IITB-Monash Research Academy

An Indian-Australian research partnership

Indian Institute of Technology Bombay | MONASH University

Project Title:	**Generative AI for understanding process-structure-property relationships in biodegradable magnesium alloys**	
Project Number	**IMURA1276**	
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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	*Artificial Intelligence and Advanced Computational Modelling*
2	*Circular Economy*
3	*Clean Energy*
4	*Health Sciences*
5	*Smart Materials*
6	*Sustainable Societies*
7	*Infrastructure*

The research problem

The traditional implant materials e.g. titanium alloys and stainless steels, demonstrate excellent mechanical properties, resistance to fatigue, wear and corrosion resistance. However, these properties differ from those of human bones, and thus can cause stress shielding. Moreover, in cases where these are used as temporary implants (e.g., plates, wires, screws), a second surgery is typically required to remove the implant after the tissues have healed, which increases the healthcare cost. This further imposes an increased risk of local inflammation as well as the physical irritation due to the rigidity of these traditional implant devices.

Magnesium (Mg) alloys are very attractive as materials for temporary implant devices due to their excellent bio-compatibility and mechanical properties being similar to those of natural bone. Recently, magnesium and its alloys have attracted increasing interest as innovative biodegradable materials, particularly for their potential use as temporary orthopaedic implants. Magnesium is not only biocompatible but also essential to human metabolism and the degradation products of magnesium are not toxic to the human physiology.

Despite highly advantageous properties of Mg alloys, they have not been commonly used as body implants because Mg alloys suffer rapid degradation and concurrent generation of undesirable amounts of hydrogen gas even in a mildly corrosive medium such as simulated body fluid (SBF).

In this project we plan to discover mechanisms via which Mg alloys degrade in body fluids, using generative artificial intelligence (GenAI). GenAI will be used for hypothesis development that can be validated via existing literature data. The proven hypothesis can be further used for discovery of the next generation biodegradable Mg alloys based on the patient data.

Project aims

1. Deep learning / language model-based hypothesis development for process-structure-property of biodegradable Mg alloys.
2. Understanding mechanisms of corrosion / failure of Mg alloy implants.
3. Discovery of next generation biodegradable Mg alloys using AI workflows.

How skills/experience of the IITB and the Monash supervisor(s) support the proposed project

1. Prof. Raman Singh has worked extensively in the area of failure of metals due to synergistic action of mechanical loading and corrosive environment, including for bioimplant applications.
2. Prof. J. F. Nie is an expert on process-structure-property relations in metals and alloys including Mg alloys.
3. Prof. Alankar has expertise in the area of application of AI / ML for science and engineering and computational materials science.

What is expected of the student when at IITB and when at Monash?

At the time of application, the student is expected to have basic understanding of metals, their mechanical behaviour and corrosion. The students must be aware of at least one programming language. Expertise in Python will be an advantage. Knowledge of Machine Learning (ML), Deep Learning, Language Model basics e.g. NLP including the underlying mathematical framework will be helpful. At IITB, the student will go through rigorous course work in the above areas. At the same time he/she will be expected to perform extensive literature review. The major modelling part of the project will be performed at IIT Bombay. The student will perform various validation tests at Monash University.

Expected outcomes

1. A systematic study of process-structure-property relations in biodegradable Mg alloys
2. Mapping of degradation mechanisms to types of bio fluids.
3. Next generation biodegradable Mg alloys and their processing routes.

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

This project aims to understand behaviour and life of Mg in simulated physiological environment. The overarching goal is to establish the feasibility of Mg-based implants as compared to the existing implants. The project addresses the goals of biomedical cluster. It has components in advanced computational modeling theme and health sciences.

How well the IITB and the Monash supervisor(s) know each other

Prof. Raman Singh, Prof. J F. Nie and Prof. Alankar have known each other now for approximately 7 years. Prof. Alankar has submitted several proposals with Profs. Singh and Nie. Overall, 4 co-guided students have graduated so far. Prof. Alankar has met with Profs. Singh and Nie in-person. Prof. Singh and Prof. Alankar are co-supervising 3 students currently. This proposal was discussed over email between the three investigators.

Potential RPCs from IITB and Monash

Professor MJNV Prasad (expert in process-structure-property relations) mjnvprasad@iitb.ac.in)
Associate Professor Aditya Paranjape (expert in Machine Learning, biological systems, aditya.paranjape@monash.edu)

Capabilities and Degrees Required

An ideal candidate should have a BTech or BE or Masters in Mechanical Engineering, Aerospace Engineering, Civil Engineering or Materials Engineering with a strong inclination towards programming, mathematics, machine learning, statistics, probability.

Necessary Courses

A few tentative courses are as following:
MM 713 Aqueous Corrosion and its Control
CSO604 Natural Language Processing and Generative AI
CS772 Deep Learning for Natural Language Processing
CS725 Foundations of Machine Learning
CS726 Advanced Machine Learning

Potential Collaborators

Hospitals, doctors. We have not contacted yet.

K**eywords** relating to this project to make it easier for the students to apply.

Biomedical implants, Mg alloys, process-structure-property relations, Generative AI, Deep learning, machine learning