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Hydrogen Effects on Dislocation Dynamics and Metal Plasticity

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Overview

- Dislocation dynamics (DD) primer
- Adding hydrogen effects to DD
- Simulations with hydrogen effects

Dislocation dynamics

- Simulate motion of dislocation lines in an elastic medium

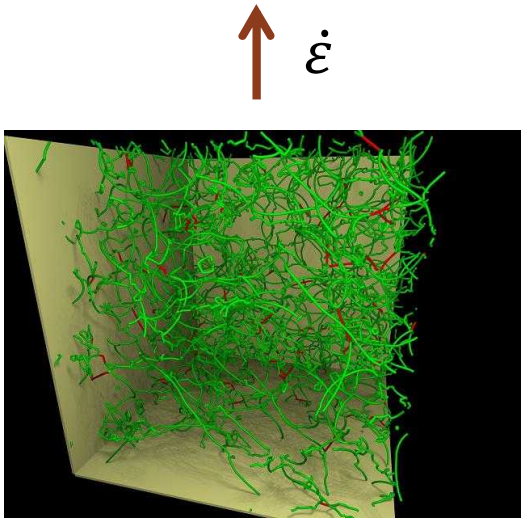
- Physics controlled (primarily) with:
  - Driving force calculation
    - Elastic interactions
    - Applied stresses

      .
      .
      .
  - Mobility law

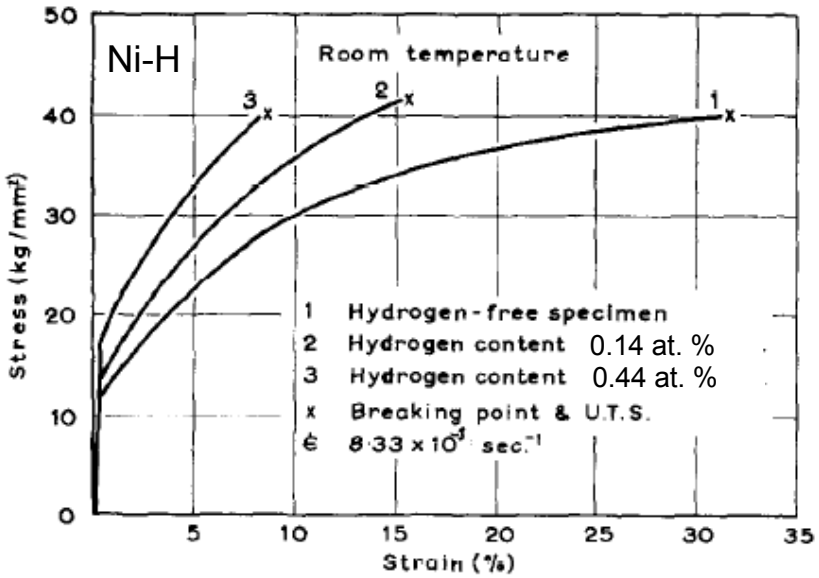
$$B\mathbf{v} = \boldsymbol{f}_{el} + \boldsymbol{f}_{app} + \cdots$$

Drag Coefficient

- To date, models primarily developed for *pure metals*

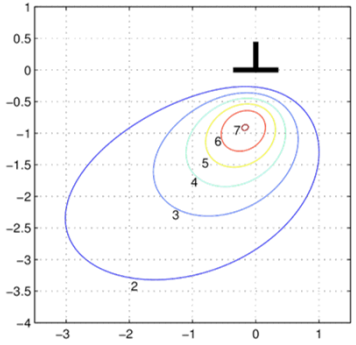


From paradis.stanford.edu

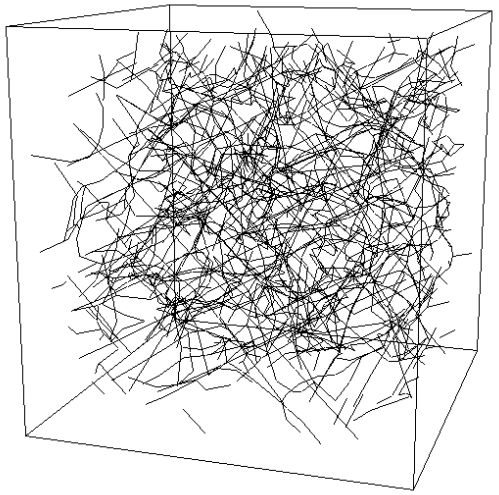


From Boniszewski and Smith, 1963

Adding H-Effects to Dislocation Dynamics



Overall approach



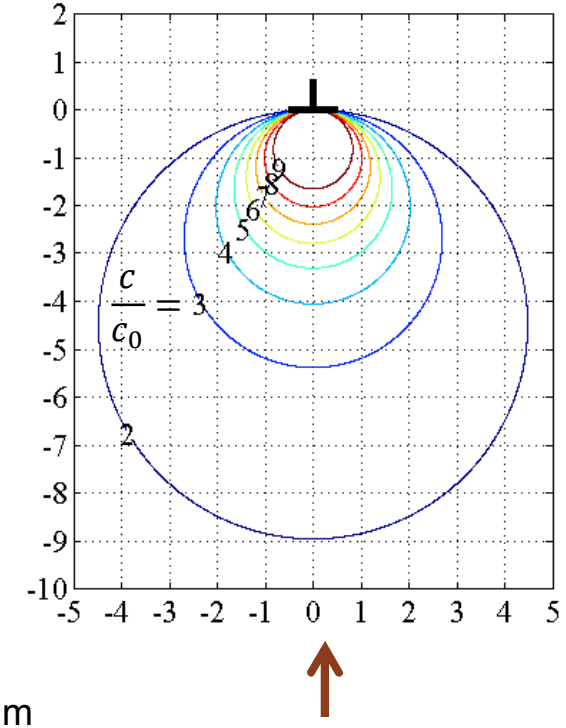
- Interested in large-scale work hardening

- Full simulation of hydrogen field infeasible
  - Large number of lattice sites (~1x10^{10}/ μm^3)
  - Dislocation stress fields highly nonlinear
    - Very fine computational grid required

- Our approach: Study solute effects on isolated dislocations
    - Use **force calculation** and **mobility law** to incorporate effects

Solid solution model

- H atoms occupy interstitial lattice sites
  - Excess volume ΔV
  - Dilatational misfit only
  - No modulus change
- Characterized by concentration field, $c(\boldsymbol{r})$
- Chemical potential:
  - Free energy cost of a solute



$$\mu = E_f + p_d \Delta V + k_B T \ln\left(\frac{c}{c_{max} - c}\right)$$

Formation Energy | Interaction Energy | Configurational Entropy

Equilibrium Concentration

$$c = \frac{c_{max}}{1 + \frac{c_{max} - c_0}{c_0} \exp[p_d \Delta V / k_B T]}$$

Diffusion Equation

$$\frac{\partial c}{\partial t} = -\nabla \bullet \mathbf{J}$$

$$\mathbf{J} = -\frac{\boldsymbol{D}c}{k_B T} \nabla \mu$$

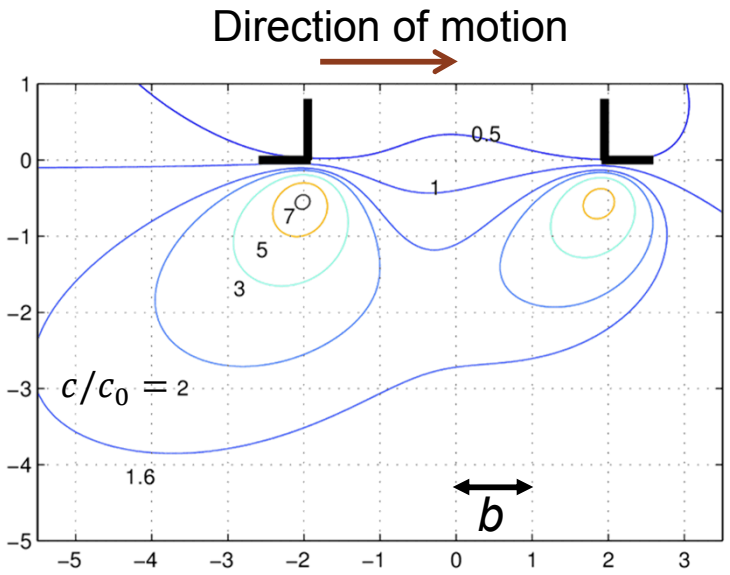
H effects on dislocations

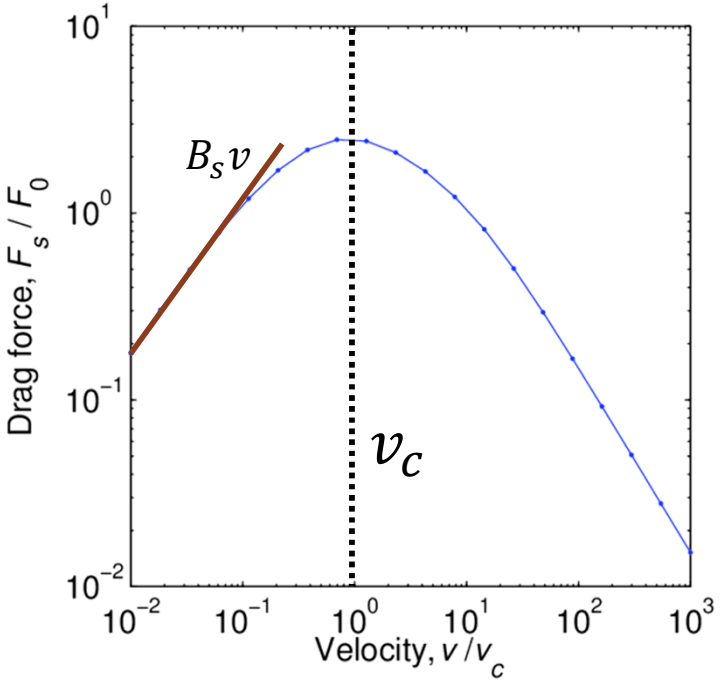
- Hydrogen (solutes) affect dislocations on multiple ways

Effect	Force Calculation	Mobility Law	Other
Reduction in dislocation-dislocation interactions	X		
Line tension change	X		
Cross-slip rate change			X
Drag force exerted by atmosphere		X	

Solute drag

- Using finite differences, solve for steady-state concentration and drag force
  - Considered both perfect and extended dislocations





Low velocity regime ($v \ll v_c$)

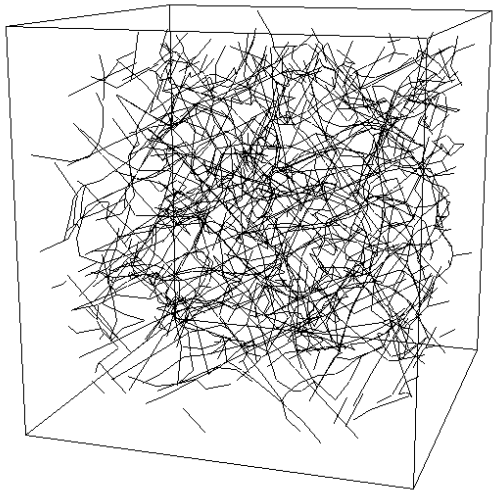
$$F_s \approx B_s(\theta) v$$

Character Angle

Hydrogen Mobility Law

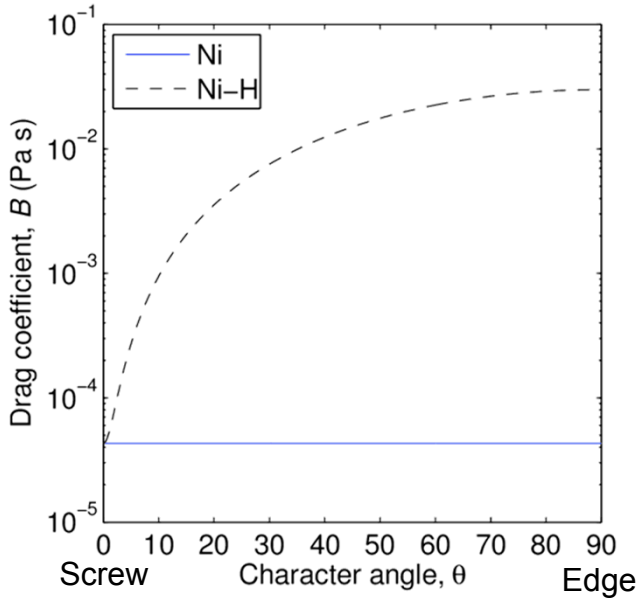
$$(B_s(\theta) + B_{ph})\mathbf{v}_i = \sum \boldsymbol{f_i}$$

DD Simulations with H-Effects



Case: Ni-H at 800 K with 1 at. % H

H-Effect on Force Calculation	Value
Edge-Edge elastic interaction change	-3.4%
Edge line energy change	-4.8%



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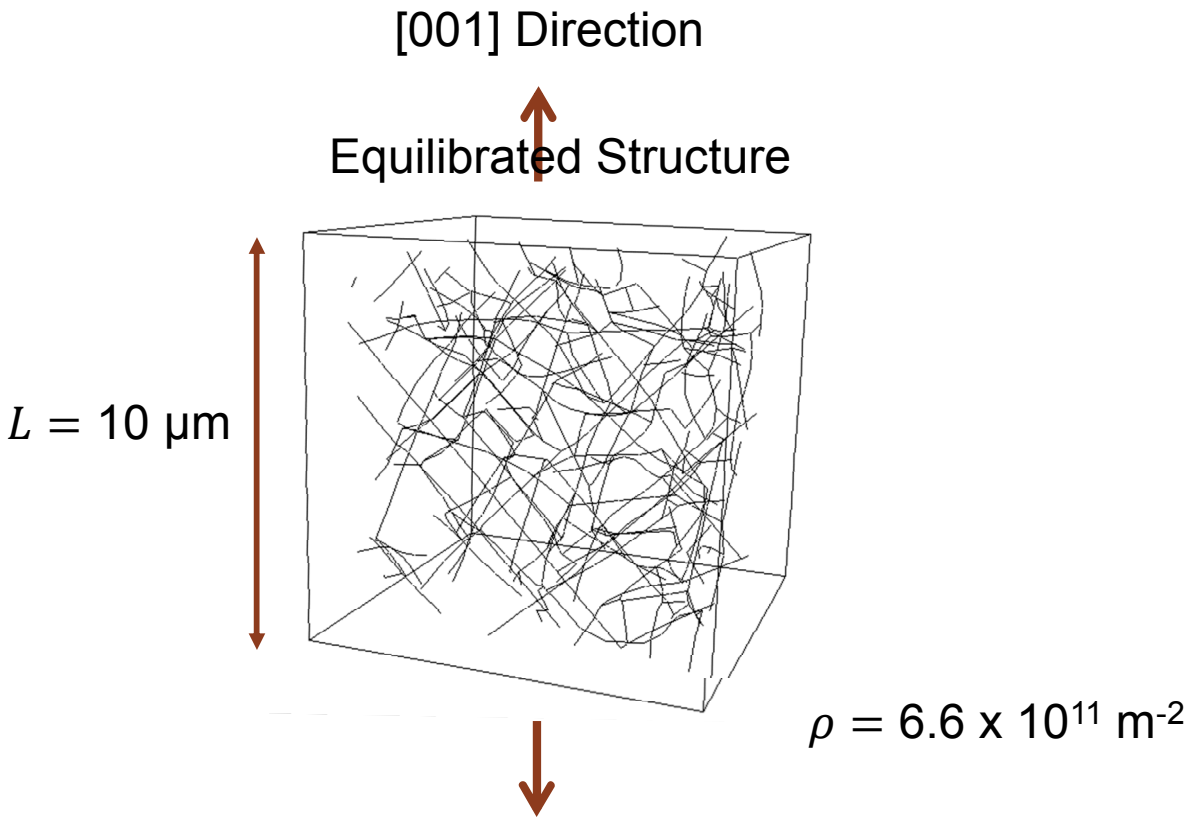
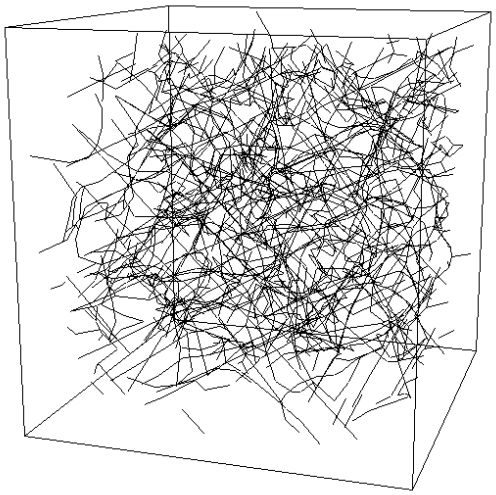
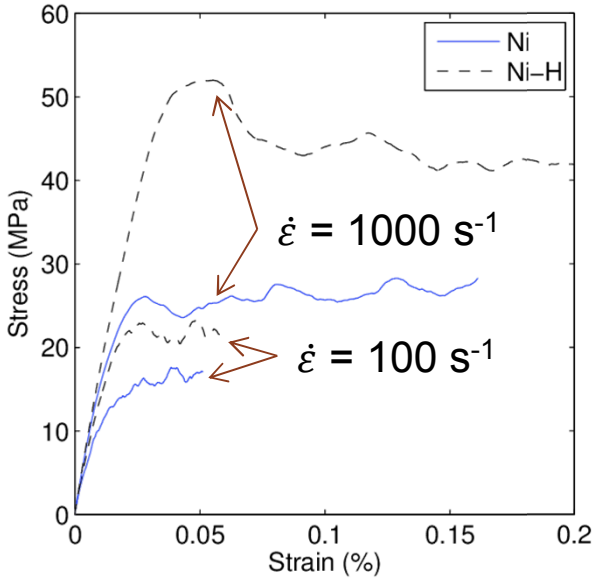
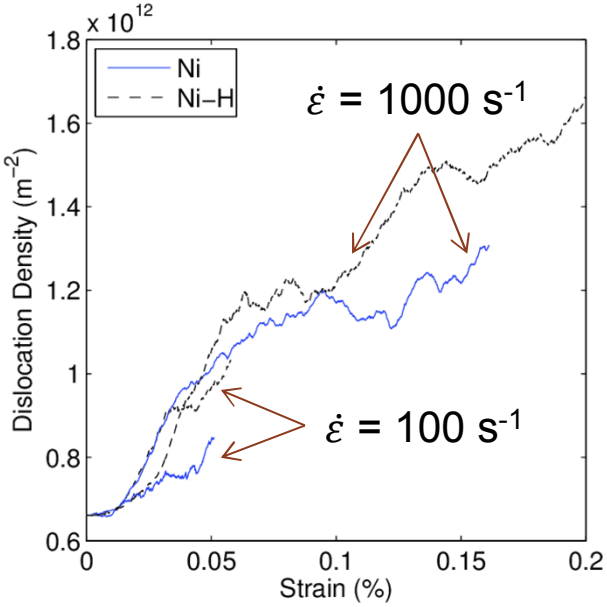


Ni-H Results

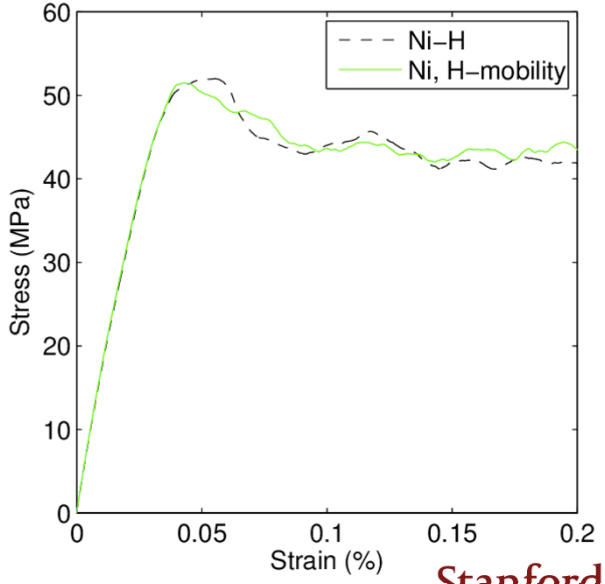


Ni-H at 0.2% strain





- Behavior dominated by drag force change



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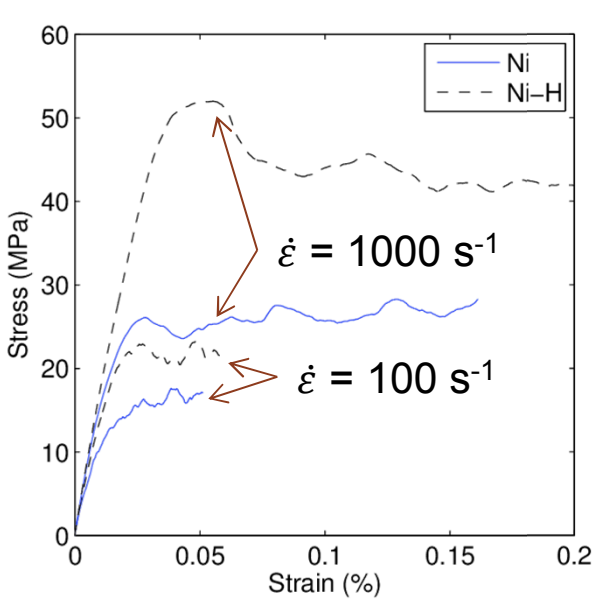
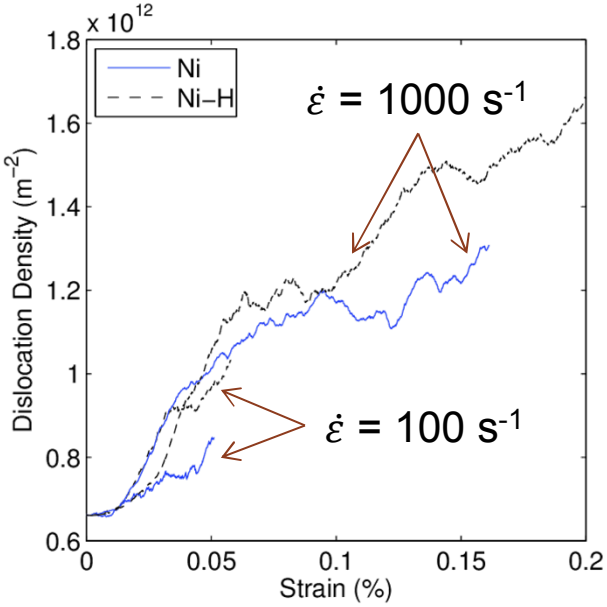
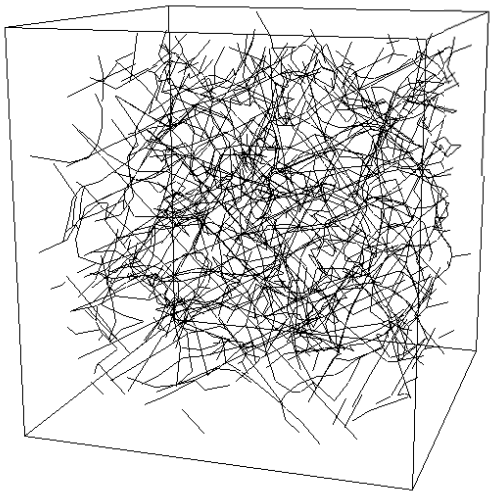
Ni-H Results







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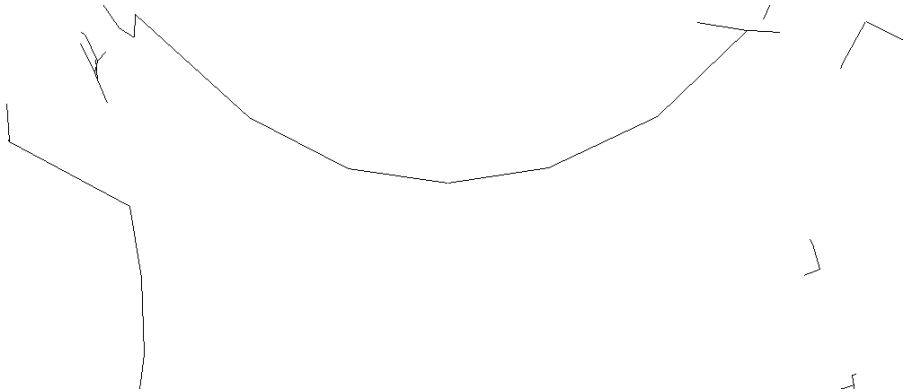

Ni-H

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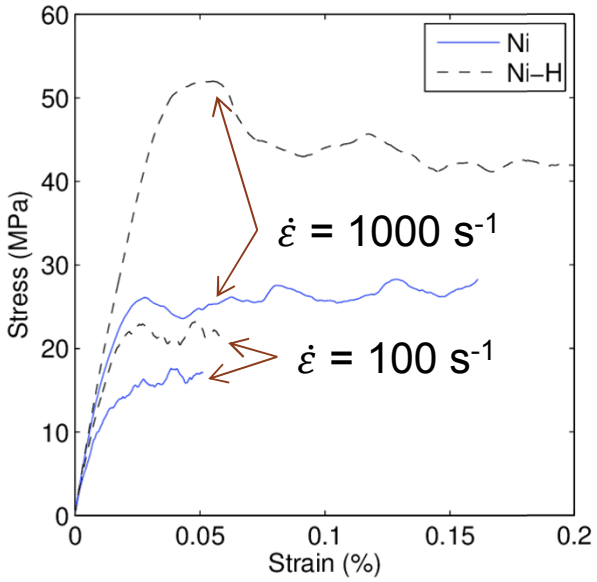

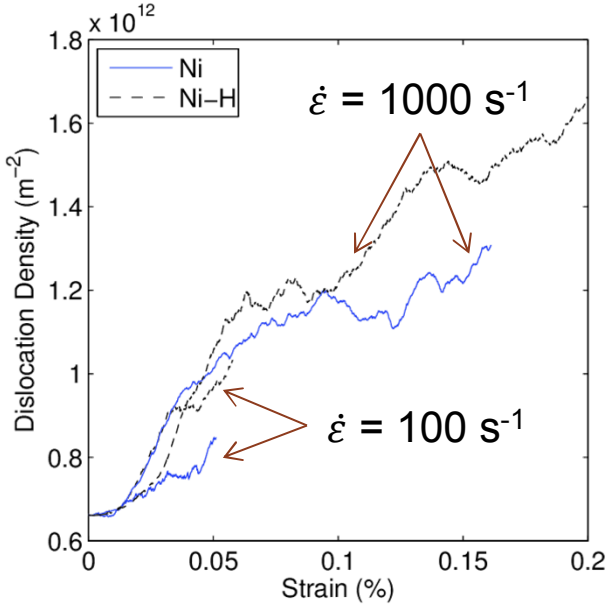

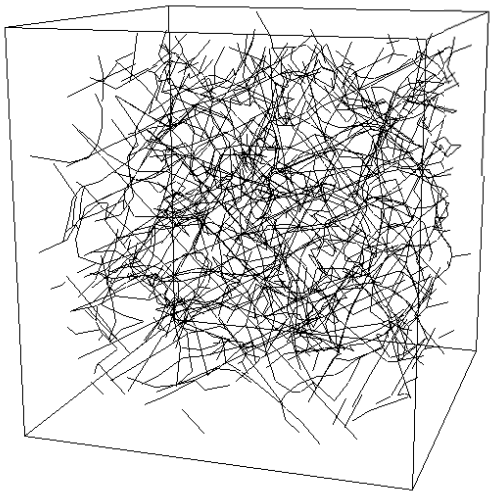

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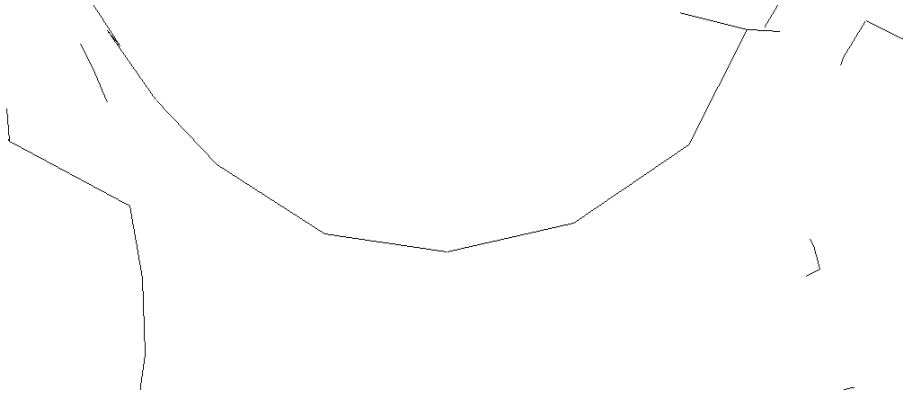

Ni-H

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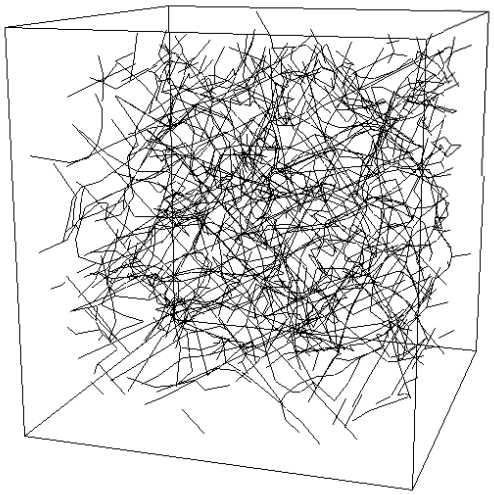

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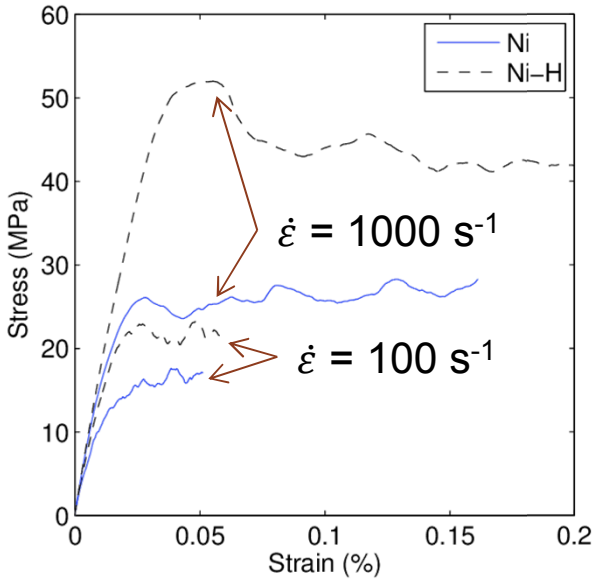

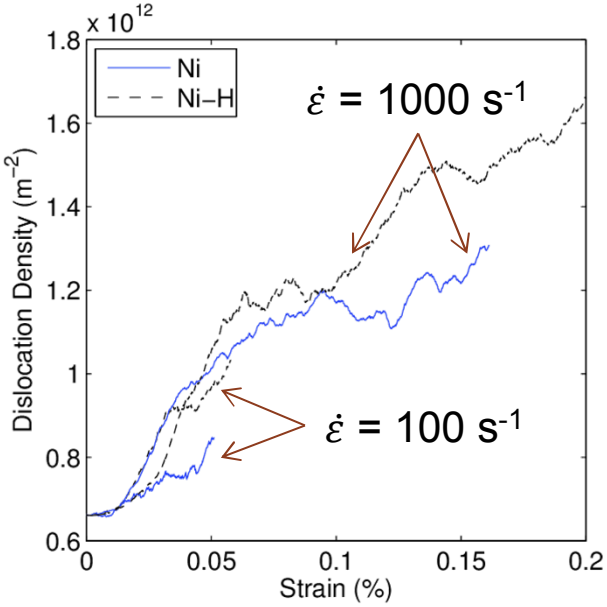

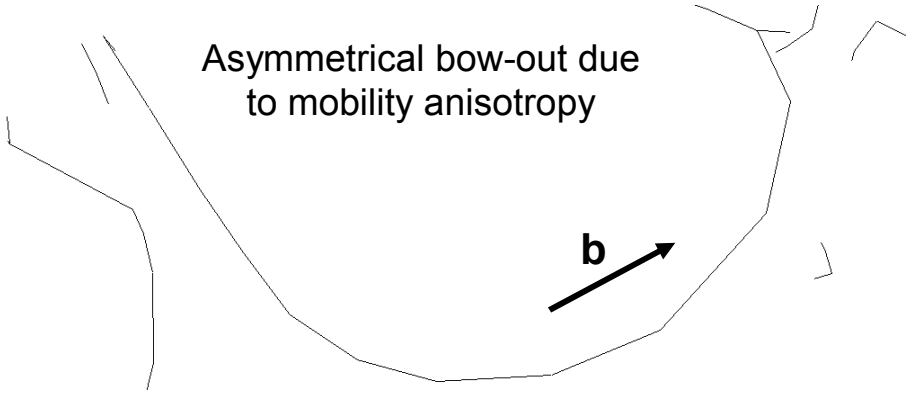

Ni-H

Conclusions

- Including hydrogen (solutes) in DD simulations requires consideration of multiple effects
- Classical continuum model useful approach for assessing effects
- Future work: Consider different diffusion regimes
  - Fast diffusion vs. dynamic strain aging vs. slow diffusion
- R. B. Sills and W. Cai, *Solute drag on perfect and extended dislocations,* In-Preparation for JMPS.