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Hydrogen embrittlement along grain boundaries in nickel based on MD simulation

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Grain boundary fracture and decohesion session
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Sandia National Laboratories

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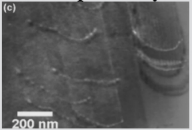
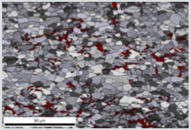
Hydrogen-assisted degradation limits structural performance

Hydrogen-enhanced local plasticity



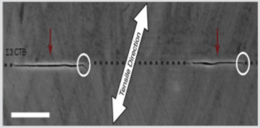
Ferreira, Acta Mater, 1998

Brittle hydride



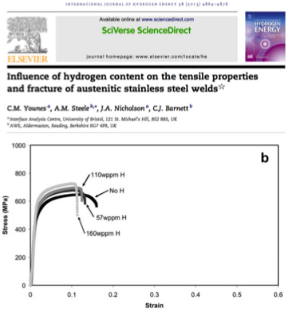
Kumar, J. Nucl. Mater, 2010

Hydrogen-assisted decohesion

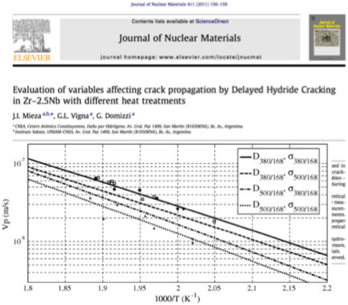


Seita, Nature Comm, 2015

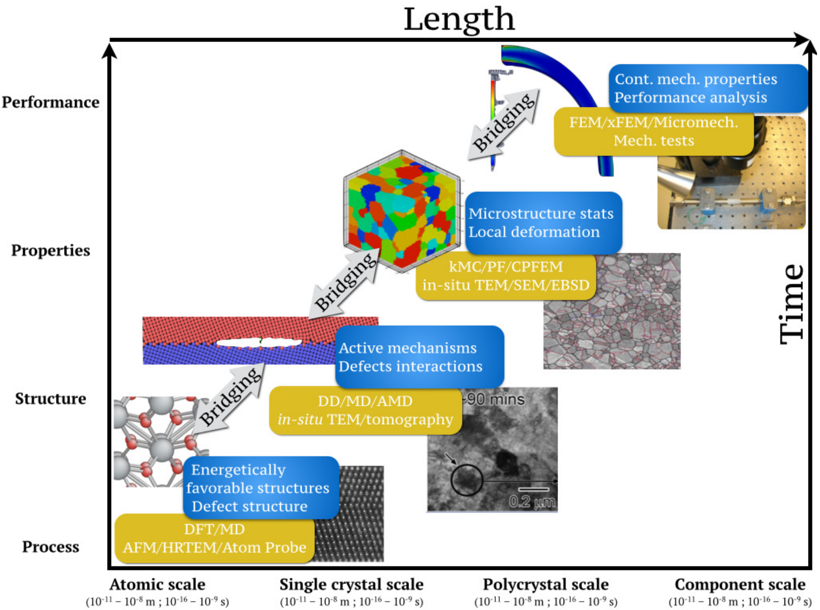
Loss of ductility



Hydride cracking



Challenges in modeling hydrogen embrittlement...



Challenges in modeling hydrogen embrittlement...

Length

A muti-scale, multi-physics approach to H-induced intergranular fracture requires understanding (among others):

- **Bulk kinetics of impurity elements (atomistic scale)**:
  - Trapping mechanisms.
  - Solubility.
- **How dislocation interactions with grain boundaries affect fracture of interface (grain scale).**
- **Relationship between solute coverage and reversible fracture work for range of boundaries (continuum scale).**
- **Reliable computational tool**:
  - Remain computationally tractable.
  - Amenable to implementation in current codes.

Atomic scale (10^{-11} – 10^{-8} m ; 10^{-16} – 10^{-9} s)
Single crystal scale (10^{-11} – 10^{-8} m ; 10^{-16} – 10^{-9} s)
Polycrystal scale (10^{-11} – 10^{-8} m ; 10^{-16} – 10^{-9} s)
Component scale (10^{-11} – 10^{-8} m ; 10^{-16} – 10^{-9} s)

Today's reflection and overview

1. **Where hydrogen matters...**
2. **Steady-state crack propagation using atomistic simulations**
   - Deriving a statistical traction–displacement relationship along GBs from atomistic simulations
   - Study of H embrittlement
3. **Perspective and summary**
   - Reality check

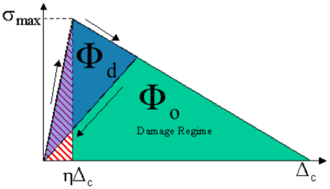
MD simulation are recast to obtain an average continuum traction–displacement relationship to represent cohesive zone interaction along a characteristic length of the grain boundary interface for the cases of ductile and brittle decohesion.

- Deriving decohesion models of hydrogenated GB from atomistic simulations.
- Extract traction–displacement relationship through a statistically meaningful approach.
- Example of crack propagation for lateral twin GB ($\Sigma 3$ (112) GB).

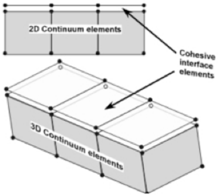
Classical continuum models for interfacial decohesion

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

Needleman (1987)



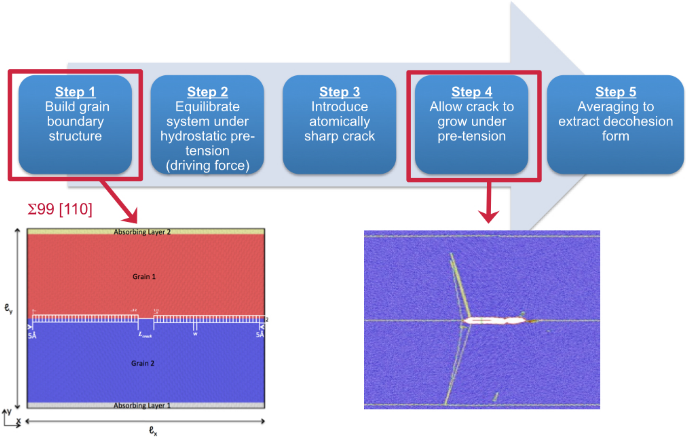
Zhou and Zhai (1998)



Scheider (2008)

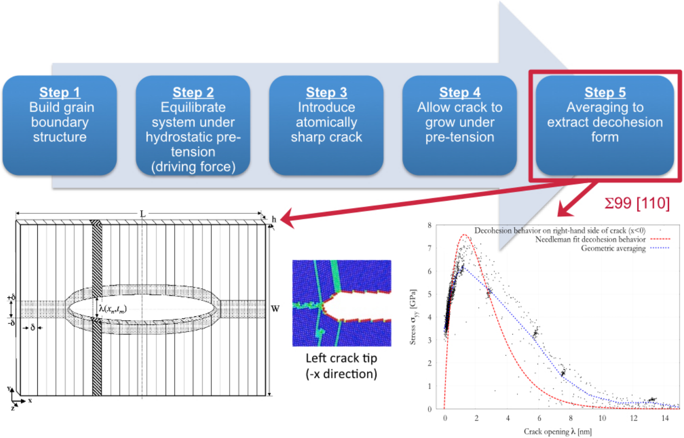
- Traction-separation decohesion potentials have been proposed to allow for predictive simulation of crack propagation path.
- Limitations to be addressed by atomistics:
  - Do not account for dissipative mechanisms, such as dislocation nucleation and structural rearrangement at the interface during separation.
  - Lack detailed information necessary to distinguish between interfaces with differing degrees of coherency, roughness or impurities.

Fracture simulation approach using MD (1/2)



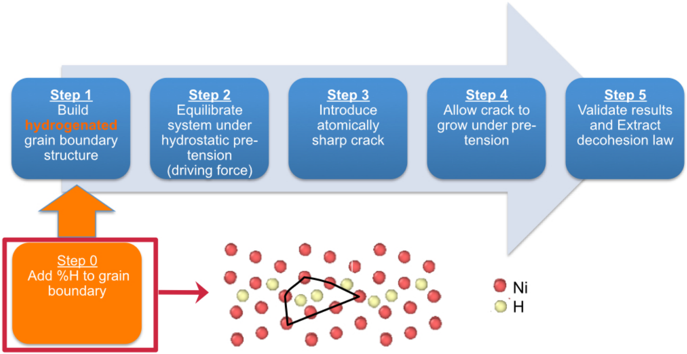
- Avoids having to artificially assign a boundary velocity!
- Work originally proposed by V. Yamakov et al. (2006).

Fracture simulation approach using MD (2/2)



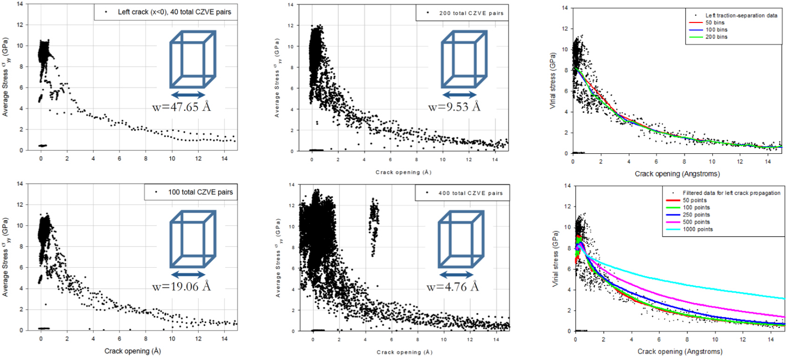
- Takes a statistical mechanics rather than a deterministic approach to T–Δ

Adding hydrogen to the GB



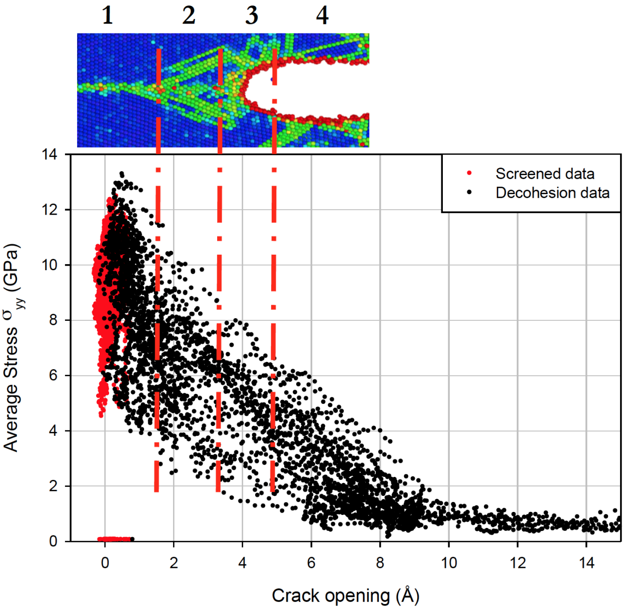
- Use Monte Carlo simulations to identify the sites and equilibrium coverage of H in a Σ 3 (112)[110] STGB
- A range of under and over saturated H coverages are examined with respect to thermodynamic equilibrium
  - 0%H $\rightarrow$ 100% H relating to "favorable sites" occupied.
  - $0\mathrm{H}/\AA^2 \rightarrow 0.198\mathrm{H}/\AA^2$ coverages along the GB.

Statistical approach to extract traction-separation relationships

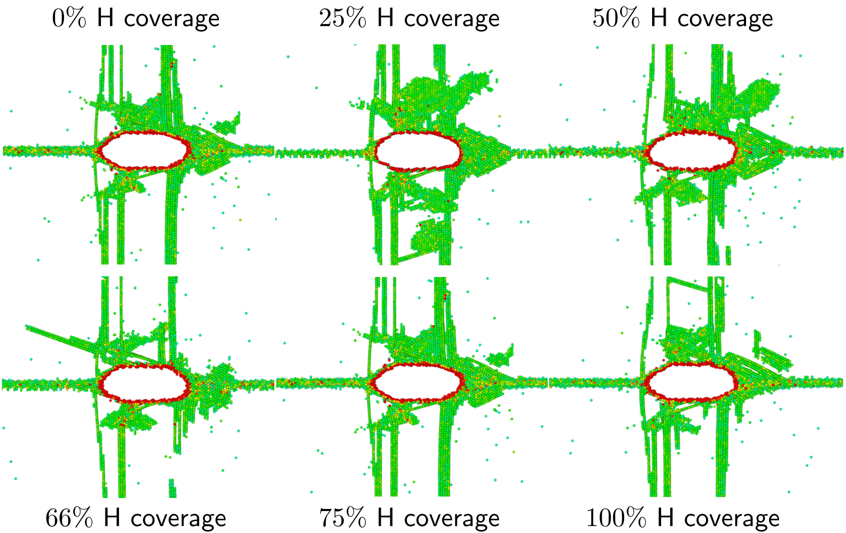


- CZVEs too large do not provide sufficient data for statistical averaging, CZVEs too small capture dislocation nucleation processes far ahead of the crack tip.
- Using data from too many CZVEs ahead of the crack tip influences the peak in the traction-separation relationship.
- Using running average technique points to best capture the decohesion peak and fit the long range CTOD data.

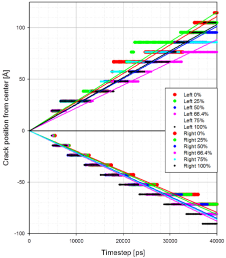
Deconvolution of the elastic and decohesion behavior

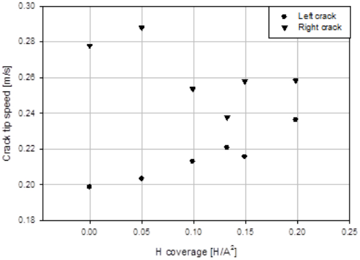


Crack tip plasticity: Hydrogen saturation at the grain boundary influences both the structure of the grain boundary and dislocation nucleation during crack propagation



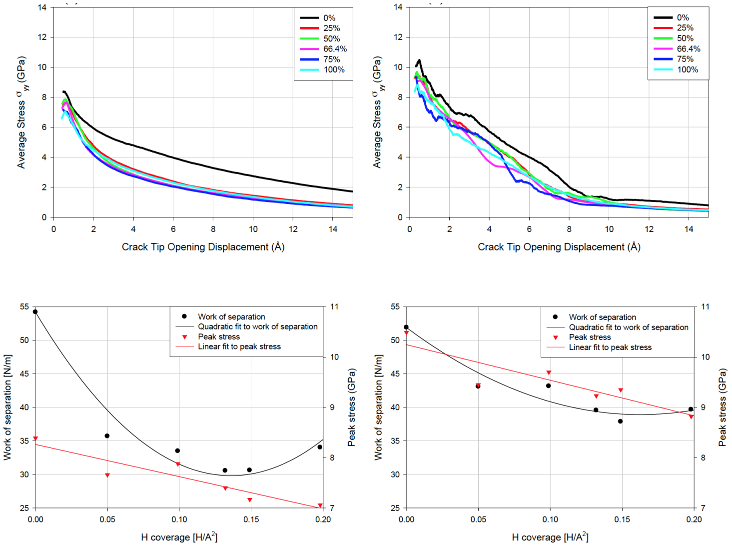
Asymmetric of crack propagation in opposite directions along GB indicates multiple mechanisms at play





- Crack propagation is “steady state” over the simulation time observed.
- In one direction, the crack propagates in a brittle manner by cleavage (crack tip velocity generally increases with increasing H concentration).
- In the other direction, the propagation is ductile (crack tip velocity generally decreases with increasing H concentration).

Traction-separation relationships clearly illustrate the role of H on the GB embrittlement



Immature elements of H embrittlement modeling...

- **Multiple length scales and mechanisms at play simultaneously:**
  - Need to link lower length scales results to meso models to describe mechanical properties over higher length scales and to incorporate scale effects in more realistic way.
  - H diffusion and trapping are stochastic by nature and so are some of the deformation mechanisms associated with their mechanical behavior: **integration of fractal and/or stochastic behaviors into models**.
  - Interplay between hydrogen-induced mechanisms such as HID and HELP, and the structure of the grain boundary relative to the lattice crystallography is a critical aspect of hydrogen embrittlement
- **Verification and validation:**
  - Dedicated experiments at relevant length/time scale.
  - "Extreme environments" have limited/no data available: **data gap interpolation**?

Summary

- Information gleaned from atomistic studies can be directly used in higher length scale formulations for intergranular fracture, through the proposed atomistic analog to a continuum cohesive zone model element.
- Careful attention needs to be paid to the statistical approach used to extract the traction–displacement relationship.
- Asymmetric crack propagation in the two opposite directions along the grain boundary.
  - In one direction, the crack propagates in a brittle manner by cleavage.
  - In the other direction, the propagation is ductile.
- Work of separation generally decreases with increasing H saturation until a minimum is reached around the equilibrium H saturation.
- Peak stress during decohesion decreases with increasing H concentration.