

An Indian-Australian research partnership

Project Title: **Selective phase crystallization using nucleating agents in isotactic polypropylene-based nanocomposites**

Project Number **IMURA0352**

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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

Isotactic polypropylene is an important industrial polymer that crystallizes in both alpha (equilibrium and monoclinic) and beta (metastable and hexagonal) forms. Often, the beta-phase is the more desirable because of its superior mechanical properties, and its concentration in the crystallizing melt is usually enhanced by addition of beta-specific nucleating agents. However, the exact mechanisms of beta-phase nucleation in the presence of beta-nucleating agents are poorly understood. Here, we propose to use dicarboxylic acid based salts as nucleating agents to enhance beta-phase nucleation in isotactic polypropylene-based nanocomposites with carbon nanotubes and graphene as the filler phases. In addition, we propose to utilize molecular dynamics simulation to investigate the crystallization of isotactic polypropylene in the presence of dicarboxylic acid salts and carbon-based nanofillers

Project aims

1. To study the morphology of the nanocomposites in the presence of nano-filler via TEM and SEM
2. To study the phase behaviour of the nanocomposites using X-ray diffraction
3. To investigate the crystallization of isotactic polypropylene from melt using molecular dynamics simulations

Expected outcomes

Highlight the expected outcomes of the project

1. Mechanism of beta-phase nucleation on a dicarboxylic acid based nucleating agent
2. Utilization of the dicarboxylic acid based salts as both dispersants and nucleating agents
3. Enhancement of beta-isotactic polypropylene in carbon nano-filler based composites

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.

The research area in the field of carbon nanotubes and graphene (graphene oxide) based polymer nano-composites can be considered as sub-research area of 'Nanotechnology'. The project aims to simultaneously disperse carbon nanotubes (graphene oxide) at the nanometer length-scale and enhance nucleation of a specific polymer phase, with the aim of achieving superior mechanical and thermal properties.

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.

1. We are looking for 1 Ph.D. students in this project who will be involved with both molecular dynamics simulations and experiments; candidates who have worked in the area of polymer composites involving carbon nanotubes/graphene would be desirable. The candidate should also demonstrate a good mathematical aptitude and basic understanding of numerical modelling.
2. M.Tech in Polymer/Fiber Science/Materials Science & Engineering/Chemical Engineering
3. M.Sc in Physics, Chemistry with 2-3 years research experience

Please provide a few key words relating to this project to make it easier for the students to apply.

Polymer Crystallization, Carbon Nanotubes, Graphene, Polymer Nanocomposites, Molecular Dynamics Simulations