IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	Modeling of Hydrogen Assisted Crack Nucleation	
Project Number	**IMURA0849**	
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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 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 7XXX alloys in presence of hydrogen.
2. Effect of hydrogen on crack nucleation activity.
3. Various modes of transport and preferred sites for hydrogen in 7XXX alloys.

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 7XXX aluminium alloys. 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. Preferred sites or hydrogen and its interaction with various microstructure features will be studied at various length scales beginning from single vacancy to grain boundaries. This effort makes extensive use of molecular dynamics, phase-field and crystal plasticity finite element modelling.

Capabilities and Degrees Required

List the ideal set of capabilities:

1. Analytical skills
2. Willingness to learn and work hard
3. Microstructure Characterization using SEM
4. Crystal Plasticity or MD simulations or Phase Field Modeling
5. Advanced Numerical Methods

A candidate with training in mechanical or materials engineering but with keen interest in simulations as well as experimental investigation of role of microstructure on mechanical properties.

Potential Collaborators

General Electric, ISRO, CSIRO, Boeing, Hindustan Aeronautics Ltd. We have not contacted any yet.

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.

Modelling and Simulation, Metallurgy, Materials Chemistry/Science, Computational Fluid Dynamics and Mechanics