Hydrogen Effects on Edge Dislocation Mobility in Iron by Molecular Dynamics

Ángel Alberto Izquierdo Sánchez,
Dr Adrian Oila, Dr Alasdair Charles

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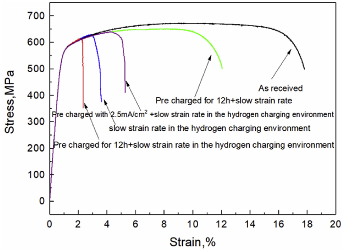
Presentation Outline

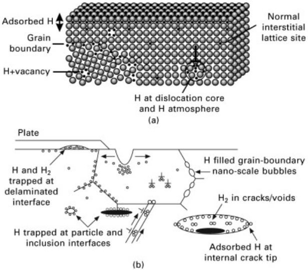
- Introduction (Hydrogen Embrittlement)
- Simulation Method
- Results:
  - Dislocation Mobility in Fe
  - H effects on Stress Field
  - Dislocation Mobility in Fe with H
- Conclusions
- Further Work

The Hydrogen Embrittlement Problem

- HE reduction of ductility of metals and alloys
- **HE importance:** Energy, transport and aerospace industries affected
- HE needs to be understood for clean energy technologies
- Mechanisms are still unclear

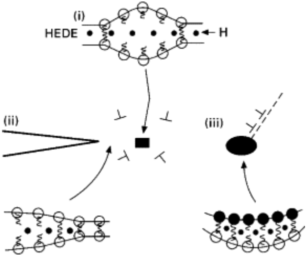


X80 steel on different H environments, C. Zhou et al. *Int J Hydrogen Energ*, 44, 22547-22558, 2019

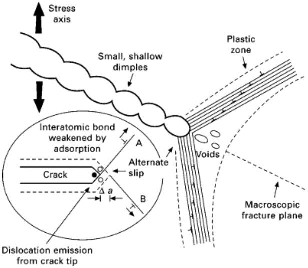


Hydrogen-metal interactions, *S.P. Lynch, Stress Corrosion Cracking, Woodhead Publishing, 2011*

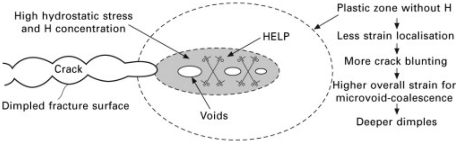
Proposed HE Mechanisms



Hydrogen Enhanced Decohesion (HEDE)



Adsorption-Induced Dislocation Emission (AIDE)

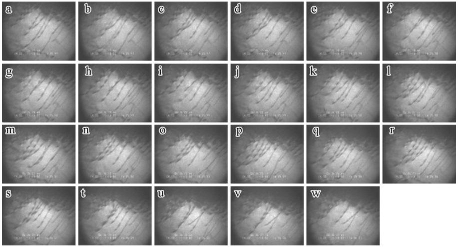


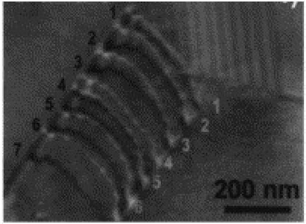
Hydrogen Enhanced Localised Plasticity (HELP)

HE mechanisms, *S.P. Lynch, Stress Corrosion Cracking, Woodhead Publishing, 2011*

HELP Concepts

i) Increased dislocation mobility (both edge and screw) in presence of hydrogen
ii) Reduction of the equilibrium separation of dislocation pile-ups
iii) Change in obstacle-dislocation interactions





Effects of Hydrogen on dislocation dynamics. I. M. Robertson et al. *Metall Mater Trans A*, 46, 2323-2341, 2015

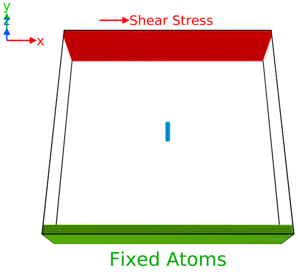
MD Simulation Methods

Aim: Test HELP concept i) using Molecular Dynamics Simulations.

- Time and length scales in MD simulations are in the order of ns and nm
- Hydrogen needs time to diffuse and reach equilibrium positions
- High mobility of H in BCC Fe ($D = 10^{-9}\,\mathrm{m}^2/\mathrm{s}$ at 300 K) allows simulation of diffusion-dominated processes
- Simulation temperature was chosen as 500 K to allow faster diffusion

MD Simulation Methods

- LAMMPS code was used for all simulations http://lammps.sandia.gov/
- Fe–H interactions were described by the EAM potential developed by Ramasubramaniam et al. (*Phys. Rev. B*, 79, 174101, 2009)
- A $\frac{1}{2}\langle 1\,1\,1\rangle$ edge dislocation was simulated resulting in a dislocation density of $6.6 \times 10^{-6}\,\mathrm{mm}^{-2}$

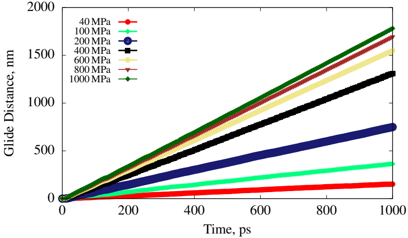


Simulation cell containing a Periodic Array of Dislocations

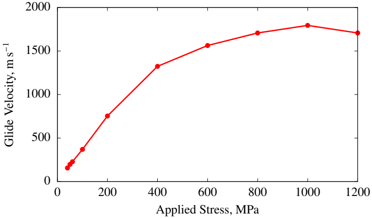
	X	Y	Z
CO	[1 1 1]	$[1\,\bar{1}\,0]$	$[1\,1\,\bar{2}]$
Dimensions (nm)	39.5	38.5	28
BC	periodic	non-periodic	periodic

Simulation domain. CO: Crystallographic Orientation, PBC: Boundary Conditions

Results: Dislocation Velocity in BCC Fe

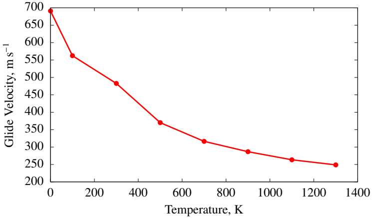


Linear relationship between dislocation core position allows estimation of glide velocity



Linear relationship up to $\tau < 300$ MPa. High free flight velocity. Average velocity depends on interactions with defects.

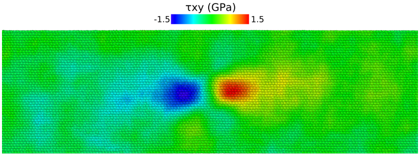
- Glide velocity follows viscous drag dynamics $v = \frac{\tau b}{B}$
- The viscous drag coefficient $B = 4.71 \times 10^{-8} T$ (Pa s)



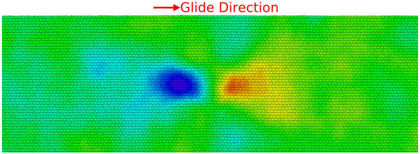
Glide velocity decreases with temperature, due to lattice vibrations

Results: H Effects Stress Field

- H atoms change the stress field around the dislocation core
- According to HELP, in directions with reduced stress field, glide will be eased
- Adding 0.025 at.%H, resulted in a slight reduction τ_{xy} stress component
- Glide should be facilitated



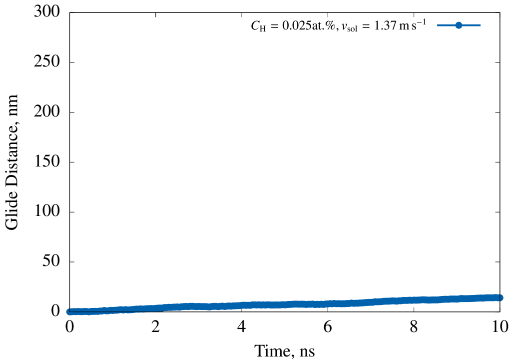
Stress around the dislocation core in Fe: Maximum $\tau_{xy} = 1.5$ GPa



Stress around the dislocation core in Fe with H solutes: Maximum $\tau_{xy} = 1.3$ GPa

Results: Dislocation Glide Velocity in Fe/H

- Adding 0.025at.%H, results in reduction of the glide velocity to $v = 1.37\,\mathrm{m\,s^{-1}}$ due to solute drag effects



Glide distance versus time for different hydrogen concentrations at applied shear stress of 100 MPa

Results: Dislocation Glide Velocity in Fe/H

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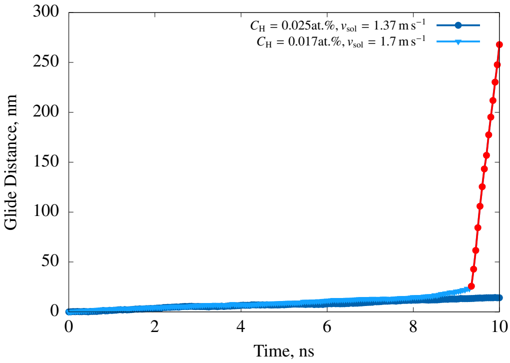
- With 0.017at.%H, dislocation cores break free from H atoms and glide at higher velocities



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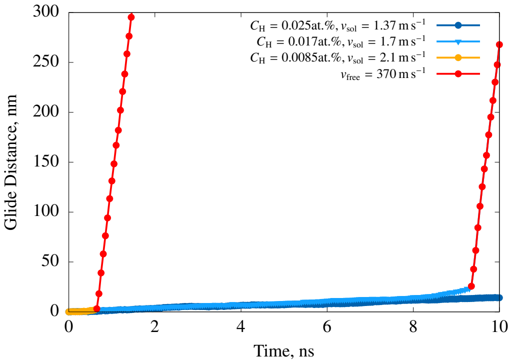
- With 0.017at.%H, dislocation cores break free from H atoms and glide at higher velocities
- Dislocations can escape H clouds more easily at lower H concentrations



Glide distance versus time for different hydrogen concentrations at applied shear stress of 100 MPa

Results: Dislocation Glide Velocity in Fe/H

(FeH glide)

Conclusions

- H atoms modify the stress field around dislocation cores. However, it is not important enough to promote dislocation mobility
- H atoms reduce edge dislocation mobility due to solute drag mechanism
- Reducing H concentration increases glide velocity in the solute drag regime
- TEM observations of enhanced dislocation mobility are unlikely to be caused by merely dislocation core – hydrogen interactions.

Further Work

Further work includes:

- Effects of hydrogen on pinning effects of obstacles to dislocations
- Can Hydrogen facilitate the movement of dislocations through obstacles?

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