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. We intend to first experimentally investigate effect of hydrogen on mechanical behaviour. This investigation will be followed up by microstructure characterization using SEM, EBSD, TEM and atom probe. Based on the identification of key mechanisms of failure, we will formulate multiscale mechanics model following crystal plasticity-phase-field framework. For estimation of material parameters and for understanding experimental observation, small scale simulation methods i.e. molecular dynamics and /or DFT may be used.

Project aims

1. Mechanical characterization of a 7XXX alloy as a function of process condition, temperature, strain, strain-rate and hydrogen.
2. Understanding microstructure with help of EBSD, TEM and atom probe tomography.
3. Modeling of hydrogen embrittlement and its effect on mechanical behaviour using multiscale modelling technique viz. molecular dynamics, phase-field, crystal plasticity.
4. 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. Effect of processing conditions on hydrogen emrittlement susceptibility.
4. 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 density function theory, 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, EBSD, TEM, Atom Probe.
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 simulation as well as experimental investigation of role of microstructure in mechanical properties, including existing skills or genuine interest in learning characterisation techniques such as SEM, TEM and EBS.

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