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February 2018

Multi-scale modelling for energy storage devices

MANIFEST Researcher Workshop

Samuel J. Cooper, Dami Taiwo, Vladimir Yufit, Farid Tariq, Enrique Ruiz-Trejo, Antonio Bertei, Ann Huang, Barun Chakrabarti, Moshiel Biton, Nigel P. Brandon

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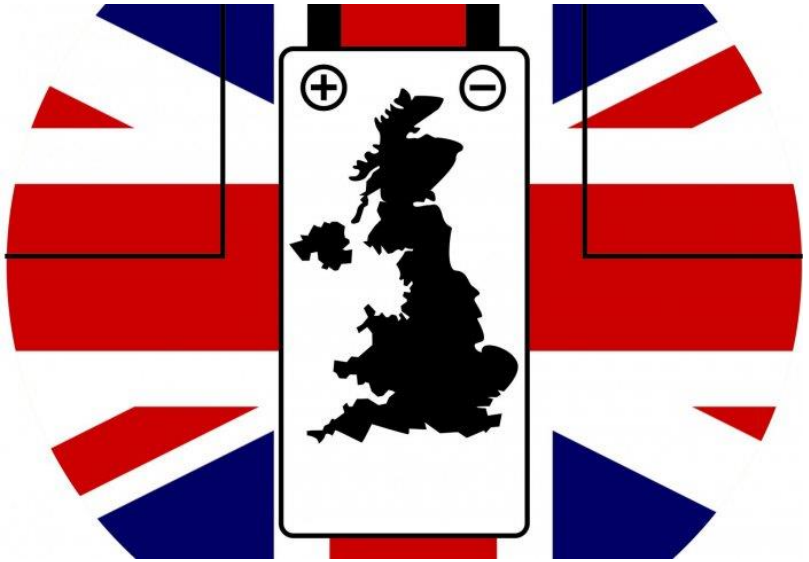
Faraday Challenge

- 4 Fast-start projects starting 2018
  - **Multi-scale modelling** - Imperial
  - **Solid state batteries** - Oxford
  - **Degradation** - Cambridge
  - **Recycling** - Birmingham



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Multiscale modelling

- Lead by Greg Offer at Imperial
- Consortium includes:
  - **Imperial** – Greg Offer (PI), Billy Wu, Monica Marinescu, Aron Walsh, Sam Cooper, Jacqueline Edge (PM)
  - **Bath** – Saiful Islam, Benjamin Morgan
  - **UCL** – Paul Shearing, Dan Brett
  - **WMG** – Emma Kendrick, Dhammika Widanalage, James Marco
  - **Lancaster** – Harry Hoster, Dénes Csala
  - **Oxford** – Dave Howey, Charles Monroe, Colin Please, Jon Chapman
  - **Southampton** - Chris Skylaris, Dennis Kramer

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Multiscale modelling

- 5 Expeditions
  - XP1 - COLDSTART (Lithium intercalation at low T)
  - XP2 - CELLDO (Cell model with defined parameterisation approach)
  - XP3 - BATPACK (Pack level models with thermal coupling)
  - XP4 - ROMCon (Reduced order models for battery control)
  - XP5 - LONGTERM (Bridge the atomistic and continuum models)
- 5 Cross Cutting activities
  - CC1 - PHYSMAT (Fundamental Physics & Materials Science)
  - CC2 - MATHS (Mathematical Methods and Solvers)
  - CC3 - VISDAM (Visualisation & data management)
  - CC4 - TEST (Parameterisation & validation)
  - CC5 - PEACE (Parameter estimation & analysis continuum models)

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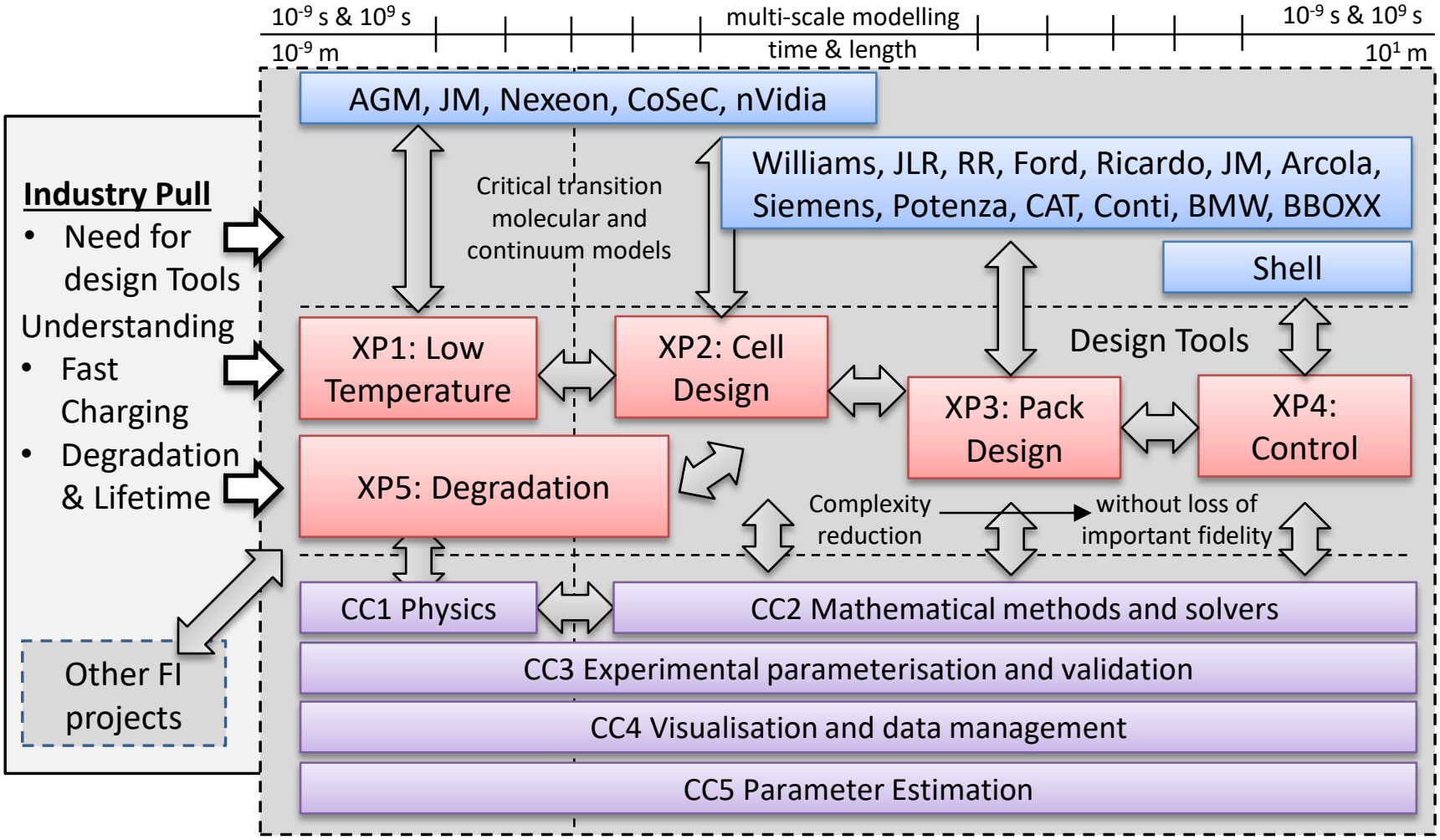

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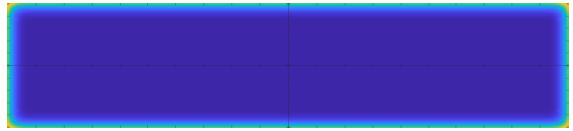
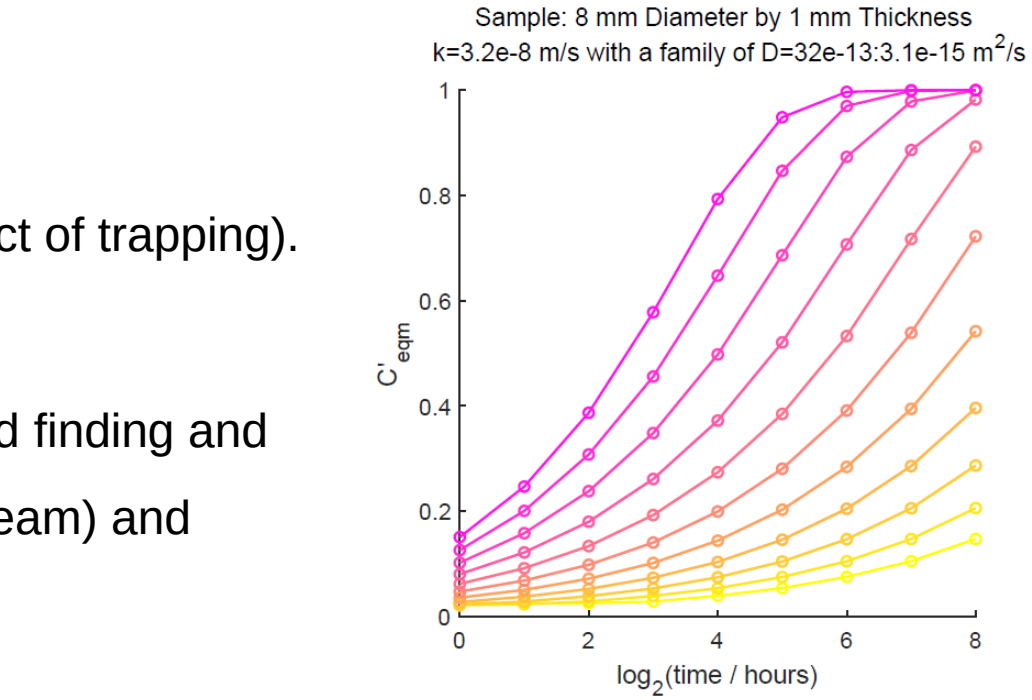
Individual contribution

- PDRA – Novel isotopic approach to characterising solid state diffusion and surface exchange processes.
- PhD – Materials stability (impact of trapping).
- Responsibility to communicated finding and assumption up (to continuum team) and down (to atoms team).





Innovate UK

- 6 project starting at Imperial in collaboration with industry
  - **ABLE** – M-KOPA, Denchi Power
  - **ATESTS** – Rolls Royce
  - **BATMAN** – Perkins, AVID tech.
  - **CoRuBa** – Fergusson's Advanced Composite Technology
  - **IMPACT** – Arcola, Reaction Engines, Flint Engineering Brunel
  - **THT** – Thermal Hazard Technology

Innovate UK

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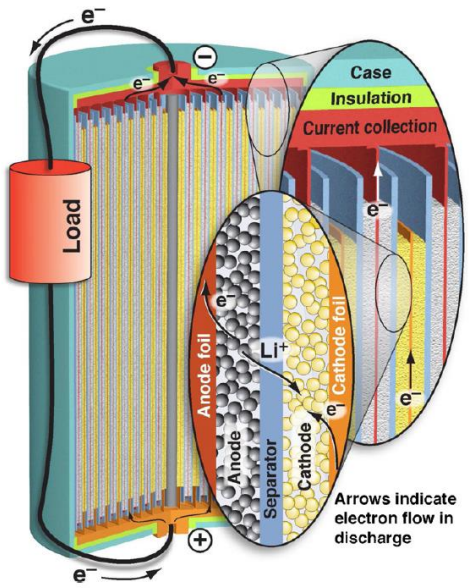
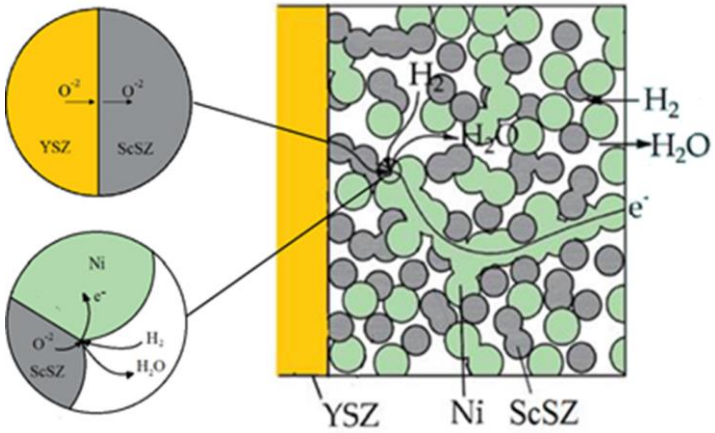
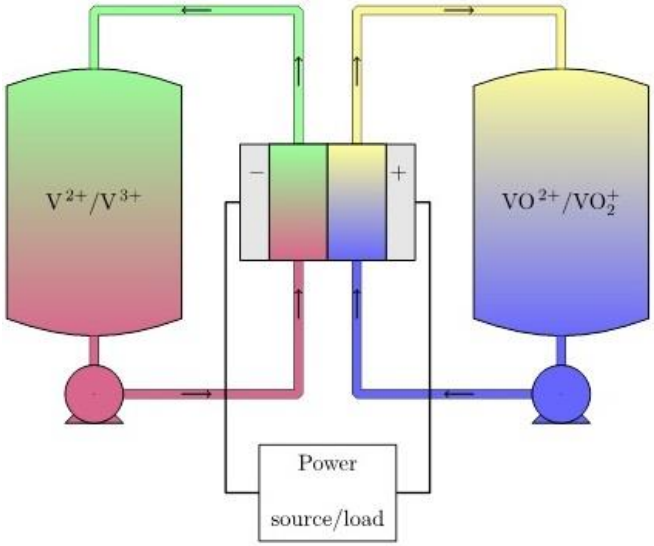
Looking for a job?

- We’re currently looking for 12 postdocs and many PhDs!
  - Please get in touch and I can point you in the right direction

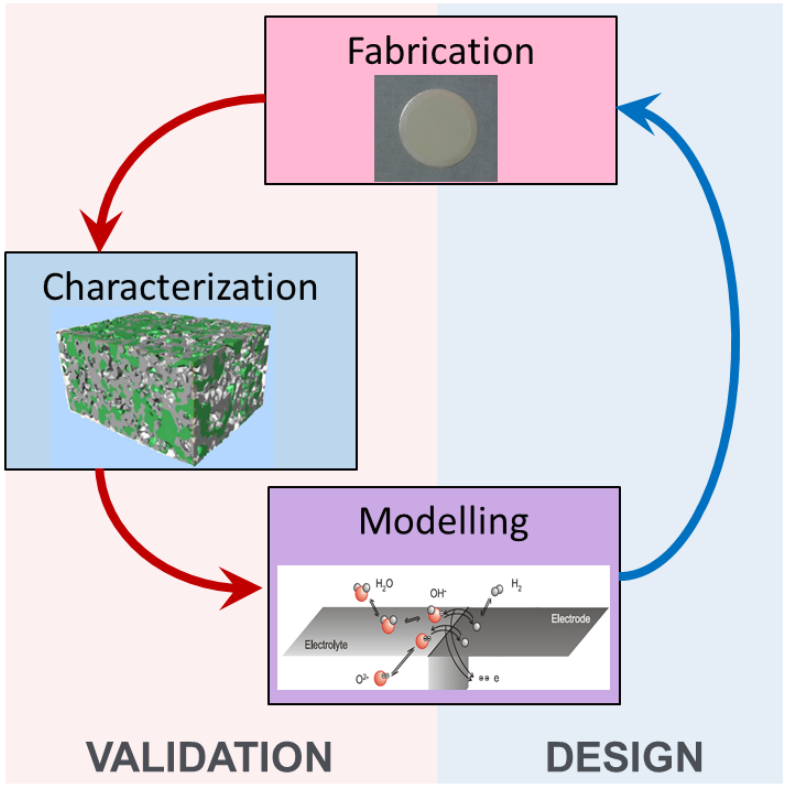
Batteries and fuel cells







Model-based design approach



Electrode microstructure for

Performance optimisation ↓

Bulk properties
- volume fractions
- connectivity
- area per unit volume

Degradation ↓

Local hot spots
Structural evolution

3D Imaging Facilities

- **Lab X-ray CT*** unit with high-efficiency flat panel detector.
- Up to **1 µm** spatial resolution.
- Capability to incorporate in-situ rigs for dynamic experiments.

- Access to **FIB-SEM tomography** equipment.
- High spatial resolution (<10 nm for FIB imaging).
- Better suited for nanostructured material analysis.

**From energy storage capital grant : EPSRC Capital for Great Technologies call - Grid-Scale Energy Storage*

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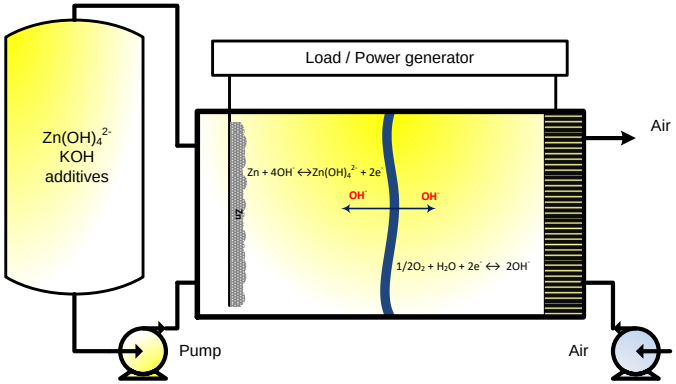
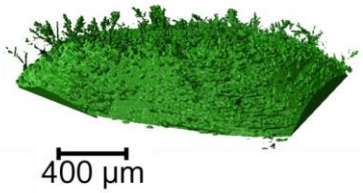
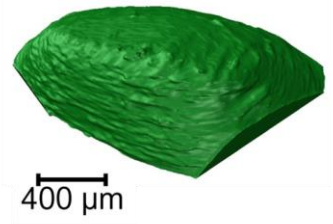
Zinc-based flow batteries – Morphological degradation of Zn

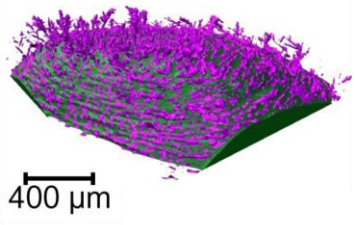




Zinc tip as deposited

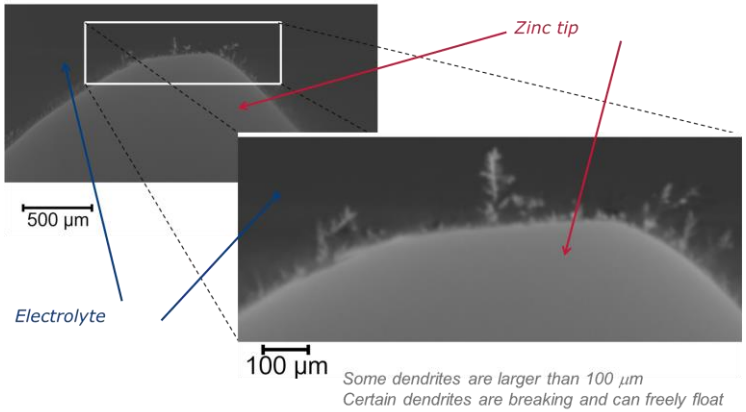


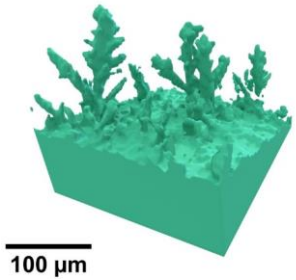
Bare zinc tip before deposition

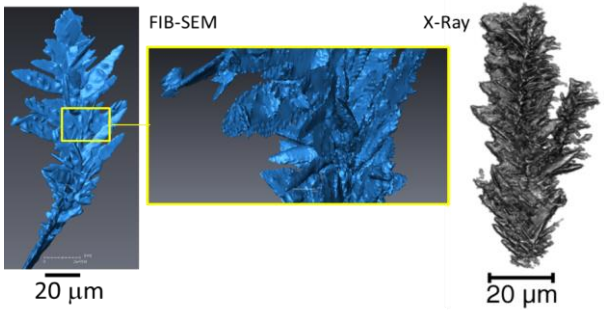


Zinc tip with dendrites "emphasized"

Surface area of the bare tip	Surface area of the tip with dendrites	Surface increase ratio
$4.43*10^6$ µm²	$6.31*10^6$ µm²	1.42



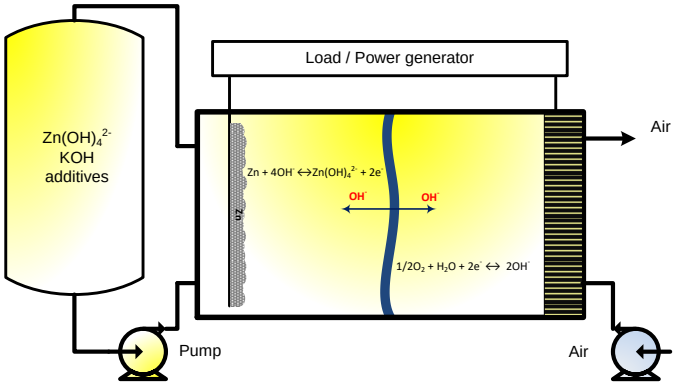


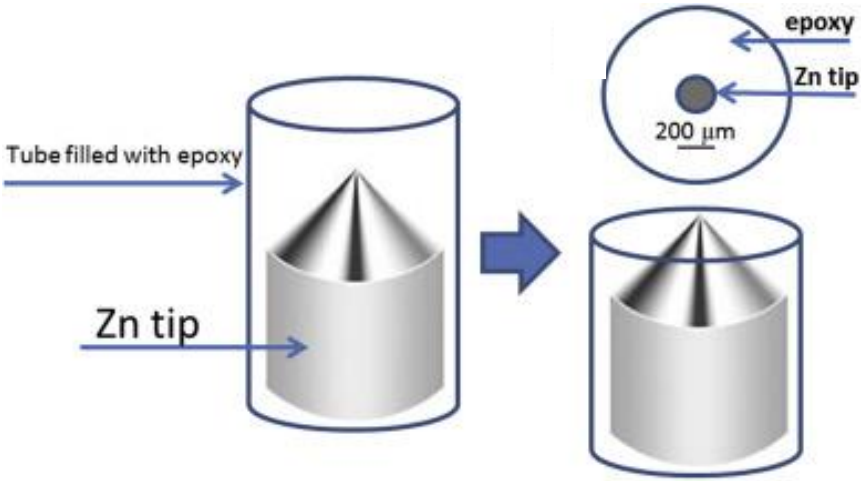


Zn dendrite formation during the first charge

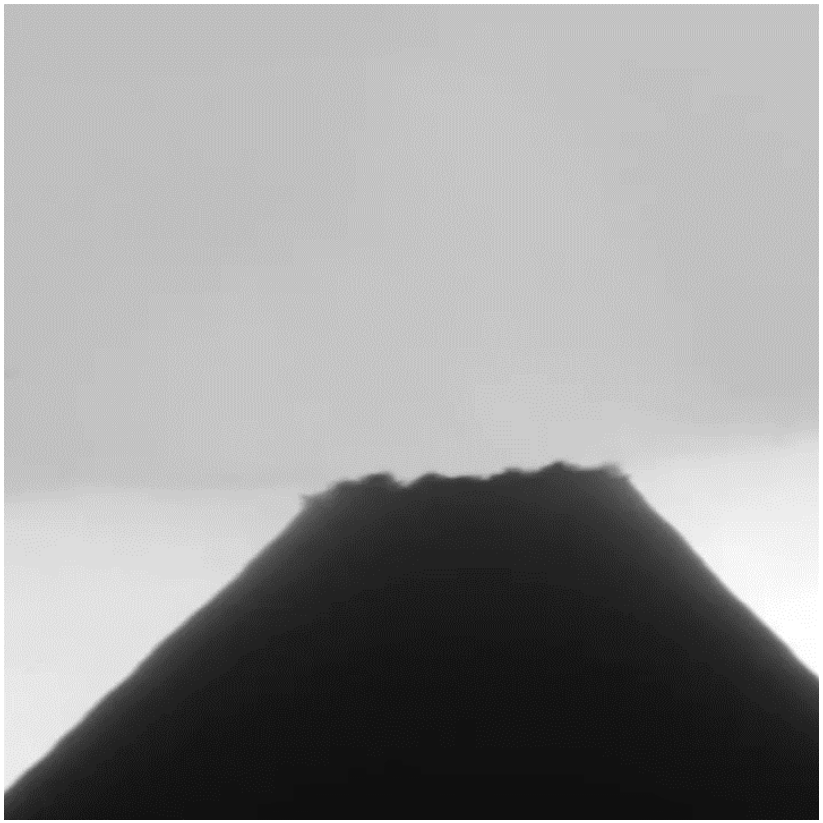
M. Biton,F. Tariq,V. Yufit, Z. Chen,N. Brandon, *Acta Materialia* **2017**, *141*, 39-46

Zinc-based flow batteries – Morphological degradation of Zn





In-situ observation of Zn dendritic growth



M. Biton,F. Tariq,V. Yufit, Z. Chen,N. Brandon, *Acta Materialia* **2017**, *141*, 39-46

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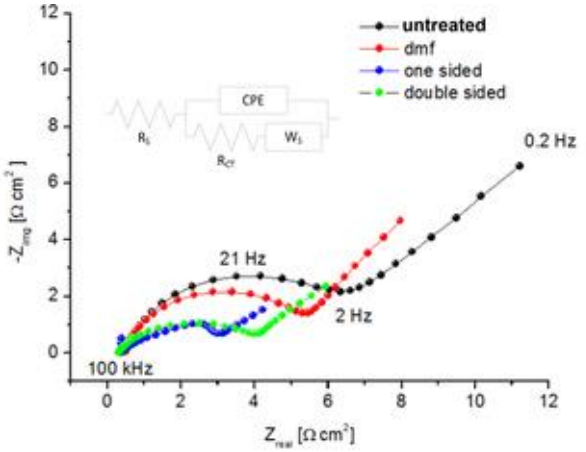
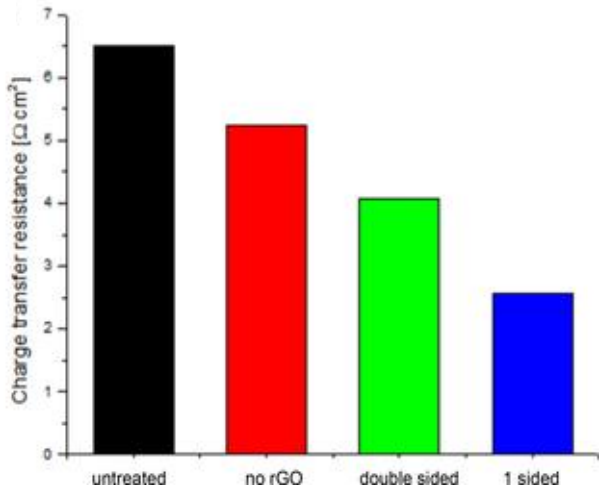
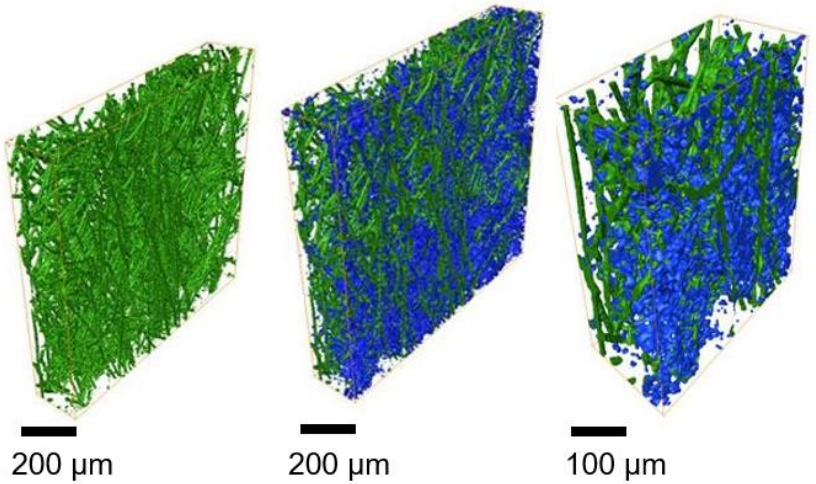
Vanadium redox flow batteries – Carbon paper modification





No rGO Single side rGO Double side rGO



	Total specific surface area with XCT [µm² µm⁻³]	BET specific surface area [µm² µm⁻³]
Untreated CP	**0.81**	**2.8**
One-sided	**1.01**	**5.1**
Double sided	**1.11**	**11.1**

B. Chakrabarti, D. Nir, V. Yufit, F. Tariq, J. Rubio-Garcia, R. Maher, A. Kucernak, P. Aravind, N. Brandon, *ChemElectroChem* **2017**, *4*, 194.

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Lithium-ion batteries – Thick electrodes with controlled porosity

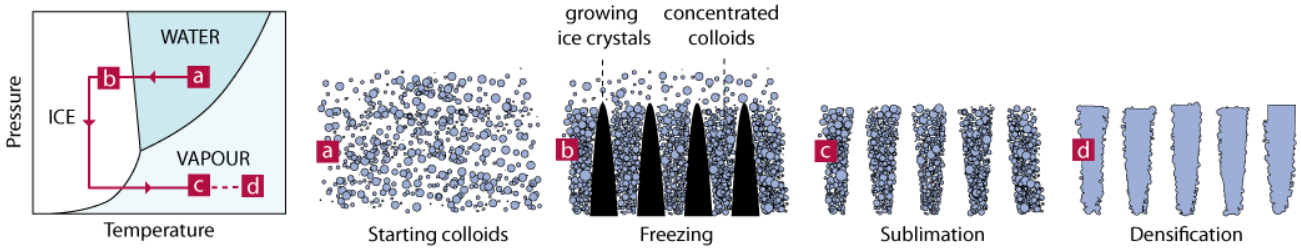
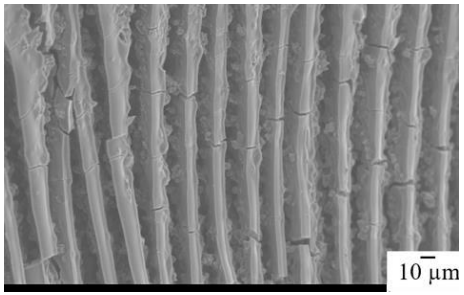


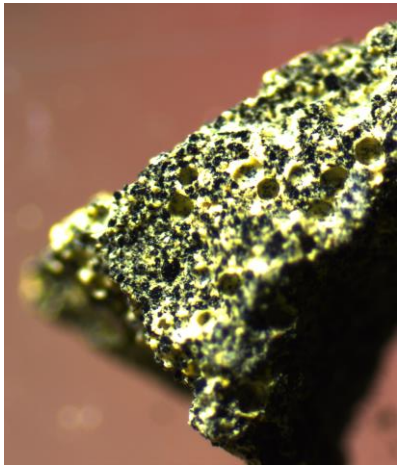
Image ref: Deville, S., Ice templating of porous materials

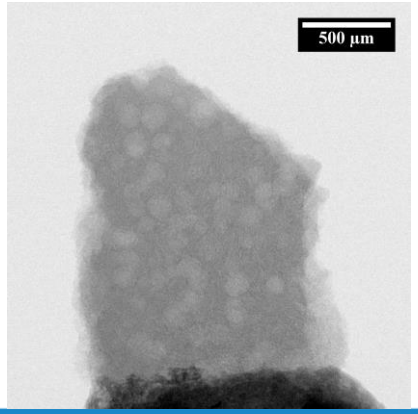
- ***In collaboration with Prof. P. Grant and Dr. A. Huang (Oxford)***
- ***Manufacture of thick high energy density electrodes***
- ***Improve battery power through microstructure control***

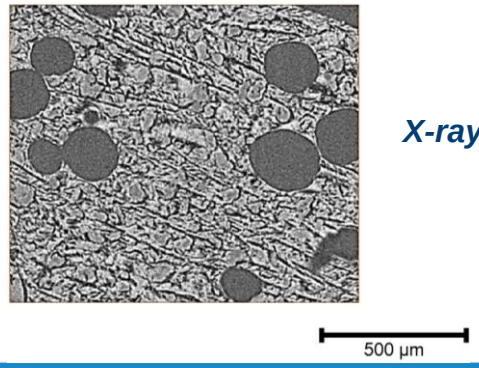


Cross section SEM

Si/SiO_X



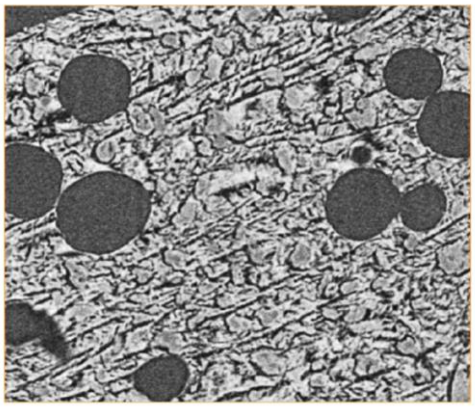


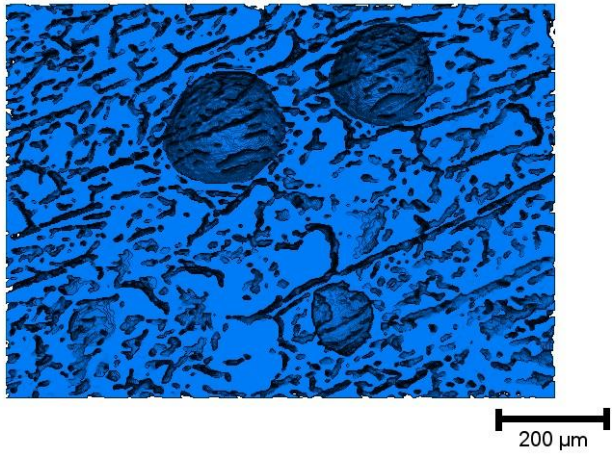


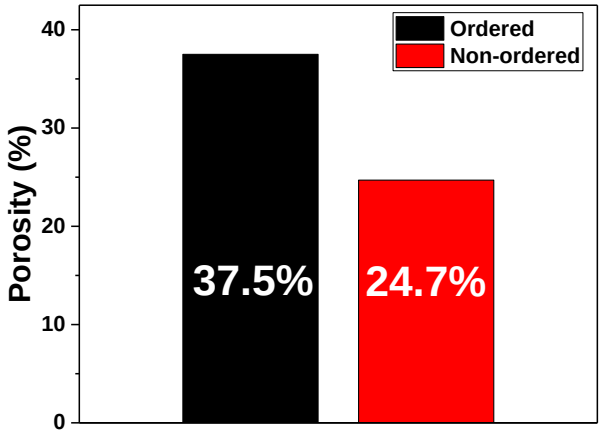
X-ray µCT

Lithium-ion batteries – Thick electrodes with controlled porosity

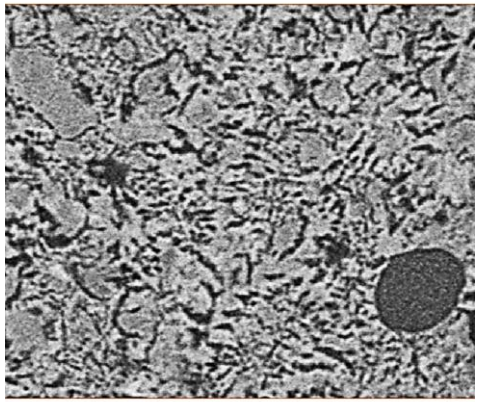
Ordered porosity

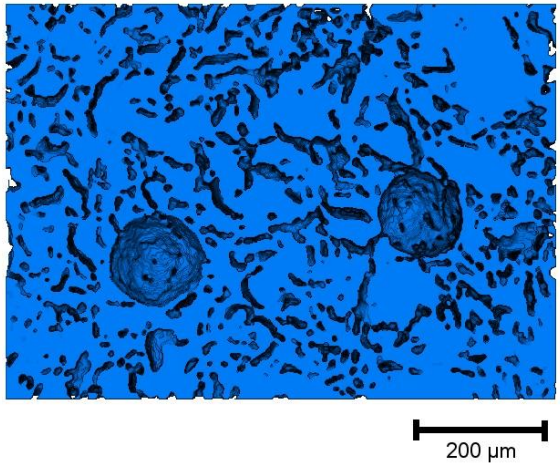


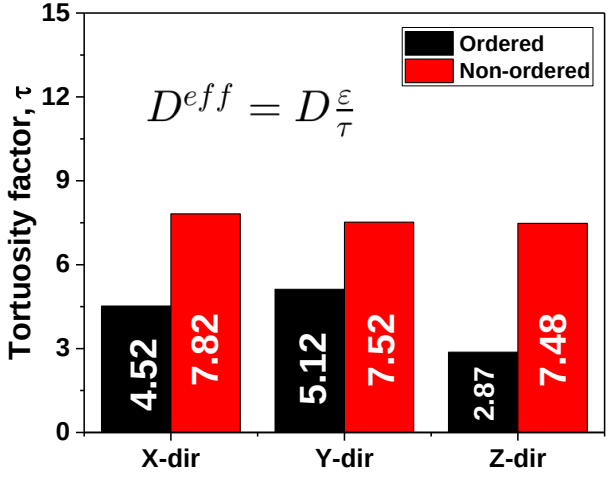




Non-ordered porosity







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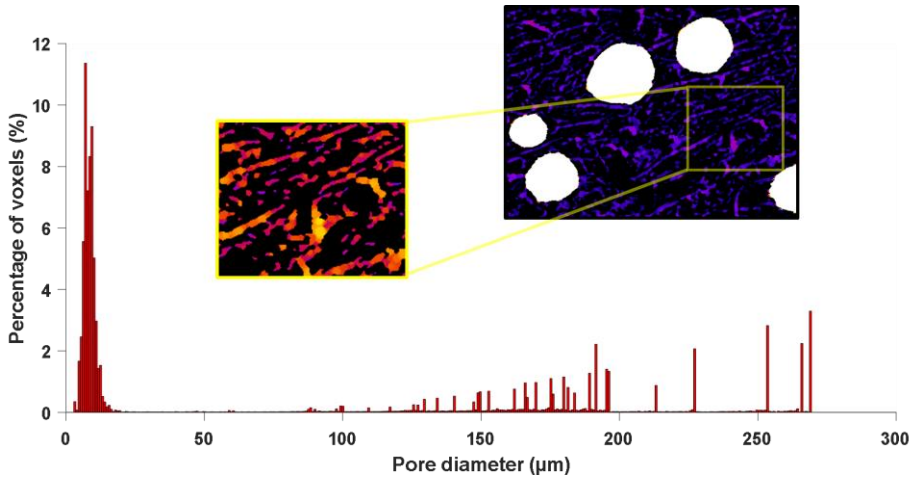
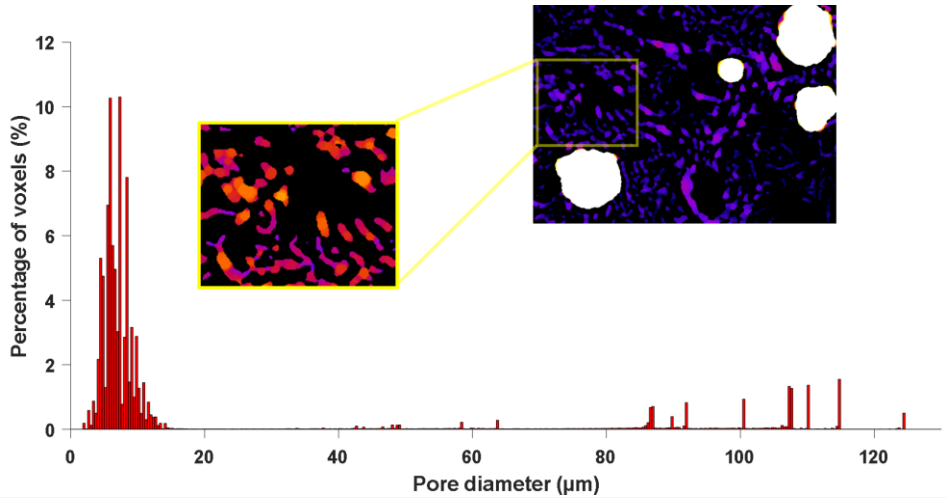
Lithium-ion batteries – Thick electrodes with controlled porosity

Ordered porosity



Non-ordered porosity



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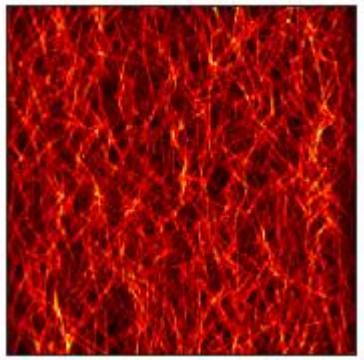
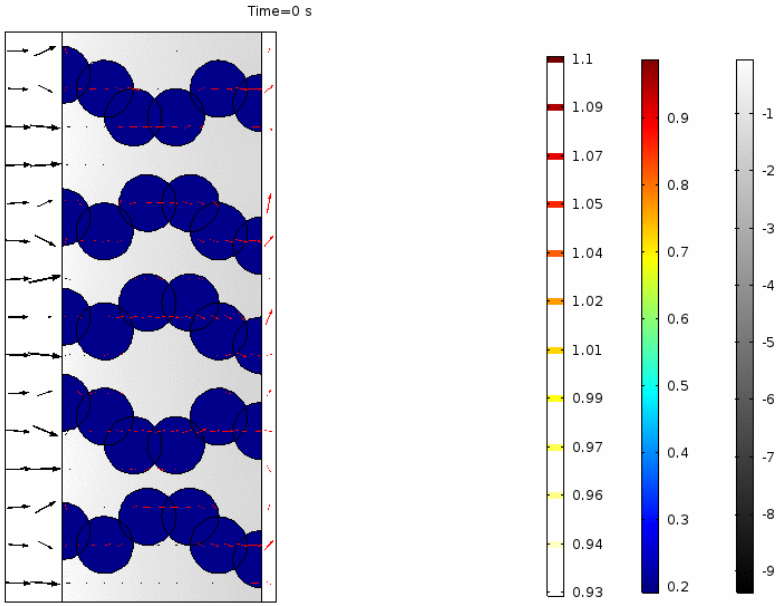
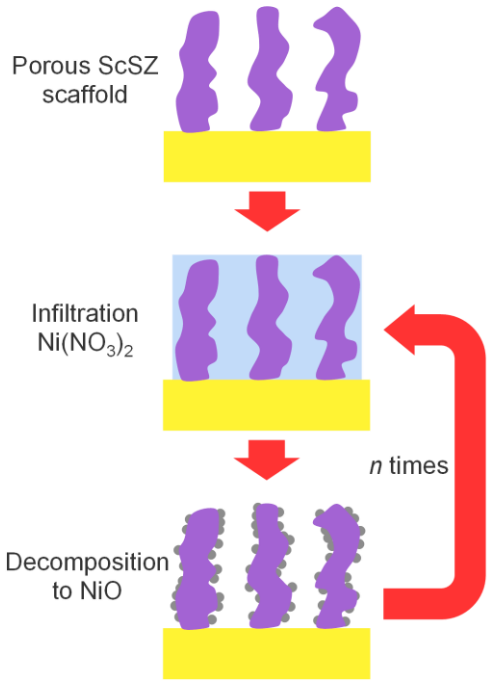
Structure electrode modelling

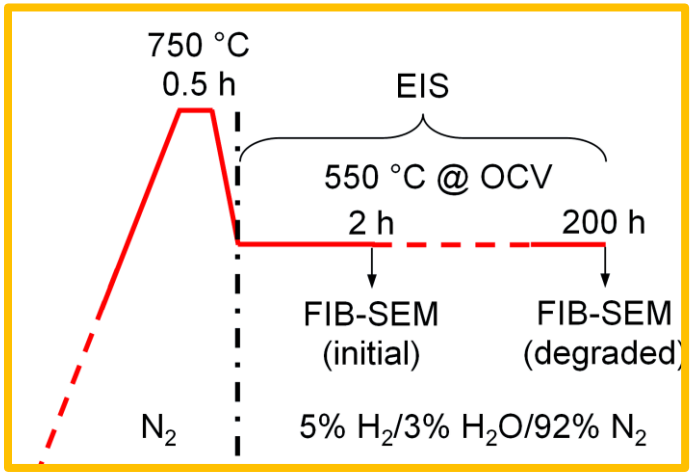


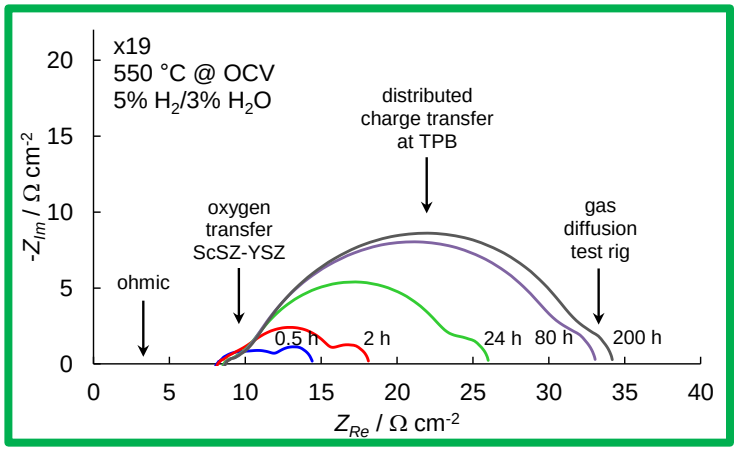
- Hierarchical electrodes fabricated by Ann Huang
- Nano-scale porosity/nanotube model - homogenised using TauFactor
- 2D model built by Antonio Bertei
  - N-P + Diffusion + B-V



Solid Oxide Fuel Cells – Microstructural degradation in NiScSZ

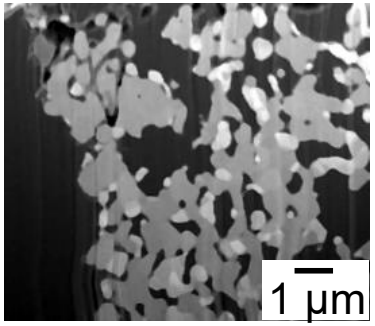




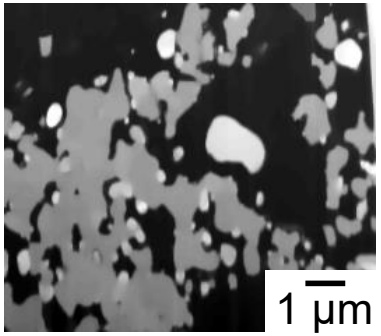


FIB-SEM

Initial anode

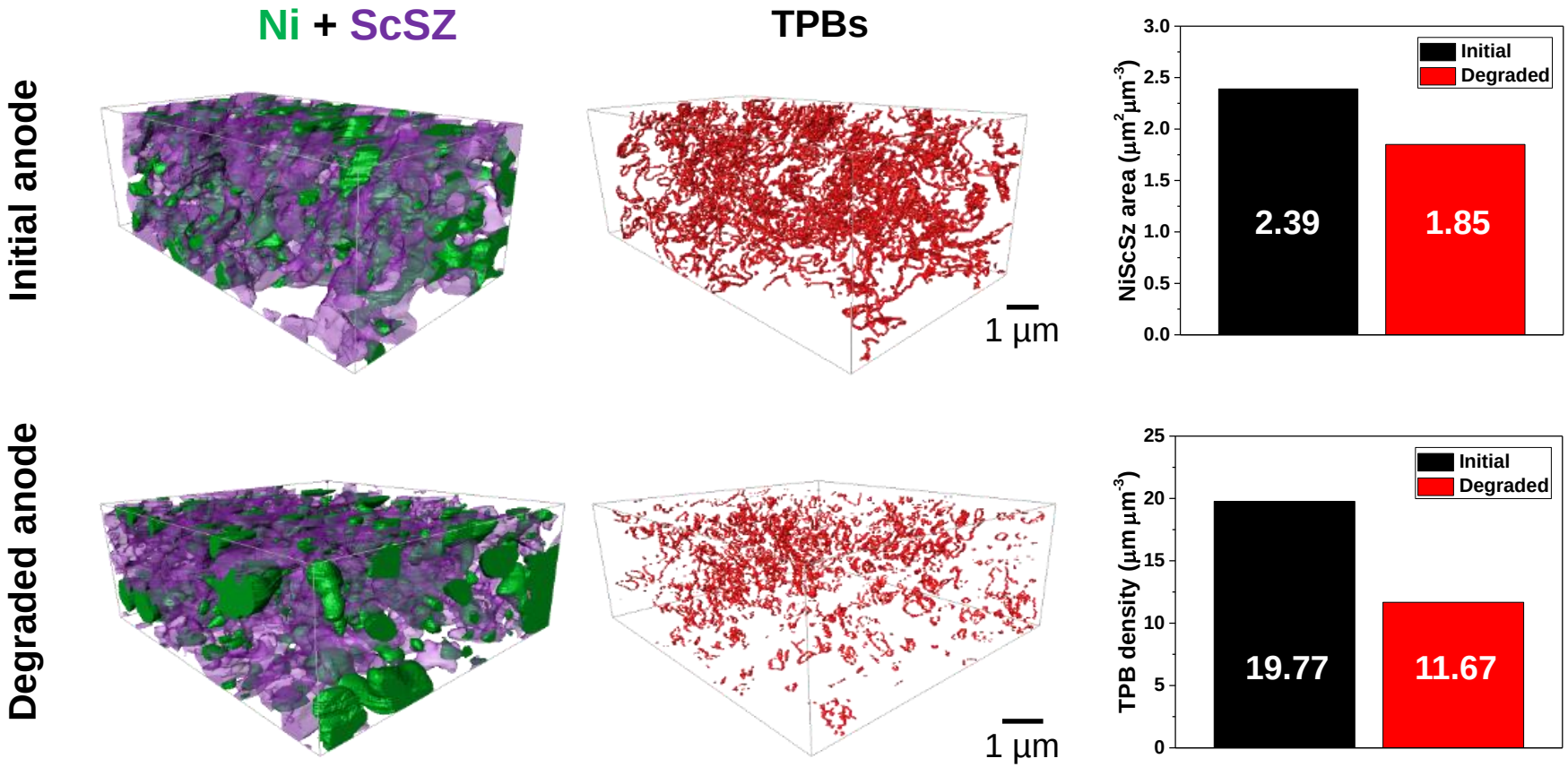


Degraded anode



A.Bertei, E.Ruiz-Trejo, K.Kareh, V.Yufit, X.Wang, F.Tariq, N.P.Brandon, *Nano Energy* **2017**, *36*, 526-536

Solid Oxide Fuel Cells – Microstructural degradation in NiScSZ



A.Bertei, E.Ruiz-Trejo, K.Kareh, V.Yufit, X.Wang, F.Tariq, N.P.Brandon, *Nano Energy* **2017**, *36*, 526-536

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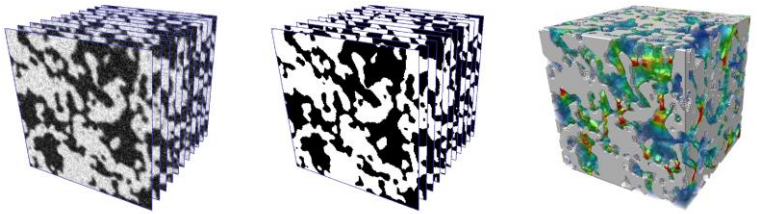
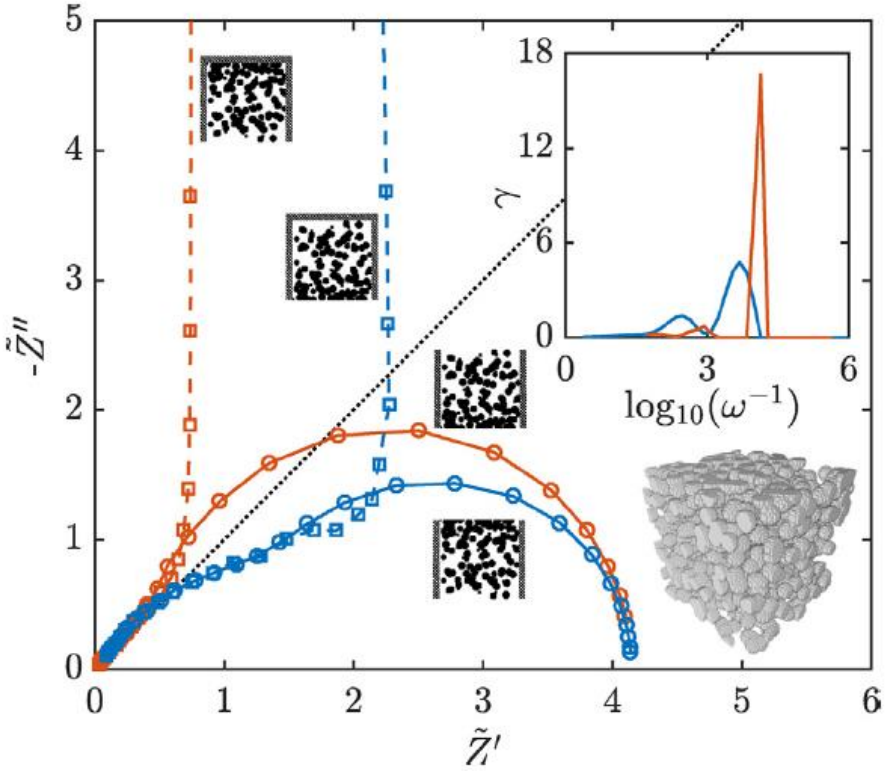
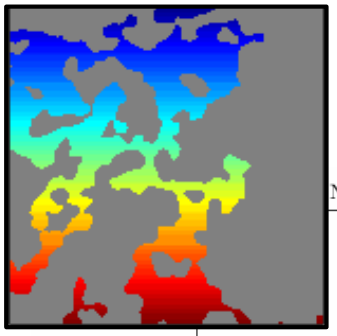
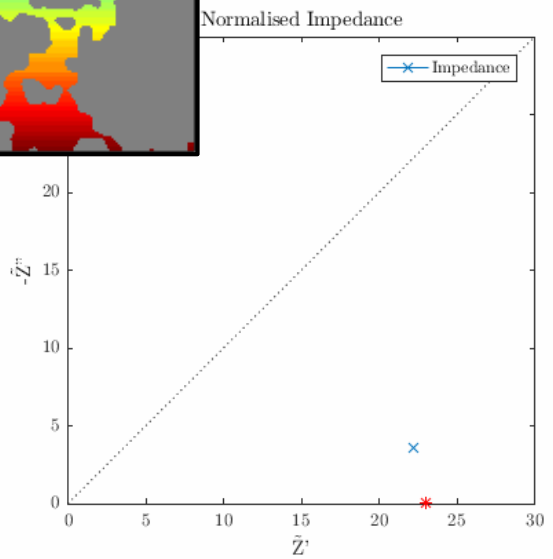
Simulated impedance









S. J. Cooper, A. Bertei, D. P. Finegan, and N. P. Brandon, "Simulated impedance of diffusion in porous media," *Electrochim. Acta*, vol. 251, pp. 681–689, 2017.

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Thank you