SAND2016-7876PE

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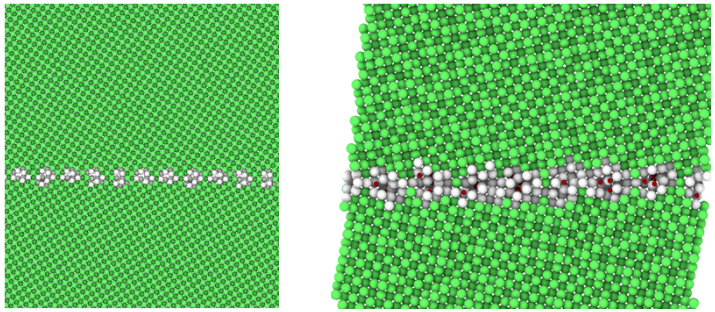
Effect of H atmospheres on grain boundary migration



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Supervised by
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Org. 6233: Structural and Thermal Analysis

SAND2016- PE

6220/6230 summer student mini-symposium
August, 16th 2016, Sandia Nat'l Labs, Albuquerque NM

Outline

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1. Hydrogen embrittlement

2. What can we learn from atomistic modeling

3. Modeling effects of H atmospheres on grain boundary migration

4. Conclusion

Hydrogen embrittlement

Image from SF Chronicle

- **Where is the H coming from?** Processing, cleaning, coatings, or simply from atmospheric conditions
- Tends to cause decreases in ductility, which in application can lead to **catastrophic failure of components** well before their expected lifetime
- "The recognition of H embrittlement in metals and alloys dates back to the nineteenth century. Yet, the atomic process of this macroscopic phenomenon remains elusive."[1]

[1]Wen-Tong Geng, Arthur J. Freeman, Gregory B. Olson , Yoshitaka Tateyama, and Takahisa Ohno (2005)

Degradation mechanisms

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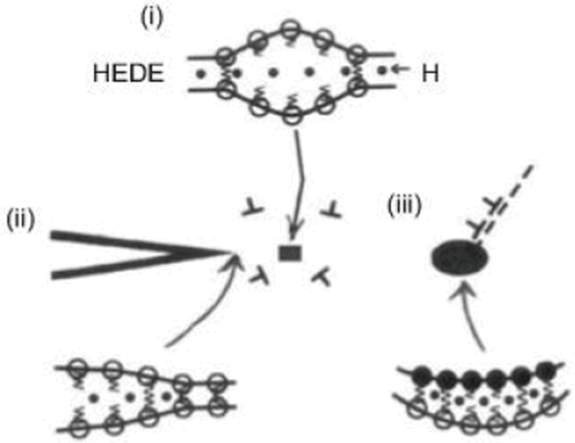
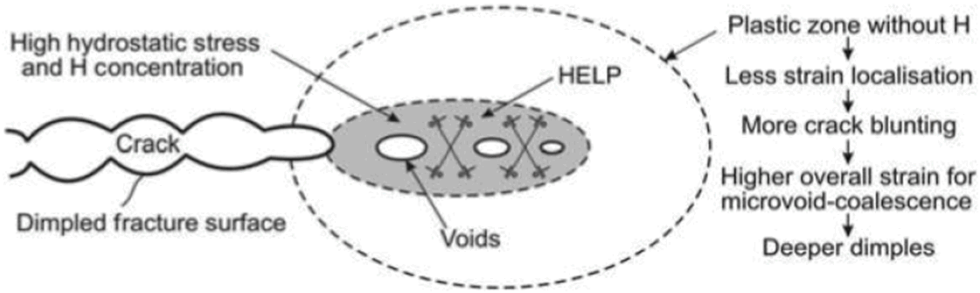
Enhanced decohesion (HEDE)



Localized plasticity (HELP)



- **Underlying principle:**
  - Segregation of H in regions with high stresses, T, solute gradients
  - Activation of multiple mechanisms depending on loading mode, temperature, H pressure etc.
- Trapping/segregation sites (single defects, precipitates, grain boundaries) play a crucial role in the degradation process:
  - Some microstructural features are **more/less susceptible to H effects**.

What can we learn from atomistic modeling

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- **What we are missing:**
  - On-going debate on why embrittlement occurs in terms of physical mechanisms
  - Measurements of H at atomic distance scales is not yet feasable with experimental techniques

- **What can atomistic simulations do:**
  - Measurements of H at atomic distance scales is not yet feasable with experimental techniques
  - Provide direct mechanistic understanding of how H interacts with defect structures in metals

Basics of molecular dynamics

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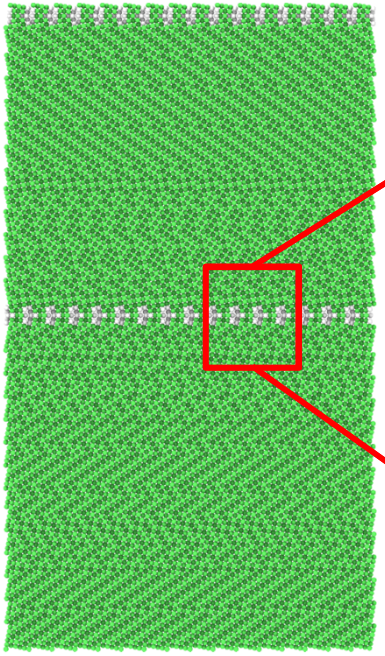
1. Start with the positions of all atoms in a system
2. Given the interaction potential between the particles and assuming they behave classically solve

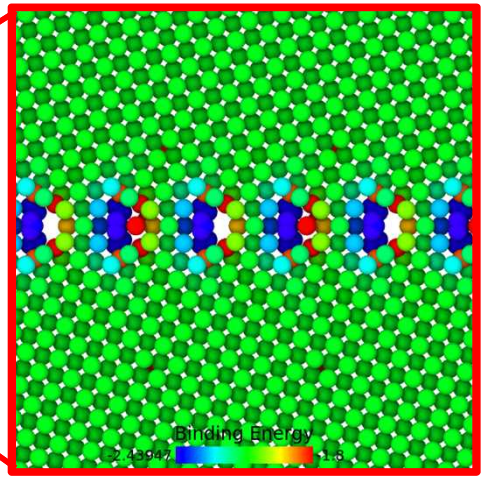
$$\mathbf{F} = m\mathbf{a}; \quad \mathbf{F} = \frac{\partial \mathbf{U}}{\partial \mathbf{x}}$$

3. Update the particle positions and repeat

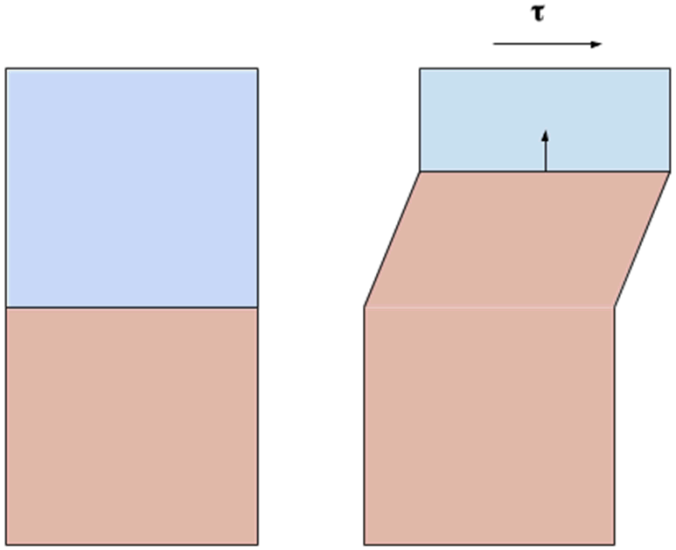
Atomistic of grain boundaries



GB construct



Segregation sites



Shear coupling GB migration

- **Segregation sites:** Grain boundaries tend to provide strong binding sites for solute atoms
- **Shear coupling GB migration:** When a shear stress is applied parallel to a GB the boundary will migrate in a perpendicular direction (almost always), this is called 'shear coupling'

Shearing of GBs

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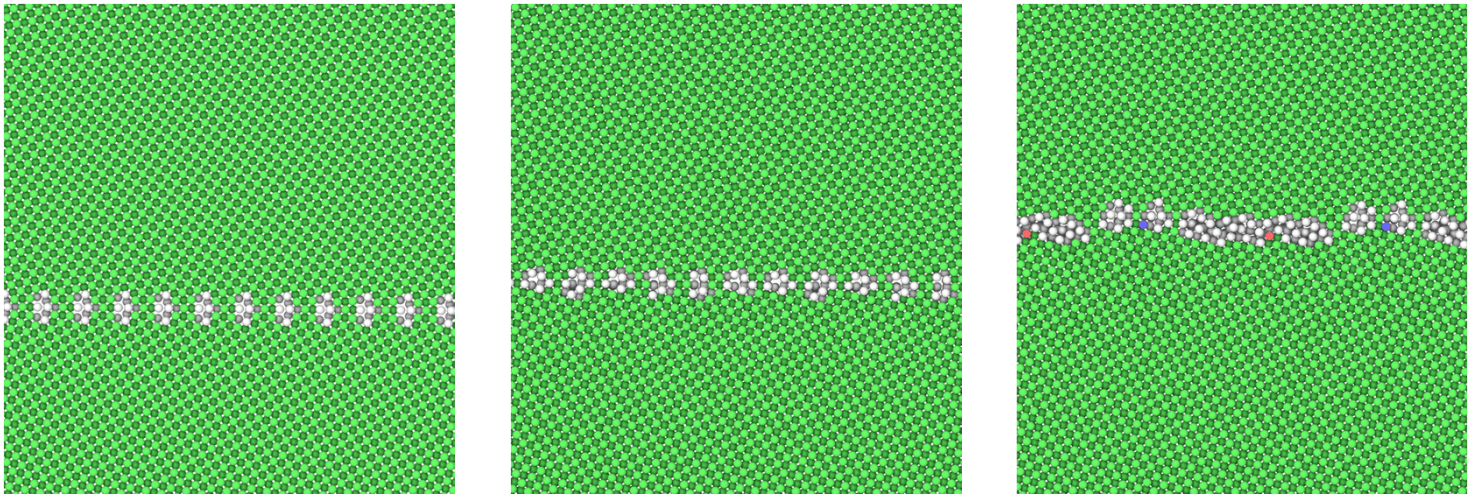
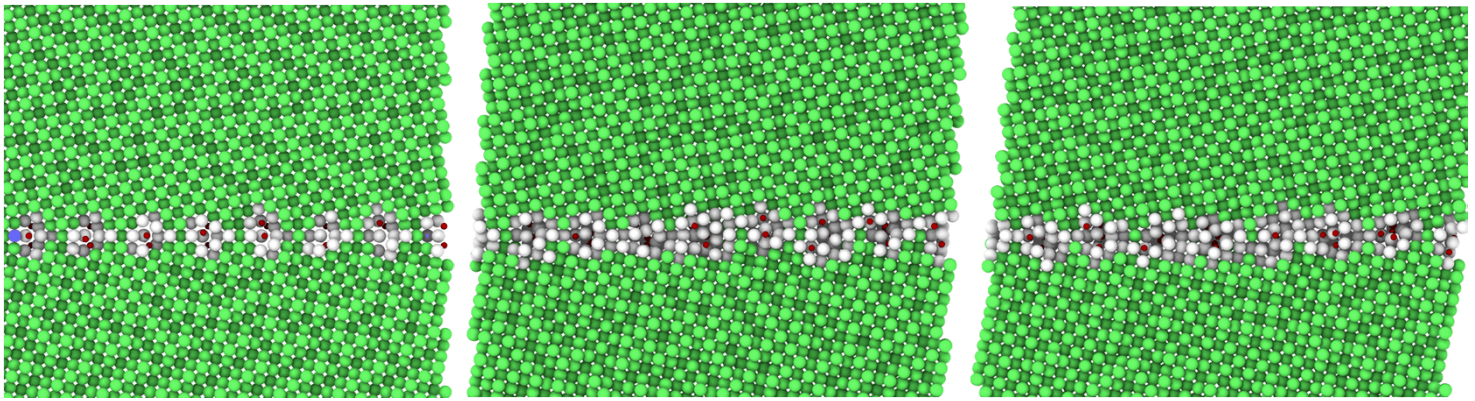
No H



Migration

With H



Suppression of migration

Discussion

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- Previous work has focused on GB migration for a specific class of GBs with no solute atoms

- **High throughput analysis of a wide variety of GB**:
  - Symmetric tilt GB
  - Assymetric
  - Twist
  - Mixed

- **Susceptibility of GB to H effects**:
  - Velocity and shear coupling as a function of background H concentration

Conclusion

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What can we learn from this study?

- Improves our understanding of H effects on plasticity
  - Microstructure evolution under harsh environments
- Provides more information to evaluate validity of the proposed mechanisms
- Manuscript in preparation

This study serves as an example of a methodology, applicable to future atomistic study of systems with introduced H atmospheres

Personal: Luke Costello

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Education:

- B.S. Oregon State University, Department of Chemistry
- M.S. University of Delaware, Department of Materials Science and Engineering
- In progress: Ph.D. Georgia Institute of Technology, Woodruff School of Mechanical Engineering

Research experience:

- Structural characterization of small molecules by gas phase electron diffraction and density functional theory (K. Hedberg, Oregon State U.)
- Silicon surface passivation with application to high efficiency silicon solar cells (R. Opila, U. of Delaware)
- Atomistic aspects of H embrittlement (D. McDowell, GaTech)