Hydrogen Effects on Edge Dislocation Mobility in Iron by Molecular Dynamics

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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

Proposed HE Mechanisms

Hydrogen Enhanced Decohesion (HEDE)

Adsorption-Induced Dislocation Emission (AIDE)

Hydrogen Enhanced Localised Plasticity (HELP)

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

**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 ($D = 10^{-9} \text{ m}^2/\text{s}$ at 300 K) allows simulation of diffusion-dominated processes.
- Simulation temperature was chosen as 500 K to allow faster diffusion.
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 $6.6 \times 10^{-6}$ mm$^{-2}$
Results: Dislocation Velocity in BCC Fe

Linear relationship between dislocation core position allows estimation of glide velocity

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

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

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 $\tau_{xy}$ 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
Adding 0.025at.%H, results in reduction of the glide velocity to \( v = 1.37 \text{ m s}^{-1} \) 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**

- Adding 0.025at.%H, results in reduction of the glide velocity to $v = 1.37 \text{ m s}^{-1}$ due to solute drag effects.
- With 0.017at.%H, dislocation cores break free from H atoms and glide at higher velocities.

![Glide distance versus time for different hydrogen concentrations at applied shear stress of 100 MPa](image)
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
- 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
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 includes:

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

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