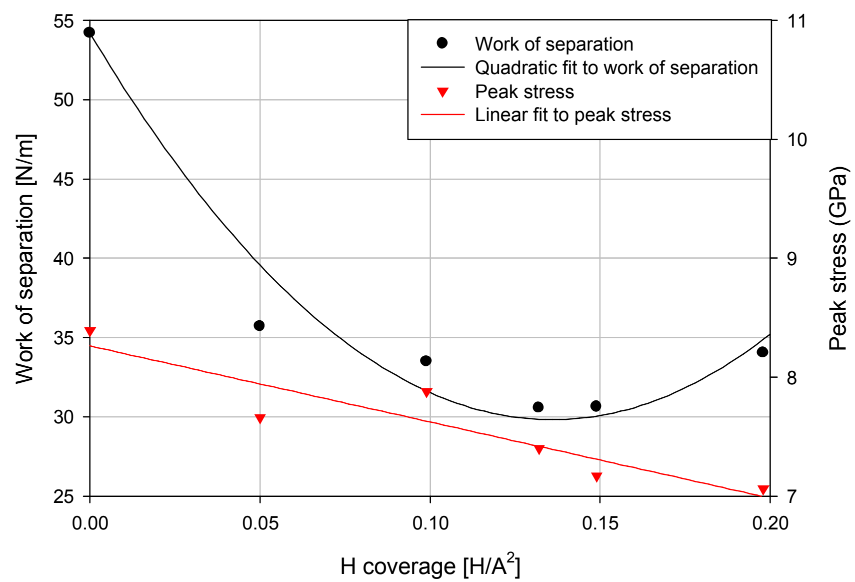


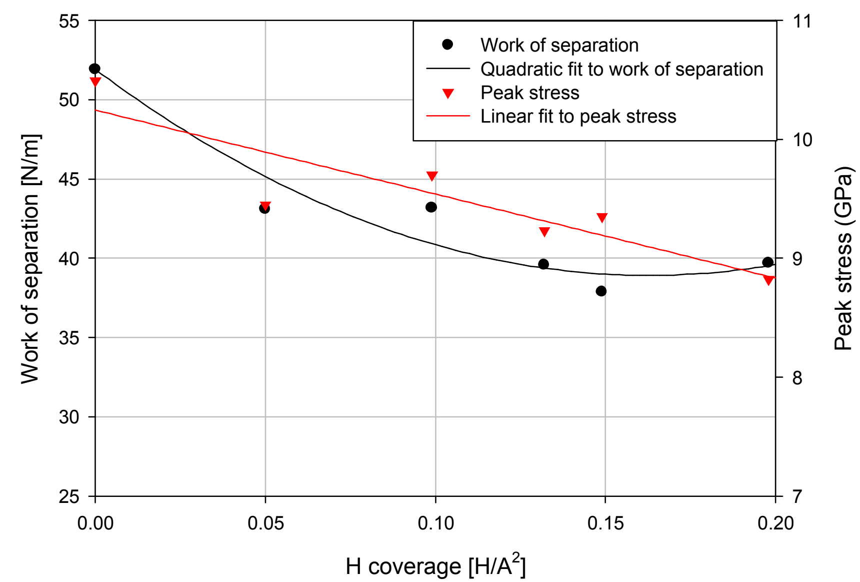
Study of Hydrogen Embrittlement





Generally, a decrease in the work of separation is observed as H coverage is increased for the Σ3 (112)[110] STGB





Conclusions

- An atomistic CZVE method following work of Yamakov et al. (2006) is implemented to study intergranular fracture

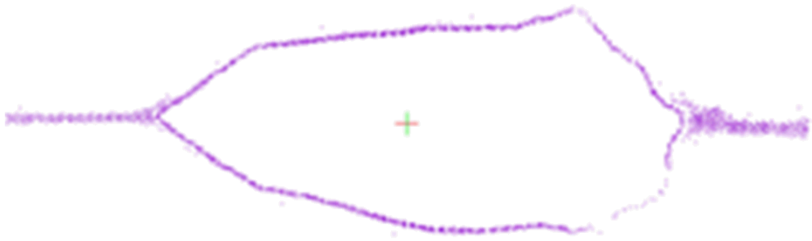
- Numerical parameters for traction-separation
  - Role of CZVE size is understood
  - Method for separating elastic and decohesion response
  - Understanding of how to best average the data

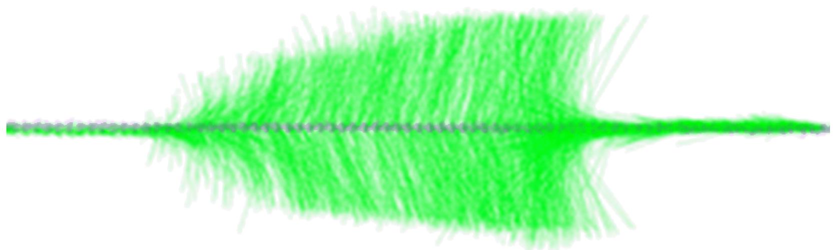
- Hydrogen embrittlement of a $\Sigma 3$ grain boundary
  - Steady-state crack growth is observed with hydrogen having a different effect on crack velocity for left and right propagations
  - Hydrogen generally decreases the work of separation of the grain boundary for both left and right propagations

Barrows, Dingreville, Spearot (2015) Materials Science and Engineering A, 650, 354-364.

Closing Comments

- Analyze the types of dislocations (twinning, slip etc.) nucleating from the hydrogenated grain boundary
- Analyze the diffusion of H along the grain boundary during crack propagation





- This methodology will be applied to many other GB systems, with carefully chosen misorientations