Project title: Investigation of hydrogen embrittlement of steels for the hydrogen transport energy future

Project ID *(optional)*: *Please leave blank*

Accept all year-round applications

Funding information: Self-funded students only

Project description:

**Introduction**

Hydrogen embrittlement (HE), the loss of the ductility due to the diffusion of atomic hydrogen in steels, has major consequences in pipelines. HE results in rapid cracking that makes it hard to detect and repair, posing a major threat for pipeline integrity. HE has been studied for more than a century, and yet the behaviour of hydrogen in steels has not been completely understood. In addition, the proposed mechanisms can only partially explain the experimental findings [1].

Computational Materials Science is becoming a very important tool, thanks to the availability of modern computing facilities which allow modelling of a great number of atoms for longer periods of time compared with two decades ago. Such advances in computing capabilities result in more accurate simulations [2], allowing major savings in the design of materials such as pipeline steel. The study of hydrogen embrittlement using computational tools is relatively novel and has an enormous potential to contribute to the understanding of the hydrogen embrittlement mechanisms.

**Project**

Hydrogen Embrittlement (HE) of High Strength Steels will be studied using a combination of computational and laboratory techniques. Density functional theory (DFT) calculations will be performed to study hydrogen adsorption in pipeline steel, calculate elastic constants and estimate diffusion coefficients of hydrogen. Molecular dynamics (MD) simulations will be carried out to elucidate crack initiation and propagation in different microstructures, and to study embrittlement. Tensile tests will be conducted on hydrogen-charged samples (cathodically or thermally charged) to evaluate the influence of HE on mechanical properties. Metallography, Optical Microscopy, Scanning Electron Microscope (SEM) and Electron Backscatter Diffraction (EBSD) will be used to examine the microstructure, grain boundaries; to study crack morphology, crack growth of HE failed samples and validate numerical results. The combination of techniques will provide a novel approach to elucidate the nature of HE in steels and help establish if the current gas transmission network could be used for hydrogen-rich gas transport in the future.

*Newcastle University is committed to being a fully inclusive Global University which actively recruits, supports and retains colleagues from all sectors of society.  We value diversity as well as celebrate, support and thrive on the contributions of all our employees and the communities they represent.  We are proud to be an equal opportunities employer and encourage applications from everybody, regardless of race, sex, ethnicity, religion, nationality, sexual orientation, age, disability, gender identity, marital status/civil partnership, pregnancy and maternity, as well as being open to flexible working practices.*

References:

 1. D. Hardie, E.A. Charles, A.H. Lopez, Hydrogen embrittlement of high strength pipeline steels, Corrosion Science, Volume 48, Issue 12, 2006, Pages 4378-4385, ISSN 0010-938X

 2. Oila, A., Lung, C. & Bull, S. J Mater Sci (2014) 49: 2383. https://doi-org.libproxy.ncl.ac.uk/10.1007/s10853-013-7942-0

Application enquires: to *Dr Alasdair Charles,* *alasdair.charles@newcastle.ac.uk**, https://www.ncl.ac.uk/swan/staff/profile/alasdaircharles.html#background*

**We will also need to link your PhD advert up to the subject keywords below so that your PhD studentship can be found on findaphd.com. Please highlight up to three relevant keywords from the lists provided below.**

**FindaPhD.com**
You can select up to **10 subject areas**.

PhD Disciplines & Subject areas

Agriculture

[ ]  agricultural sciences

[ ]  agricultural technology

[ ]  arable farming

[ ]  livestock farming

[ ]  forestry & arboriculture

[ ]  other

Anthropology

[ ]  biological anthropology

[ ]  social anthropology

[ ]  other

Architecture, Building & Planning

[ ]  architecture

[ ]  built environment

[ ]  construction management

[ ]  landscape architecture

[ ]  rural planning

[ ]  surveying

[ ]  urban planning

[ ]  other

Biological Sciences

[ ]  bacteriology

[ ]  behavioural biology

[ ]  biochemistry

[ ]  biodiversity

[ ]  bioinformatics

[ ]  biophysics

[ ]  biotechnology

[ ]  cancer biology

[ ]  cell biology

[ ]  developmental biology

[ ]  ecology

[ ]  ecotoxicology

[ ]  entomology

[ ]  environmental biology

[ ]  evolution

[ ]  genetic engineering

[ ]  genetics

[ ]  genomics

[ ]  human genetics

[ ]  immunology

[ ]  marine biology

[ ]  microbiology

[ ]  molecular biology

[ ]  molecular genetics

[ ]  neuroscience

[ ]  parasitology

[ ]  plant biology

[ ]  plant cell biology

[ ]  reproductive biology

[ ]  structural biology

[ ]  systematic biology

[ ]  virology

[ ]  zoology

[ ]  other

Business & Management

[ ]  accounting

[ ]  business

[ ]  e business

[ ]  education management

[ ]  event management

[ ]  hospitality

[ ]  human resource management

[ ]  management

[ ]  marketing

[ ]  project management

[ ]  sport management

[ ]  tourism

[ ]  other

Chemistry

[ ]  analytical chemistry

[ ]  applied chemistry

[ ]  computational chemistry

[ ]  environmental chemistry

[ ]  industrial chemistry

[ ]  inorganic chemistry

[ ]  organic chemistry

[ ]  petrochemical chemistry

[ ]  pharmaceutical chemistry

[ ]  physical chemistry

[ ]  polymer chemistry

[ ]  structural chemistry

[ ]  synthetic chemistry

[ ]  other

Communication & Media Studies

[ ]  broadcast media

[ ]  digital media

[ ]  journalism

[ ]  print media

[ ]  production

[ ]  public relations

[ ]  publishing

[ ]  other

Computer Science

[ ]  artificial intelligence

[ ]  computer architectures

[ ]  computer vision

[ ]  computer graphics

[ ]  cyber security

[ ]  data science

[ ]  human computer interaction

[ ]  internet of things

[ ]  machine learning

[ ]  networks

[ ]  quantum computing

[ ]  software engineering

[ ]  videogames

[ ]  other

Creative Arts & Design

[ ]  animation

[ ]  art

[ ]  crafts

[ ]  creative writing

[ ]  dance

[ ]  design

[ ]  drama

[ ]  fashion

[ ]  film studies

[ ]  fine art

[ ]  graphic design

[ ]  interior design

[ ]  music

[ ]  music technology

[ ]  photography

[ ]  theatre studies

[ ]  other

Economics

[ ]  econometrics

[ ]  financial economics

[ ]  macroeconomics

[ ]  microeconomics

[ ]  political economics

[ ]  other

Education

[ ]  further education

[ ]  higher education

[ ]  nursery education

[ ]  primary education

[ ]  secondary education

[ ]  special needs education

[ ]  other

Engineering

[ ]  acoustics engineering

[ ]  aerospace engineering

[ ]  atomic engineering

[ ]  automotive engineering

[ ]  bioengineering

[ ]  biomedical engineering

[x]  chemical engineering

[ ]  civil engineering

[ ]  communications engineering

[ ]  control systems

[ ]  cybernetics

[ ]  dynamics

[ ]  electrical engineering

[ ]  electronic engineering

[ ]  energy technologies

[ ]  environmental engineering

[ ]  fluid mechanics

[ ]  gas engineering

[ ]  geotechnical engineering

[ ]  integrated engineering

[ ]  manufacturing engineering

[ ]  marine engineering

[x]  mechanical engineering

[ ]  mechanics

[ ]  mechatronics

[ ]  nanotechnology

[ ]  offshore engineering

[ ]  petroleum engineering

[ ]  robotics

[ ]  solid mechanics

[ ]  structural engineering

[ ]  structural mechanics

[ ]  systems engineering

[ ]  thermodynamics

[ ]  other

Environmental Sciences

[ ]  climate science

[ ]  hydrology

[ ]  marine sciences

[ ]  meteorology

[ ]  pollution

[ ]  soil science

[ ]  other

Finance

[ ]  actuarial science

[ ]  banking

[ ]  financial management

[ ]  insurance

[ ]  investment

[ ]  taxation

[ ]  other

Food Sciences

[ ]  food hygiene

[ ]  food production

[ ]  other

Forensic and Archaeological Sciences

[ ]  archaeological science

[ ]  forensic science

[ ]  other

Geography

[ ]  agricultural geography

[ ]  cultural geography

[ ]  economic geography

[ ]  environmental geography

[ ]  geographical information systems gis

[ ]  historical geography

[ ]  human geography

[ ]  marine geography

[ ]  physical geography

[ ]  political geography

[ ]  remote sensing

[ ]  social geography

[ ]  transport geography

[ ]  urban geography

[ ]  other

Geology

[ ]  applied geology

[ ]  geochemistry

[ ]  geophysics

[ ]  geoscience

[ ]  geotechnology

[ ]  hydrogeology

[ ]  marine geology

[ ]  palaeontology

[ ]  seismology

[ ]  volcanology

[ ]  other

History & Archaeology

[ ]  african history

[ ]  american history

[ ]  ancient history

[ ]  archaeology

[ ]  asian history

[ ]  australasian history

[ ]  british and irish history

[ ]  economic history

[ ]  european history

[ ]  heritage studies

[ ]  history

[ ]  history of art

[ ]  history of religions

[ ]  history of science

[ ]  medieval history

[ ]  military history

[ ]  modern history

[ ]  russian history

[ ]  social history

[ ]  world history

[ ]  other

Information Services

[ ]  information security

[ ]  information systems

[ ]  librarianship

[ ]  other

Languages, Literature & Culture

[ ]  african studies

[ ]  american studies

[ ]  asian studies

[ ]  australasian studies

[ ]  chinese

[ ]  danish

[ ]  dutch

[ ]  english language

[ ]  english literature

[ ]  european studies

[ ]  finnish

[ ]  french

[ ]  german

[ ]  italian

[ ]  japanese

[ ]  middle eastern studies

[ ]  norwegian

[ ]  portuguese

[ ]  russian

[ ]  spanish

[ ]  swedish

[ ]  other

Law

[ ]  criminal law

[ ]  commercial law

[ ]  contract law

[ ]  property law

[ ]  other

Linguistics & Classics

[ ]  ancient greek

[ ]  celtic studies

[ ]  classics

[ ]  latin

[ ]  linguistics

[ ]  other

Materials Science

[ ]  ceramics

[ ]  glass

[x]  metallurgy

[ ]  polymers

[ ]  textiles

[ ]  other

Mathematics

[ ]  applied mathematics

[ ]  applied statistics

[ ]  computational mathematics

[ ]  data analysis

[ ]  engineering mathematics

[ ]  mathematical modelling

[ ]  medical statistics

[ ]  operational research

[ ]  probability

[ ]  pure mathematics

[ ]  statistics

[ ]  stochastic processes

[ ]  other

Medicine

[ ]  anatomy

[ ]  audiology

[ ]  biomechanics

[ ]  cardiology

[ ]  complementary medicine

[ ]  dentistry

[ ]  endocrinology

[ ]  epidemiology

[ ]  neural engineering

[ ]  neurology

[ ]  nutrition

[ ]  ophthalmology

[ ]  optometry

[ ]  pathology

[ ]  pharmacology

[ ]  pharmacy

[ ]  physiology

[ ]  physiotherapy

[ ]  podiatry

[ ]  radiology

[ ]  speech science

[ ]  tissue engineering

[ ]  toxicology

[ ]  other

Nursing & Health

[ ]  adult nursing

[ ]  community nursing

[ ]  counselling

[ ]  dental nursing

[ ]  environmental health

[ ]  health informatics

[ ]  medical nursing

[ ]  mental health nursing

[ ]  midwifery

[ ]  occupational health

[ ]  occupational therapy

[ ]  paediatric nursing

[ ]  paramedical science

[ ]  surgical nursing

[ ]  other

Philosophy

[ ]  ethics

[ ]  metaphysics

[ ]  philosophy of science

[ ]  other

Physics

[ ]  acoustics

[ ]  astronomy

[ ]  astrophysics

[ ]  chemical physics

[ ]  computational physics

[ ]  electromagnetism

[ ]  environmental physics

[ ]  experimental physics

[ ]  medical physics

[ ]  nuclear physics

[ ]  optical physics

[ ]  particle physics

[ ]  quantum mechanics

[ ]  solid state physics

[ ]  space science

[ ]  theoretical physics

[ ]  other

Politics & Government

[ ]  development studies

[ ]  government

[ ]  international relations

[ ]  politics

[ ]  public policy

[ ]  other

Psychology

[ ]  child psychology

[ ]  clinical psychology

[ ]  community psychology

[ ]  counselling psychology

[ ]  developmental psychology

[ ]  educational psychology

[ ]  forensic psychology

[ ]  health psychology

[ ]  neuropsychology

[ ]  occupational psychology

[ ]  organisational psychology

[ ]  psychotherapy

[ ]  sport psychology

[ ]  other

Sociology

[ ]  criminology

[ ]  disability studies

[ ]  gender studies

[ ]  socio economics

[ ]  social work

[ ]  other

Sport & Exercise Science

[ ]  sport coaching

[ ]  sport development

[ ]  sport performance

[ ]  sport technology

[ ]  sport therapy

[ ]  other

Theology & Religious Studies

[ ]  divinity

[ ]  religious studies

[ ]  theology

[ ]  other

Veterinary Sciences

[ ]  animal welfare

[ ]  veterinary dentistry

[ ]  veterinary medicine

[ ]  veterinary nursing

[ ]  veterinary nutrition

[ ]  veterinary pathology

[ ]  other