IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	Understanding the integrity/stability of 'alloying reaction' based anode materials for Na-ion batteries via *in-situ* investigations and mathematical modelling	
Project Number	**IMURA0757**	
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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*

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	*Advanced computational engineering, simulation and manufacture*
3	*Clean Energy*
5	*Nanotechnology*

The research problem

Advanced and sustained electrochemical energy storage (EES) technology is deemed as one of the most promising avenues to address the ever increasing concerns associated with depletion of fossil fuel and rising levels of environmental pollution. Among the advanced EES, Li-ion battery system has been the most sought after technology. However, limited, localized and relatively expensive reserves of lithium precursors have necessitated looking beyond Li-ion battery technology. Accordingly, sodium ion battery system is emerging as the most promising alternative, especially for large scale applications like grid energy storage and storage of energy harvested from renewable sources [1,2]. However, the major obstacle towards the development of Na-ion battery technology is the larger ionic radius of Na^+ (~1.02 Å), as compared to that of Li^+ (~0.76 Å), which renders the most commonly used anode material for Li-ion battery, *i.e.*, graphitic carbon and its variants, not suitable for Na-ion battery [1-4]. This mandates extensive research activities directed towards identification and development of suitable anode material for the upcoming Na-ion battery system; which is presently at its infancy.

In the last few years, a few alloying reaction based materials (primarily, Sb, Sn and SnSb intermetallic) [5,6] have been explored as possible anode materials for Na-ion batteries. Surprisingly, silicon (Si), which otherwise has the highest theoretical Li-storage capacity [7], was initially believed to be 'inactive' towards electrochemical Na-storage [8,9]; thus causing lack of interest towards exploring Si as one of the potential anode materials for Na-ion batteries. By contrast, some of the very recent studies conducted at IIT Bombay have established beyond doubt the possibility of Na-storage in Si [10,11].

Nevertheless, similar to the case of usage of alloying reaction based materials (especially Si) in the Li-ion system, considerable cyclic instability or capacity fade upon repeated sodiation/de-sodiation cycles have been recorded [10,11]. The primary cause for this is the huge volumetric changes associated with Na-insertion/removal; which lead to severe stress developments, concomitant fracture/disintegration and loss of contact with current collector. In addition to capacity fade with increasing cycle number, the stresses also reduce the Na-storage capacities in a more direct sense (as studied for the case of Li-ion batteries [12]), with the fracture of the active materials also contributing towards the irreversible capacity (or coulombic inefficiency) in each cycle. Accordingly, for successful usage of Si (or other alloying reaction based materials like Sn) as anode material for the upcoming Na-ion system, the above issue needs to be better understood and addressed for this system; which, at this stage, is fair to say is relatively unexplored.

References

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Project aims

Against the above backdrops, this proposed research aims at developing better insights into the stress developments in Si and Sn based anode materials for Na-ion battery and contributing towards addressing the same in scientific, as well as technologically viable, terms. As a first step, the stress developments in such anode materials will be investigated in real-time (*i.e.*, *in-situ*) during electrochemical cycling. In this context, it needs to be mentioned here that the set-up/expertise needed for the above is present at few the

research laboratory in the world, including ours. The extent of sodiation and desodiation will also be investigated in real-time via *in-situ*) synchrotron X-ray diffraction and Raman experiments. The investigations will be performed with systematic variations of the dimensions of the active electrode materials (from sub-micron to nanoscaled levels). The results obtained via basic electrochemical experiments and the different *in-situ* studies will be analysed in correlation with each other. The usage of nanoscaled buffer/interlayers (such as graphene) between the anode active material and current collector on the electrochemical performance and stress developments will also be explored. Better understanding of the stress developments during sodiation/de-sodiation will be obtained via detailed mathematical modelling and numerical simulations. A theory coupling sodium diffusion to large, plastic deformation of the anode materials will be developed inspiring from the state of the art in modelling lithium-ion batteries. Numerical implementation of the theory will be carried out using the finite element method in order to solve relevant boundary value problems of various geometries, such as the cyclic sodiation of thin films accounting for the presence of a buffer. Model predictions will be compared to the experimental results obtained via *in-situ* monitoring of the stress developments.

Overall, the knowledge gained via the comprehensive/systematic sets of experimental, modelling and computational studies will eventually be used to develop high capacity and stable anode materials for the Na-ion battery system. This is expected to address one of the major issues associated with the upcoming Na-ion battery technology; thus contributing significantly towards the overall scenario of energy storage (in more precise terms; via successful development of a more sustainable advanced electrochemical energy storage technology).

Expected outcomes

The project aims at developing detailed/critical understanding of the major issues concerning the cyclic instabilities (or fairly rapid capacity fade with electrochemical cycling) of the relatively unexplored 'alloying reaction' based anode materials (such as Si, Sn; of varying dimensions) for Na-ion batteries via comprehensive and systematic sets of electrochemical measurements, associated innovative *in-situ* experiments and advanced continuum mechanics modelling.

The effects of the presence of nanoscaled buffer/interlayers on the above aspects will also be investigated with a bid to achieve considerable improvement in the performance of such electrode materials.

The obtained results and understanding will then be used to design and develop high capacity, yet highly stable, anode material for the upcoming and relatively more sustainable Na-ion battery technology; thus addressing one of the bottlenecks towards the successful development of the same.

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

In a broader perspective, the presently proposed project is based on application of **nanomaterials** (such as thin films of Si/Sn, layered 2D materials like graphene) and **nanotechnology** (such as development of multi-layered thin films, electrochemical-mechanical *in-situ* studies with nanostructured materials and interfaces etc.) towards improvements in the electrochemical **energy storage** technology. In other words, contributing significantly towards the developments of **sustainable** energy storage technology. Such concerned improvements (based on the overall objective of the project) are essential for rendering the energy storage technologies suitable for applications related to storing of energy 'harvested' from renewable sources like *solar energy* (which is needed for *controlling environmental pollution* and also in light of the *depletion of fossil fuels*) and *grid energy storage* (which is needed for allowing the large scale usage of the *cleaner*, but intermittent, *renewable sources of energy* like solar and wind) in a relatively economical-cum-sustainable manner. Finally, a key aspect of this project is to investigate the stress generation mechanisms and associated plasticity and damage using advanced continuum modelling and finite element simulations. The project will also investigate the atomic structure and stress-generation mechanisms of the interfaces using density functional theory or molecular dynamics simulations. These methods require state-of-art massively parallel high performance computing systems, consequently addressing the theme of **advanced computational engineering**.

Capabilities and Degrees Required

The student should ideally have a basic degree in areas related to Mechanical Engineering and/or Metallurgical/Materials Engineering (including Ceramic Engineering). The modelling component of the project requires a strong background in solid mechanics, numerical methods (in particular the finite element methods) and good analytical and programming skills. Candidates having a CPI of > 7.5/10 (or overall % of 75%) in the qualifying examination/degree are likely to get preference. Similarly, candidates having some previous research experience during Master's program or as research/project associate might get preference.

Potential Collaborators

Prof. Prita Pant (Metallurgical Engineering and Materials Science, IIT Bombay), Prof. Sagar Mitra (Energy Science and Engineering, IIT Bombay), Prof. M. Aslam (Physics, IIT Bombay), Prof Douglas R. MacFarlane (School of Chemistry, Monash), Prof. Nikhil Medhekar (Materials Science and Engineering, Monash)

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.

Energy, Energy Storage, Energy Materials ;
Nanotechnology, nanoscience ;
Novel Batteries and Fuel Cells;
Modelling and Simulation