IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**MACHINE LEARNING FOR INSIGHTS INTO GRAPHENE NANOPLATELET-POLYMER COMPOSITE COATINGS FOR CORROSION RESISTANCE**	
Project Number	**IMURA1154**	
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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)*	
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2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*	2	*Circular Economy*
3	*Math, CFD, Modelling, Manufacturing*	3	*Clean Energy*
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*	4	*Health Science*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*	5	*Smart Materials*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*	6	*Sustainable Societies*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*	7	*Infrastructure*
8	*HSS, Design, Management*		

The research problem

This project aims to synthesise, characterise and test novel graphene composite coatings to improve the corrosion resistance, and develop an insight of coating performance by using machine learning based methods. Corrosion of metallic components cause economic losses, and its effective mitigation such as by novel coatings is technologically, commercially and socially very attractive. The composite coatings developed for this proposal will utilise the unique and notable properties of graphene and its derivatives such as graphene nano platelets (GNPs). In the proposed work, polymer-based composite coatings will be modified by adding GNPs to significantly improve the corrosion resistance of common engineering alloys such as steels. The investigation has four parts:

(i) To establish the ability of some common derivatives of graphene (graphene functionalised with -COOH, amine and fluorine groups) to form mechanically and chemically stable composites.

(i) To find suitable resin (epoxy/silane) as a matrix for composite for required mechanical properties and corrosion resistance, and

(ii) To establish the effective/durable corrosion resistance of the graphene derivative-based composite coating.

(iii) Utilize machine learning (ML) for insight of coating development as well its degradation and performance.

In the past decade, several experimental studies have been performed on the development of functionalised graphene-based nanoplatelets (GNPs) containing composite coatings for corrosion resistance. A few of them have provided improvements in corrosion resistance whereas others have not been successful. For example, Krishnamoorthy et al [1] prepared a paint composite by incorporating graphene oxide sheets in an alkyd resin. that improved corrosion resistance of the galvanized iron by an order of magnitude in an aggressive chloride environment similar to sea water. Chang et al [2] reported polyaniline (PANI)/graphene composite coatings to improve the corrosion resistance of steel in sea water, by up to an order of magnitude; and the resistance increased with the content of the graphene-based materials in the composite. However, it was necessary to suitably functionalise the graphene nanomaterial used in this study. The mechanism of the considerable further improvement in corrosion resistance due to polymeric coatings upon incorporation of GNPs into the polymer matrix lies in the ability of GNPs in creating a tortuous path for the corrosive species while permeating through the coating. In fact. a similar mechanism has been well-known in the case of polyaniline/clay-containing composites sheets (PACCs). However, the composite coatings with GNPs have been demonstrated to outperform the composite with polyaniline/clay-containing sheets (PACCs), as result of the former providing more tortuous paths for the corrosive species, as evidenced by the permeability data. Another study [3] has also supported the tortuous path mechanism due to sheets/exfoliates of graphene-based materials. There have been further studies on the composites containing GNPs (e.g., graphene nanosheets [4], graphene oxide (GO) [5], reduced graphene oxide (rGO) [6]). However, these systems have not produced as impressive corrosion resistance. In order to understand the reasons for such variabilities and mitigate them, it is proposed to utilize the modern tools available with machine learning (ML), at synthesis as well its degradation of the composite coatings.

The aforementioned challenge of designing novel composite coatings based on graphene calls for an efficient optimization framework. Experimental approach reveals the fundamental observations. However, that may be limited due to preparation, repeatability and tedious nature of the trial-and-error based investigation. This approach is not only expensive but also is associated with large uncertainty around finding the target property or process. Thus, the required number of experiments need to be strategically reduced by using suitable algorithms. In designing graphene based composite coatings containing GNPs, the primary design parameters are matrix material and its characteristics, GNPs size, GNP distribution, matrix-GNP interface characteristics and corrosion species. Similarly the objective function be chosen to be direct i.e. corrosion rate or indirect e.g. degree of tortuosity of corrosion path for various species, architecture of the composite or internal structure and desired mechanical properties. This sets up a multifaceted optimization problem in which apart from the known inputs and output variables, several unknowns may also play critical role. Thus, classical optimization methods may not yield the desired coating architecture, especially when the data may not be in abundance. As noted by McDonald et al [7], large polymers show more complicated and less predictable structure-property relationships than alloys due to the greater number of variables which dictate their properties in the former-namely, composition, molecular mass, inter- molecular forces, and architecture. This is usually not the case in small molecule polymers.

The concept of machine learning offers many flavours for novel design complex materials [8]. The most common problems where both input variables and outcomes are known, can be addressed by using supervised machine learning [9]. In supervised machine learning, the model is shown several examples for learning. Neural network models, random forests [10], Gaussian process regression [11] are a few such methods. The model is chosen based on availability of data, interpretability and several other factors e.g. ease of application. For examples, random forest model based framework is usually associated with a feature selection method by using which one can rank the most important features i.e. factors that affect the output. This is an important exercise since this also leads to order reduction of the numerical setup which otherwise becomes computationally expensive. Overall, supervised learning can be used for identifying matrix material and next generation GNPs. For such data-driven machine learning models, data is usually available from dedicated databases. For polymers see ChemNetDatabase in Ref. [12] and Ref. [13] that can be useful for the matrix material. Another class of machine learning called unsupervised learning can be employed for corrosion species path which is related to the network of size, size distribution of network of GNPs in the matrix.

References

(1) K Krishnamoorthy et al, Graphene Oxide…., ***Carbon***, 72 (2014) 328.

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(3) M Yi et al, Exploring few-layer graphene and graphene oxide as fillers to enhance the oxygen- atom corrosion resistance of composites, ***Phys. Chem. Chem. Phys.***, DOI: 10.1039/c4cp00114a

(4) J Han et al, Microstructure and anti-wear and corrosion performances of novel UHMWPE/graphene-nanosheet composite coatings deposited by flame spraying**, *Polym. Adv. Technol.***, 24 (2013) 888.

(5) S Mayavan et al, Graphene ink as a corrosion inhibiting blanket for iron in an aggressive chloride environment, ***RSC Adv.***, 3 (2013) 24868.

(6) M Zhang et al, Two-dimensional transparent hydrophobic coating based on liquid-phase exfoliated graphene fluoride, ***Carbon***, 6 (2013)149.

(7) S M McDonald, et al, Applied machine learning as a driver for polymeric biomaterials design, ***Nature Communications***, 14 (2023), 4838.

(8) R Ramprasad et al. Machine learning in materials informatics: recent applications and prospects, ***npj Computational Materials***, 3(2017), 54 (2017).

(9) Aurelien Geron, **Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems**, Third Edition, O'Reilly.

(10) G S Thoppil et al., Hierarchical machine learning based structure–property correlations for as–cast complex concentrated alloys, ***Computational Materials Science***, 216 (2022), 111855.

(11) G S Thoppil et al., Bayesian approach for inferrable machine learning models of Process-Structure-Property Linkages in Complex Concentrated Alloys, ***Journal of Alloys and Compounds***, 171595.

(12) https://poly.chemnetbase.com/polymers/PolymerSearch.xhtml?dswid=-429

(13) https://pppdb.uchicago.edu

Project aims

The Objectives of the project are:

(i) To establish the ability of some common derivatives of graphene (graphene functionalised with -COOH, amine and fluorine groups) to form mechanically and chemically stable composites.

(iv) To find suitable resin (epoxy/silane) as a matrix for composite for required mechanical properties and corrosion resistance, and

(v) To establish the effective/durable corrosion resistance of the graphene derivative-based composite coating.

(vi) Utilize machine learning (ML) for insight of coating development as well its degradation and performance.

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 polymers, graphene, their derivative materials and their corrosion behavior. The student must be willing to perform experiments and modeling both. Basic understanding of statistics, probability and machine learning will be advantageous. Some programming experience in Python language programming language is an asset. 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 corrosion tests and failure analysis at Monash University, including under the synergistic action of mechanical loading and corrosive fluids.

Expected outcomes

1. Machine learning based structure-property correlations for polymer-GNP composites for corrosion and mechanical properties.

2. Design/composition of a suitable resin (epoxy/silane) as a matrix for composite for required mechanical properties and corrosion resistance.

3. Database of polymer-GNP based composite coating materials focusing on corrosion resistance.

4. A machine learning model addressing the above.

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

This project aims to to establish the ability of some common derivatives of graphene (graphene functionalised with -COOH, amine and fluorine groups) to form mechanically and chemically stable composites. Such composites have found applications in engineering and biomedical domain.

Potential RPCs from IITB and Monash

Associate Professor Vijayshankar Dandapani (expert in Corrosion v.dandapani@iitb.ac.in)
Associate Professor Wenyi Yan (expert in Mechanical Properties of Alloys, wenyi.yan@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 analytical methods. Experience in at least two of the following three criteria is desired: 1. Background in experimental methods, 2. Background in corrosion; 3. Expertise in programming (Python, C, C++, Fortran).

Necessary Courses

A few tentative courses are as following:
MM713: Aqueous Corrosion and its Control
ME793: Multiscale Materials Informatics, Discovery and Design
AE649: Finite Element Method

Potential Collaborators

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.

Corrosion, mechanical behavior, biomedical implants