

An Indian-Australian research partnership

Project Title: **Laser Assisted Evaporation for Imaging of Biological Specimens Using Graphene-Enabled Atom Probe Tomography**

Project Number **IMURA0821**

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IITB Department:
Mechanical Engineering

Research Clusters:

Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? <i>(Please nominate JUST <u>one</u>. For more information, see www.iitbmonash.org)</i>		Highlight which of the Academy's Theme(s) this project will address? <i>(Feel free to nominate more than one. For more information, see www.iitbmonash.org)</i>	
1	Material Science/Engineering (including Nano, Metallurgy)	1	Advanced computational engineering, simulation and manufacture
2	Energy, Green Chem, Chemistry, Catalysis, Reaction Eng	2	Infrastructure Engineering
3	Math, CFD, Modelling, Manufacturing	3	Clean Energy
4	CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control	4	Water
5	Earth Sciences and Civil Engineering (Geo, Water, Climate)	5	Nanotechnology
6	Bio, Stem Cells, Bio Chem, Pharma, Food	6	Biotechnology and Stem Cell Research
7	Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng	7	Humanities and social sciences
8	HSS, Design, Management	8	Design

The research problem

Define the problem

Atom probe tomography (APT) is the only technique capable of offering 3D chemical measurements with near atomic resolution has recently been applied to imaging biological cells by coating the specimen with a graphene layer. The graphene layer is coated to make the specimen conductive. Application of APT to imaging of insulating materials has been recently enabled by achieving evaporation not by direct high voltage pulsing but by thermally driven evaporation using high-power high-frequency laser pulsing. The evaporated ions and molecules reach a position sensitive detector. The impact positions and sequence of hits are employed to reconstruct their original position within the specimen and the time of flight is utilized to determine the atomic species. The optimal resolution largely depends on the evaporation process, which is largely governed by the choice of laser parameters. Therefore, the aim of this project is to understand the influence of laser parameters on the evaporation process using molecular dynamics simulations and determine the right set of operating parameters to generate optimal resolution using APT. The work would a concurrent experimental and simulation approach.

Project aims

1. *To develop an atomistic model of laser-assisted evaporation in APT of biological cells using molecular dynamic (MD) simulations*
2. *To validate and interpret the models developed using experiments*
3. *To determine the optimal laser parameters for improved resolution in APT.*

Expected outcomes

1. *Enabling the use of atom probe tomography (APT) for biological cells based on laser-assisted evaporation*
2. *Enhance the understanding of laser-assisted evaporation using computational models (MD simulations), which could enhance the understanding of laser-matter interaction of graphene and biological cells.*

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

1. *The research would lead to the development of a novel atom probe tomography (APT) for insulating materials based on laser-assisted evaporation. The technique would have wide applications in materials science and nanotechnology.*
2. *The project also deals with developing atomic scale simulations to capture the evaporation process involved in APT of biological cells. A significant part of the work would involve modeling & simulation.*

Capabilities and Degrees Required

Essential skills:

*Strong background in thermodynamics, heat transfer, basic physics, mathematical modeling and computational methods
Computer programing in C/C++, Java or Fortran*

Additional skills (not mandatory):

MD simulations, solid-state physics

Qualifications:

B.Tech/M.tech in Mechanical Engineering, Materials Science and Engineering, Nanotechnology or Physics.

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.

1. Prof. Shobha Shukla (Metallurgical Engineering and Materials Science, IIT Bombay)
2. Prof. Wenlong Cheng (Chemical Engineering, Monash University)

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.

Laser-assisted evaporation, graphene, biological cells, atom probe tomography