Innovative Energy Materials: Enabling High-performance Reversible Solid Oxide Cells for a Net Zero Economy

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BACKGROUND ON REVERSIBLE SOLID OXIDE CELLS

The advantages of reversible solid oxide cells (RSOCs) over solid oxide electrolytic and solid oxide fuel cells include the possibility of on-demand production of green hydrogen and electricity in electrolysis and fuel cell mode.[1]

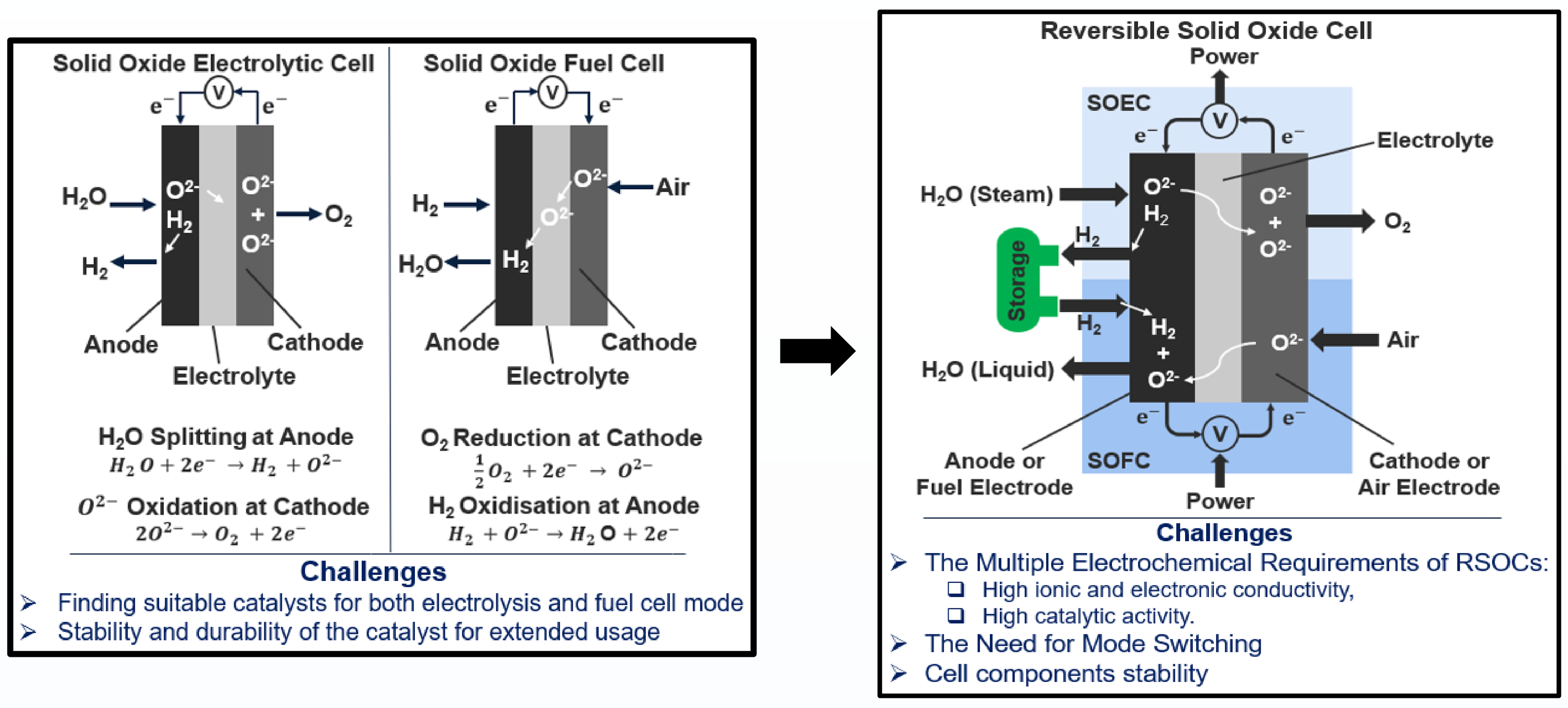


Figure 1: Challenges and materials requirements in RSOCs development

However, further development of RSOCs for commercialisation requires materials that can work efficiently as fuel cells and electrolytic cell electrodes.[2] Therefore, developing novel perovskite materials to enhance the performance of RSOCs and ensure their commercialization is beneficial to our global energy system.

OBJECTIVE OF THE RESEARCH

Exsolution entails the segregation of metallic cations to form highly active and anchored nanoparticles on the surface of a perovskite lattice – enhancing stability and other electrochemical requirements of RSOCs.[3,4] Forming such nanoparticles within the bulk of the perovskite lattice (bulk exsolution) has recently improved ionic conductivity.[3]

This research aims to develop a novel perovskite material capable of surface and bulk exsolution processes to fulfil the multiple electrochemical requirements of RSOCs.

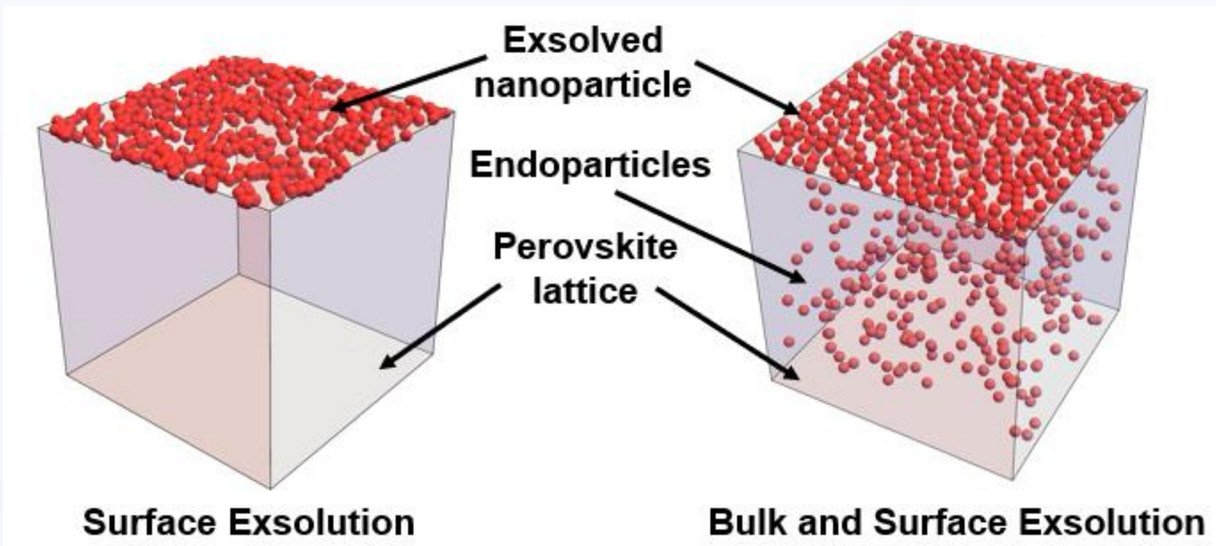


Figure 2: Schematics of surface and bulk exsolution in perovskites

A-site deficient perovskites with $(Sr,Ca)_{1-\alpha}(Ti,Fe,Ni)O_3$ stoichiometric composition that can drive B-site exsolution while attempting to revert to a stable ABO_3 perovskite stoichiometry is targeted in this research.[3]

MATERIALS AND METHOD

- **Potential precursors materials selection:** $Fe(NO_3)_3.9H_2O$, $Ni(NO_3)2.6H_2O$, $CaCO_3$, $SrCO_3$, TiO_2.
- **A preliminary study to examine parameters related to the novel perovskite synthesis:** thermal stability, decomposition temperature, decomposition products, composition, morphology and structural details of the precursor materials.
- **Detailed characterisation of the potential precursors:** thermogravimetric analysis (TGA), scanning electron microscopy (SEM) and X-ray Diffraction Analysis (XRD).
- **Selection of synthesis route:** a modified solid-state synthesis method

RESULTS

- **Important findings from the preliminary studies**

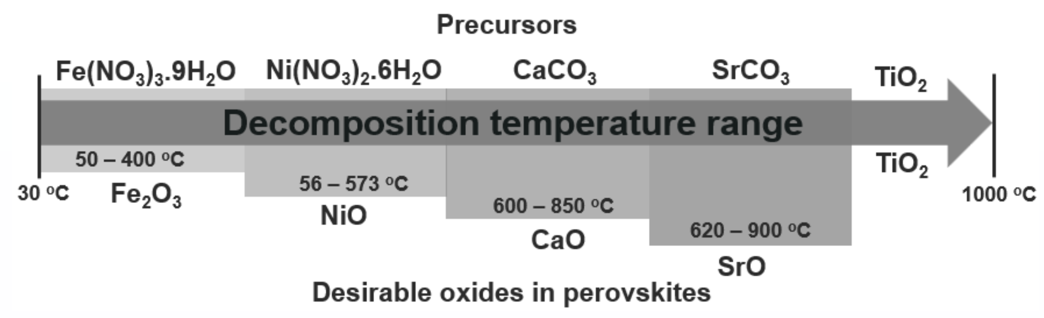
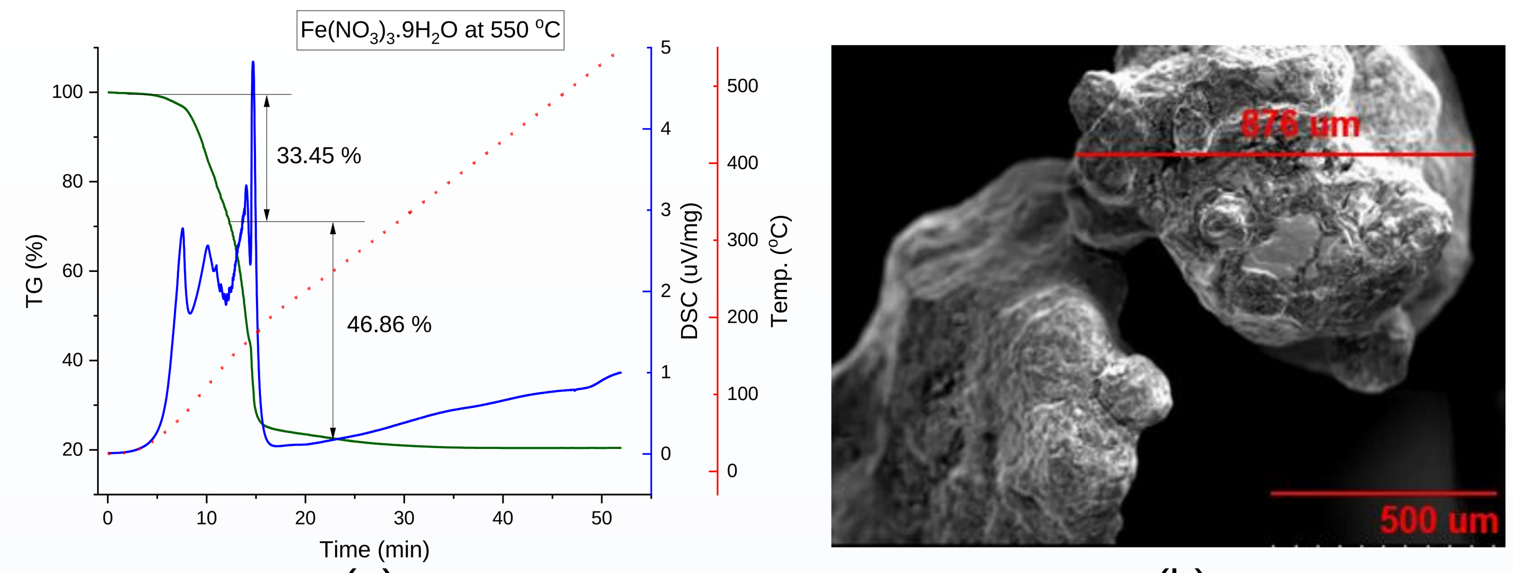


Figure 3: Key findings from TGA of the precursor materials, predicting 1000 °C as the calcination temperature for the novel perovskite



(a) (b)

Figure 4: A combined TG curve, DSC curve, and temperature response for (a) $Fe(NO_3)_3.9H_2O$ and (b) SEM image of $Fe(NO_3)_3.9H_2O$

- **Synthesis method adopted**

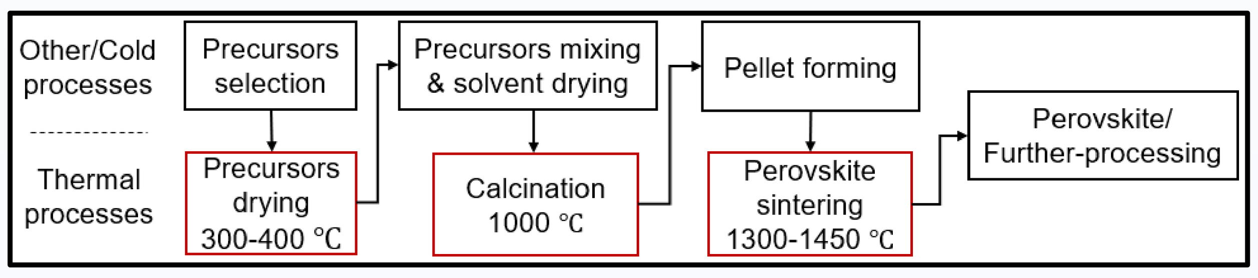
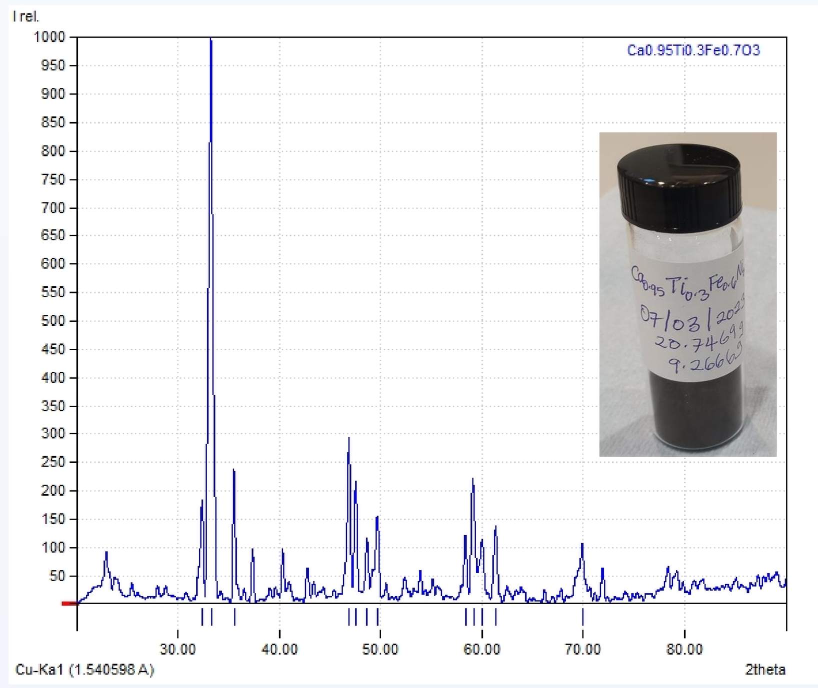


Figure 5: A simplified form of the modified solid-state synthesis method adopted based on the precursor TGA results.[5]

- **Perovskites synthesis:** two perovskite compositions have been synthesised

(a)



(b)

Figure 6: (a) $Sr_{0.95}Ti_{0.3}Fe_{0.6}N_{0.1}O_3$, and (b) XRD peaks of $Ca_{0.95}Ti_{0.3}Fe_{0.7}O_3$, synthesized

CONCLUSION AND FUTURE WORK

- The suitability of the precursor materials for the novel perovskite synthesis has been confirmed from their decomposition products.
- The perovskite synthesis process can be monitored through the precursor materials' decomposition time and temperature ranges.
- The modified solid-state synthesis method is expected to be useful for the synthesis of the novel perovskite with the desired stoichiometry.

FUTURE WORK

- Synthesis of other perovskite stoichiometric compositions;
- Detailed characterisation of synthesized perovskite materials;
- Exsolution analysis on sintered button cells;
- Modelling of the exsolution process for performance optimisation.

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ACKNOWLEDGEMENT AND CONTACT

Research Funder

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