simpleware

IMPERIAL COLLEGE LONDON

Success Story

"An ability to understand processes at work, at fine length scales, in electrochemical devices allows us to improve them. An ability to improve them is vital if we are as a species to meet increasing energy demands in areas from transport to consumer electronics, all in a clean efficient manner."

Dr Farid Tariq,
Research Associate,
Imperial College London

Thanks to:
Department of Materials and Department of Earth Science & Engineering at Imperial College London

Optimising the Design of Energy Materials

Overview

Image-based modelling helps researchers at Imperial College London to better understand the functional properties of electrochemical and other energy materials and devices such as fuel cells and batteries. Using a range of scan modalities, including FIB-SEM, micro-CT and electron microscopy, as well as image processing tools such as Simpleware and physics-based solvers, researchers can reconstruct and investigate complex 3D structures.

The design of energy materials used in everything from cars to the home can be better understood and optimised by exploring their nano/microstructures and simulating their response to a variety of different physical conditions (e.g. thermal, electrochemical, stresses).

At a Glance

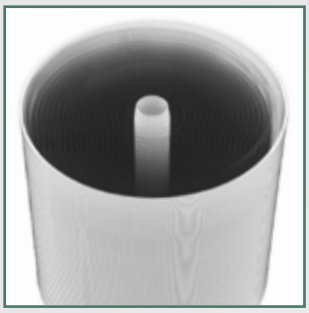
» Images of energy materials obtained at different length scales

» 3D models generated for analysis and simulation

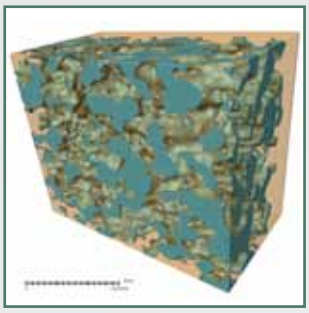
» Research enables better understanding of fuel cells, batteries, flow cells and other energy materials

OBTAINING 3D IMAGE DATA

One of the challenges faced in energy materials research involves accurately reconstructing and being able to analyse samples at the micro and nano-scale. At Imperial College London, scientists have tackled this problem by developing innovative multi-scale tomographic techniques to obtain 3D images of batteries, fuel cells and other devices. Images generated from multi-scale tomography can be investigated to quantify shape, sizes, structures and morphology, allowing for comprehensive insights into functional properties.



Micro-CT Scan of a Lithium Ion Battery

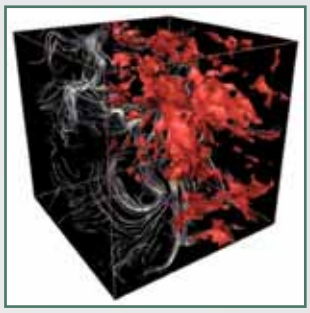


3D Reconstruction of a Solid Oxide Fuel Cell (pores green and ceramic transparent)

STUDYING CATALYST FLUID FLOW

One successful application of these techniques has been to evaluate the effect of pore size on fluid flow across large length scales in silica-alumina pellet-based catalysts. 3D image data was obtained from X-ray microtomography (XMT), dual beam-focused ion tomography (DB-FIB) and electron tomography (ET). Reconstructed images were analysed and converted at each length scale into meshes in Simpleware software, before being exported to solver ANSYS Fluent® for simulation of permeability, enabling new insights into pore size and how to optimise materials.

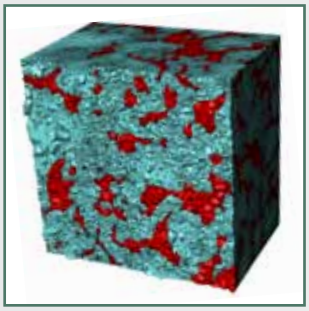
Catalyst Pellets



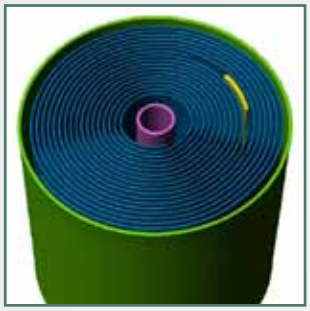
3D Fluid Flow (silver) through the Pore Structure (red) within the Catalyst Pellet

GENERATING FE/CFD MESHES

Using Simpleware software, researchers are able to convert scan data from different 3D imaging techniques into computational models suitable for finite element and computational fluid dynamics simulations. Complex nano/microstructures can be converted at different length scales into meshes that can be directly exported into physics-based solvers for the simulation of electrochemistry, fluid flow, stresses, heating and other physics.



Multi-part Mesh of the Micro-structure of a S2 Catalyst Pellet (pores in red)



Segmentation and Mesh of a Lithium Ion Battery

INDUSTRIAL APPLICATIONS

This type of image-based research has broad applications for industry, enabling researchers and manufacturers to explore the relationship between nano/microstructures and property behaviour in energy materials and devices. Potential applications include designing new fuel cells and batteries that consume less energy and are more efficient at performing their functions, making it possible for manufacturers to handle increasing consumer demands for clean and reliable power. Dr Tariq commented:

"Simpleware provides meshing of highly complex energy material structures acquired from 3D imaging methods with seamless effort and high quality output that can be used with a variety of modelling software. It forms part of the workflow that provides insights into effects which may be difficult to experimentally measure, which may be sources of performance degradation, and areas to target for microstructural optimisation."