IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Microstructure-property relationships of conductive polymers and substrates for organic solar cells – Experimental characterisation and micromechanics-based modelling.**	
Project Number	**IMURA0718**	
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Research Clusters:

Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? *(Please nominate JUST* ***one.*** *For more information, see www.iitbmonash.org)*		**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	***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*		
8	*HSS, Design, Management*		

The research problem

Solar cells made of organic semi-conductor are highly promising as a low-cost alternative to the currently used crystalline, mostly silicon-based materials. In addition to their low cost and ease of processing, organic solar cells can also be made flexible and stretchable, opening new venues for photovoltaic applications, including integration with textiles or wearable devices [Lipomi et al., Adv. Mater. 23:1771 (2011)]. In this context, the intrinsic mechanical properties of the semi-conductor polymer play a critical role. Ideally, one would like to increase the compliance and ductility of the active material while maintaining good electrical properties.

The most studied material for organic semi-conductor is a blend of p-type conjugated polymer (P3HT) and a n-type fullerene (PCBM). At the scale of the microstructure, these blends usually consist of a nanocrystalline regions of pure P3HT tied together by polymer chains and embedded in an amorphous matrix made of a mixture of P3HT and PCBM. In addition, the microstructure morphology may evolve during straining, inducing an anisotropic response, both mechanically and electrically [O'Connor et al., Adv. Funct. Mater. 21:3697 (2011)]. However, a precise understanding of the relationships between the microstructure of the semi-crystalline polymer and its mechanical and electrical properties remain mostly elusive. From a mechanics perspective, most available experimental data focus on properties like the elastic modulus and the strain at crack initiation [Savagatrup et al., Adv. Funct. Mater. 24:1169 (2014)], while the stress-strain behaviour of the conductive polymer under general loading conditions (including multiaxial and non-monotonic loading conditions relevant for stretchable photovoltaic applications) has not been well characterised and modelled. In addition, there is a fundamental gap in knowledge regarding how the mechanical and functional behaviour of the polymer relate to the microstructure and its evolution during straining.

Project aims

The general objective of this project is to develop a fundamental understanding of the deformation mechanisms of P3HT-PCBM blends. This will be achieved through a combination of experiments and modelling. The experimental component of the project will be conducted at IITB under the supervision of Dr Singh and will provide the physical basis for the model development, which will be done at Monash University under the supervision of Dr Brassart.

Specific project aims:

1) To characterise the mechanical and electrical behaviour of P3HT-PCBM blends. This will be done by considering thin films on top of an elastic substrate with well-known properties (e.g. PDMS) and subjected to various loading conditions (uniaxial, biaxial, cyclic).
2) To characterise the microstructure and how it evolves during straining.
3) To develop a micromechanics-based constitutive model for the semi-crystalline polymer. The proposed constitutive model should be able to capture the elastic-plastic response of the polymer under arbitrary loading conditions, while explicitly linking the mechanical properties to the relevant microscale features, such as the relative volume fraction of crystalline and amorphous regions and their intrinsic properties, e.g. [van Dommelen et al., J. Mech. Phys. Solids 51:519 (2003)]. The model should also be able to predict how the microstructure evolves during straining. The proposed model will be implemented as a user-subroutine (UMAT) within the finite element software Abaqus, which will enable the simulation of flexible and stretchable devices under arbitrary loading conditions.
4) To propose guidelines for the development of optimal microstructures in terms of compliance, ductility and electrical conductivity.

Expected outcomes

- New knowledge on microstructure-property relationships in P3HT-PCBM blends.
- A numerical platform for the simulation of photovoltaic devices based on semi-crystalline polymers based on which other models could be developed in the future.
- To demonstrate the enhanced stretchability and flexibility of the devices made using the recommendations of the models.

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.

Theme 1: This project involves a major modelling and simulation component that directly addresses the need to new simulation tools that can assist the manufacturing of advanced polymers with optimal properties.

Theme 3: This project will advance the field of organic solar cells by providing new knowledge and design principles for new advanced conductive polymers.

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.

- Masters or bachelors degree in mechanical engineering/materials science/metallurgy or in a related area;
- A keen interest for polymer physics and mechanics, constitutive modelling and programming;
- A strong background in solid mechanics (continuum mechanics, plasticity theory) and applied mathematics, as well as good programming abilities (e.g. Python, C/C++, Fortran). Prior experience with the finite element software Abaqus will be an asset.

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.

This project is directly related to the research of A/Prof. Chris McNeil at Monash University, which focuses on organic semi-conductor and polymer solar cells.

Select up to **(4)** keywords from the Academy's approved keyword list **(available at www.iitbmonash.org)** relating to this project to make it easier for the students to apply.

Modelling, materials, advanced computational engineering, mechanical engineering