Hydrogen in Metals

HEmS mid-term meeting

Hydrogen embrittlement: Industrial problems and research challenges

When: **Wednesday 20 April, 2016**

Where: **Dept. of Engineering Science, Parks Road, Oxford, OX1 3PJ**

Please note - This is an 'open meeting' and all information presented will be in the public domain

AGENDA

10.30 **Welcome and HEmS overview**
Alan Cocks (University of Oxford)

Industrial challenges and data management

Chair Tony Paxton (King's College London)

10.50 Review of De-Embrittlement Treatments on Steels for Aerospace Applications
Martin Rawson (Materials Engineering, Rolls-Royce Plc)

11.15 Atomistic simulations of hydrogen in bearing steels
Sebastián Echeverri Restrepo (SKF Engineering and Research)

11.40 *Hydrogen Embrittlement: Considerations for Production & Application of AHSS*
Richard Thiessen (ThyssenKrupp Steel Europe)

12.05 *HEmS Materials Information Management*
Donna Dykeman (Granta MI)

Discussion

12.45 – 13.45 **Lunch**

HEmS – Hydrogen in Metals

HEmS (Hydrogen in metals - from fundamentals to the design of new steels) is a major initiative to investigate the process of embrittlement of metals from hydrogen. The research is funded by the EPSRC and is a joint collaboration between the Universities of Oxford, Cambridge, Sheffield and Imperial and King's Colleges London. http://www.hems.ox.ac.uk/

13.45 **Ongoing HEmS Research Activities**

Chair Dave Rugg (Rolls Royce Plc)

13.45 – 14.05 *HEmS Work Package 1 - Microstructural Design*
Miles Stopher (University of Cambridge)

The Microstructural Design of Hydrogen Embrittlement Resistant Microstructures

- Microscale modelling of hydrogen migration and trapping in steels
- Understanding the role of microstructure in the hydrogen embrittlement of high strength steels
- Development of hydrogen embrittlement resistant bearing steels with vanadium
- Atomic Scale modelling and nanoscale mechanical testing of hydrogen interactions in steels

14.05 – 14.25 *HEmS Work Package 2 - Production, Characterisation & Testing*
Dan Haley (University of Oxford)

Nanoprecipitate steels for Hydrogen Resistance: Processing and Characterisation

- Production of nanoscale VC dispersion steels
- Characterisation by TEM and Atom Probe
- Development of APT methods for Hydrogen imaging

14.25 – 14.55 *HEmS Work Package 3 – Data intensive Modelling*
Tom Daff (University of Cambridge)

Data management, potential fitting and atomistic simulation

- General use of the HEmS wiki
- Data management with Grant
- Other data management projects
- DFT simulations of pure iron to train a GAP potential
- Simulations of hydrogen in iron, training a GAP potential and determining solute-solute interactions
- Simulations of hydrogen in low sigma and high sigma grain boundaries

Discussion

15.00 – 15.15 Afternoon break

15.15 – 17.00 HEmS Work Package 4 - Elucidation of Mechanisms

Erlend Davidson (Imperial College, London)

Hydrogen in Fe(100) - (self-)trapping, diffusion and quantum effects

- Self-trapping of hydrogen in iron.
- Quantum nuclear effects (diffusion and vacancy escape).
- Free energy and partition function calculations using nested-sampling

Olga Barrera (University of Oxford)

HELP and HID mechanisms: mesoscopic to continuum modelling.

- Mesoscopic modelling of HELP: Kinetic Monte Carlo model for simulation of dislocation motion in bcc Fe
- Continuum modelling of HELP (finite element modelling)
- Modelling H diffusion
- Mesoscopic modelling of HID: Interfacial decohesion in bcc Fe in presence of H
- Continuum modelling of HID at grain boundaries
- Continuum modelling of HID + HELP in dissimilar welds

James Kermode (University of Warwick – HEmS Associate)

Multiscale modelling of chemomechanical properties in metallic systems

- Requirement for precision: EAM vs DFT for metals
- The 'Learn on the Fly' approach and its extension to metallic systems
- On-the-fly machine learning of quantum mechanical forces (cf. WP3)
- Enabling modelling of complex chemistry and 3D model systems

Discussion

Scientific Posters and refreshments

HEmS
Hydrogen in Metals

Scientific Posters

Atomic Scale Characterisation of M50 Bearing Steel

Sarah Hopkin (University of Oxford)

Characterisation of Hydrogen Trapping in steel by Atom Probe Tomography

Yi-Sheng Chen (University of Oxford)

Modelling dislocation processes using the tight binding approximation

E. Luke Simpson (Kings College, London)

KMC modelling of one-half [111] screw dislocation motion in Fe

Ivo Katzarov and Tony Paxton (Kings College, London)

Hydrogen Effect on Interfacial Decohesion in bcc Iron

Ivo Katzarov and Tony Paxton (Kings College, London)

Fracture Simulations of α-Fe: Cleavage Planes and Grain Boundaries

Henry Lambert (Kings College, London)

Hydrogen induced sudden-crack at a stressed grain boundary

Siamak S. Shishvan (University of Cambridge)

QM/MM atomistic simulations: from Ni alloys to Iron

Federico Bianchini (Kings College, London)

Modelling hydrogen diffusion in martensitic steels

Andrej Turk (University of Cambridge)

HEmS Work Package 3: Data Generation, Curation and Inference

Tom Daff (University of Cambridge)

Hydrogen in and at BCC Fe(100)

Erlend Davidson (Imperial College, London)

Modelling hydrogen diffusion in martensitic steels

A. Turk, E. Galindo-Nava and P.E.J. Rivera-Díaz-del-Castillo (University of Cambridge)

Design of Hydrogen Embrittlement Resistant Steels - from Concept to Market

M.A. Stopher, D. Bombac and P.E.J. Rivera-Díaz-del-Castillo (University of Cambridge)

Hydrogen interactions with steel: effects on elastic properties of cementite

D. Bombac, M.A. Stopher, and P.E.J. Rivera-Díaz-del-Castillo (University of Cambridge)

Design of high strength steels resistant to hydrogen embrittlement for reduced emission in automotive vehicles

A. Chamisa, A. Patterson, F. Sweeney, WM Rainforth, D Haley, P. Bagot, M Moody, A Rijkenberg

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