IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	Multiscale Modeling of Hydrogen Embrittlement	
Project Number	**IMURA0918**	
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IITB Department:	Mechanical Engineering	

Research Clusters:

Highlight which of the Academy's CLUSTERS this project will address?
*(Please nominate JUST **one.** For more information, see www.iitbmonash.org)*

1	*Material Science/Engineering (including Nano, Metallurgy)*
2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*
3	*Math, CFD, Modelling, Manufacturing*
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*
8	*HSS, Design, Management*

Research Themes:

Highlight which of the Academy's Theme(s) this project will address?
(Feel free to nominate more than one. For more information, see www.iitbmonash.org)

1	*Advanced computational engineering, simulation and manufacture*
2	*Infrastructure Engineering*
3	*Clean Energy*
4	*Water*
5	*Nanotechnology*
6	*Biotechnology and Stem Cell Research*
7	*Humanities and social sciences*
8	Design

The research problem

Hydrogen embrittlement is a challenging issue in fuel-cell cars. Hydrogen may get trapped in aluminium microstructure via water vapour during initial stages of processing. Other mechanisms of hydrogen transport in aluminium alloys are not clearly understood. It is evident that hydrogen interacts with dislocations, second phase e.g. precipitates, grain boundaries and even vacancies. In a recent research work it was pointed out that hydrogen transport is affected by presence of vacancies and vice-versa. Pre-existing vacancies may help entrap more hydrogen. Moreover, hydrogen may assist generation of vacancies. It is also understood that presence of hydrogen clusters at interfaces may result into delamination of interfaces. However, it has not been systemically studied how all the aforementioned mechanisms collectively participate towards nucleation of cracks and ultimate failure. Based on, various mechanisms understood via experiments as reported in literature, we intend to formulate a multiscale mechanics model following crystal plasticity-phase-field framework. For estimation of material parameters and for understanding experimental observation, small-length scale simulation methods i.e. molecular dynamics may be used.

Project aims

1. Modeling of hydrogen embrittlement and its effect on mechanical behaviour using multiscale modelling technique viz. molecular dynamics, phase-field coupled crystal plasticity.
2. Understanding effect of hydrogen embrittlement as a function of heterogeneity and local strain energy
3. Experimental investigation of hydrogen embrittlement

Expected outcomes

1. Multiscale model of mechanical behaviour of aluminium alloy in presence of hydrogen.
2. Effect of hydrogen on crack nucleation activity.
3. Various modes of transport and preferred sites for hydrogen in aluminium alloy

How will the project address the Goals of the above Themes?

The objective of this project is to understand impact of hydrogen on mechanical behaviour of an aluminium alloy. We intend to understand and model the effect of hydrogen via combining the modelling and experimental efforts. We will model the hydrogen transport and storage in aluminium using multiscale modelling technique. Effect of hydrogen on fracture behaviour will be explored.

Capabilities and Degrees Required

An ideal candidate should have a BTech or BE or Master in Mechanical Engineering, Aerospace Engineering, Civil Engineering or Materials Engineering with a strong inclination towards advanced mathematics, numerical methods, continuum mechanics, non-linear elasticity. Experience in at least two of the following three criteria is desired: 1. Background in mechanics of materials; 2. Expertise in numerical methods for PDEs (finite element methods); 3. Expertise in programming (Python, C, C++, Fortran)

Potential Collaborators

Fuel cell companies, GE, Thermal power, Nuclear Power.

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

Hydrogen embrittlement, Fracture, Crack nucleation, Data Science, Computational Mechanics