IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Nanostructure Stabilization in Energy Materials**	
Project Number	**IMURA0399**	
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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

Nanostructured materials are used in several energy-related fields such as photovoltaics, batteries, fuel cells, and hydrogen storage due to their attractive properties. However, nanostructured materials are, very unstable owing to their large fraction of high-energy intercrystalline regions also called as grain boundaries. Stabilizing nanoscale structures in these materials is a major challenge, and is proving to be a bottleneck in utilizing these promising materials for industrial-scale applications. One way of stabilizing the nanostructured materials is by adding a second component to the matrix through alloying.

In the present project, energy-related nanomaterials will be synthesized by electrodeposition. The structural characterization and compositional analysis at nano-scale will be performed using High Resolution Transmission Electron Microscope (HRTEM). The segregation tendency of the second component atoms to the grain boundaries of matrix and its contribution to the grain size and nanostructural stability will be investigated. Using advanced computer simulation techniques, the atomic interactions between second component and the matrix will be studied and related to the segregation tendency. Finally, thermodynamic and kinetic models for the nanostructural stabilization will be established.

Project aims

Define the aims of the project

The aims of the project are to understand the fundamental aspects of the

(i) segregation tendency of the second component atoms to the grain boundaries of matrix using HRTEM

(ii) role of segregation tendency in nanostructural stabilization using computer simulations

These aims will be directed towards preparing promising energy-related materials

Expected outcomes

Highlight the expected outcomes of the project

The following outcomes are expected from the present project

(i) some thermodynamic/kinetic models to explain nanostructural stabilization

(ii) investigation of the applicability of these models in preparing better energy-related materials

(iii) a possible set of guidelines for designing stable nanostructured materials

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.

Nanostructured materials of interest to Clean Energy storage and conversion will be studied in the present project with the aim of tailoring these materials toward high stability. Advanced Computational Tools will be used to understand a few fundamental aspects at atomic level related to structural stability of these materials.

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.

The candidate should hold any degree from B.E., B.Tech., M.E., M.Tech. or M.Sc. in any of the disciplines: Metallurgical Engg., Materials Science and Engg., Chemical Engg., Physics or Chemistry and related disciplines.

Exposure to computer programming, preferably using Fortran, Knowledge about computer simulations can be an added advantage.

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.