

An Indian-Australian research partnership

Project Title: **Atomistic Simulations of Nanoscale Precipitate Interfaces in Structural Materials**

Project Number **IMURA0435**

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IITB Department:

Energy Science and Engineering

Research Academy 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

The research problem

Define the problem

Nanoscale precipitates are key features of the microstructures of many natural and artificial materials. In particular they govern the properties of a technologically significant class of materials, from high-strength light alloys and stabilised zirconia ceramics to biomaterials such as artificial bone. Yet understanding, let alone designing, the microstructures of such materials remains a formidable challenge. The recent experimental discovery in structural aluminium alloys of a new class of embedded interfaces with unusual

structures offers the prospect of determining the atomic-scale mechanisms of precipitation. In this project we will apply advanced computer simulation techniques to characterise the atomic-scale structure, thermodynamics and kinetics of embedded interfaces in key model aluminium alloys. Particular attention will be placed on investigating the effect of segregation at these interfaces.

Project aims

Define the aims of the project

Expected outcomes

Highlight the expected outcomes of the project

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

Describe how the project will address the goals of one or more of the 6 Themes listed above.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.

Potential Collaborators

Please visit the IITB website www.iitb.ac.in OR Monash Website www.monash.edu to highlight some potential collaborators that would be best suited for the area of research you are intending to float.