

FAISAL, N., RAJENDRAN, V., PRATHURU, A. and HOSSAIN, M. 2023. Materials for molten salt facing parts: challenges and opportunities for nuclear thermochemical cycle electrolysis. Presented at the 5th International conference on structural nano composites 2023 (NANOSTRUC 2023), 24-26 May 2023, Nicosia, Cyprus: [virtual event].

Materials for molten salt facing parts: challenges and opportunities for nuclear thermochemical cycle electrolysis.

FAISAL, N., RAJENDRAN, V., PRATHURU, A. and HOSSAIN, M.

2023

5th International Conference on Structural Nano Composites

NANOSTRUC 2023

Novel Materials for Future

24-26 May 2023

Nicosia, Cyprus

<https://nanostruc.info/>

Materials for molten salt facing parts: challenges and opportunities for nuclear thermochemical cycle electrolysis

Nadimul Faisal, Vinooth Rajendran, Anil Prathuru, Mamdud Hossain

School of Engineering, Robert Gordon University, Aberdeen, UK

One of the important challenges is to develop coating materials for thermochemical containment vessels and pipes that encounters the highly corrosive and harsh environment produced by the molten salt at high temperature. The aim of this review is to summarise structural and coating materials (mainly thermally sprayed) that can withstand thermochemical cycle corrosive environment. This review presents findings published in the scientific literature related to high temperature aggressive corrosion of materials, specifically geared towards nuclear thermochemical cycles leading to hydrogen production. Data related to materials, composition, synthesis have been gathered. Corrosion environment data such as environment, test time, test results have been reviewed. Structure-property relations of different materials reviewed as a part of this exercise will aid in the material selection process for future development. The overall assessment based on the evidence from previous investigations in this area is that none of the high-performance structural materials (coating, substrates) are likely to survive for an extended period in the high temperature corrosive environment. However, there are means and methods which could be considered to have sustainable coating-substrate assembly and extended lifetime. This review presents challenge and assess opportunities that will warrant efficient hydrogen production with stable thermochemical structure for operation at molten salt reactor (MSR) nuclear plants (e.g., thermochemical electrolysis leading to water splitting and hydrogen production) as well as other power plants, boilers, and waste incinerators.

NANOSTRUC

5th International Conference on Structural Nano Composites
NANOSTRUC 2023
Novel Materials for Future
24-26 May 2023
Nicosia, Cyprus
(ONLINE)

Materials for molten salt facing parts: challenges and opportunities for nuclear thermochemical cycle electrolysis

Nadimul Faisal, Vinooth Rajendran, Anil Prathuru, Mamdud Hossain

School of Engineering, Robert Gordon University, Aberdeen, UK

N.H.Faisal@rgu.ac.uk

@nh_faisal



Acknowledgements



H E N R Y . . .
R O Y C E . . .
I N S T I T U T E

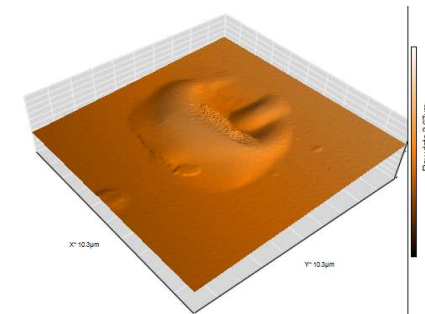
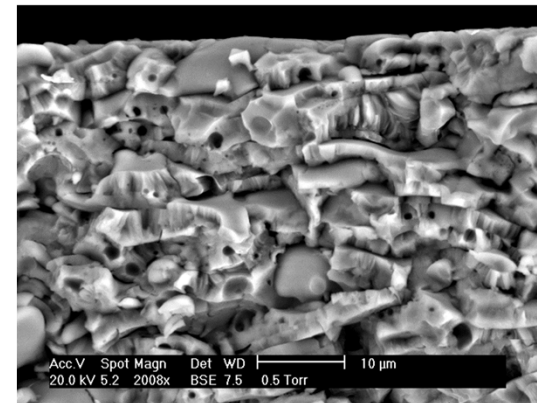
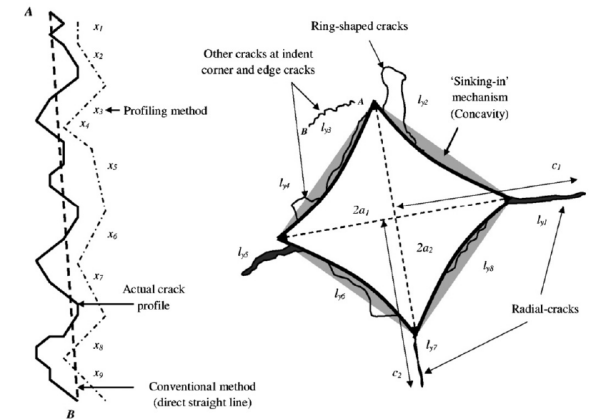
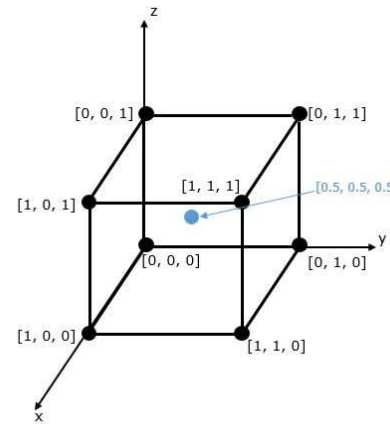
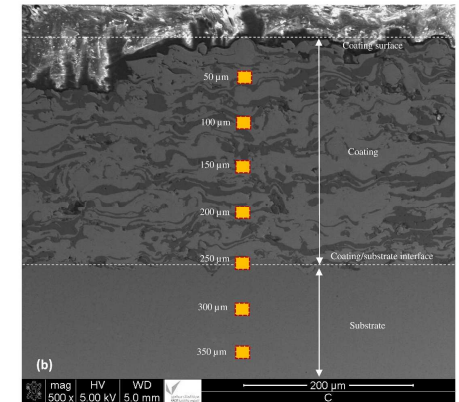
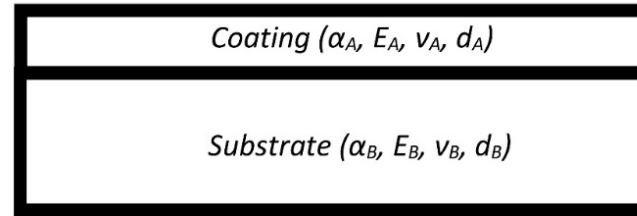
Acknowledgements

(partners, sponsors, collaborators, colleagues) – thermal spray coatings

- International Advanced Research Centre for Powder Metallurgy and New Materials - ARCI (Surface Engineering Division; Prof Shrikant Joshi@Univ West, Mr D S Rao, Mr K R C Soma Raju, Dr G Sivakumar, Mr D Sen)
- Heriot-Watt University (Dr Rehan Ahmed, Prof Bob Reuben, Prof John Steel)
- Monitor Coatings Ltd (Dr Bryan Allcock)
- Science and Technology Facilities Council (Neutron beamtime; Dr Anna Paradowska@ANSTO, Dr Shu Yan Zhang, Dr Tung Lik Lee, Dr Joe Kelleher, Dr Saurabh Kabra)
- Alfaisal University (Dr Mattheus Goosen)
- Saudi Aramco (Wear resistant coatings, SOFC coatings)
- The Carnegie Trust for the Universities of Scotland (MD simulation)
- Robert Gordon University (Dr Anil Prathuru, Dr Nazmi Sellami, Dr Firdaus Muhammad-Sukki, Dr Sheikh Islam, Prof John Steel, Dr Andrei Petrovski, Jordan Davidson, Alexander Muir, Chris Pegg, Adam White, Chloe Pearson)
- London South Bank University & Cranfield University (Dr Saurav Goel, Prof Hari Upadhayaya)
- University of Nottingham (Dr Tanvir Hussain, Dr Federico Venturi, Mr Tunji Owoseni)

Interest & Motivation

- Developing new applications using thermal spray coatings
- Sensor-based analysis: micromechanical degradation of materials (coatings, thin films, structural materials)
- Corrosion monitoring (electrochemical, acoustic emission)
- Hydrogen as new energy vector



Substrate shape & size during thermal spraying

Google Search: Ball valve thermal spray coatings



Valve Coating: Gas-Tight Tungsten ...
kemetico.com



HVOF coating | Thermal spray | Surfac...
surfacetechology.co.uk



Valve Coating: Gas-Tight Tungsten ...
kemetico.com



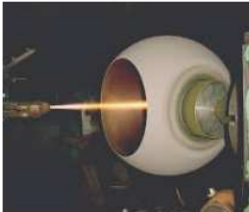
HIGH VELOCITY SPRAY HVOF (High Ve...
coating-ball.com



Introduction to Thermal Spray and ...
metallisation.com



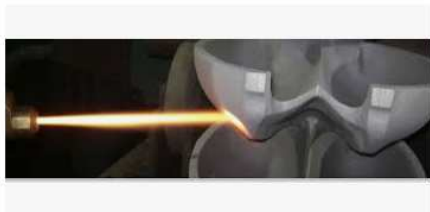
Valve Coating: Gas-Tight Tungsten ...
kemetico.com



Thermal spray coatings to protect b...
ee.co.za



Oil & Gas Thermal Metal Spraying ...
alphatek.co.uk



hvoF coatings for metal seated gate ...
spraymet.com



Tungsten carbide coating pro...
kemetico.com



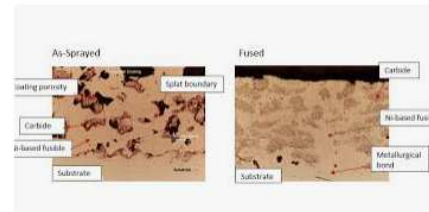
Spraying sand tooling turntable-LJIJ...
ljipt.com



Ball Seated Ball Valves for Severe S...
copelandvalve.com



HVOF Thermal Spraying for Va...
youtube.com



The Use of Thermal Spray Coatings for ...
empoweringvalves.com



Introduction to Thermal Spray and ...
metallisation.com



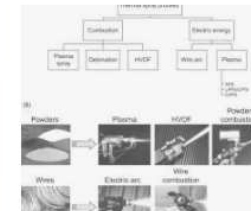
Spraymet thermal spray and cladding ppt ...
slideshare.net



Understanding Metal-Seated Ball Valve ...
thermalspray.com



Meccanica Gervasoni - Offshore ...
offshore-technology.com



Thermal Spray Coatings - Science...
sciencedirect.com



Is a Metal-seated Ball Valve f...
pinterest.com



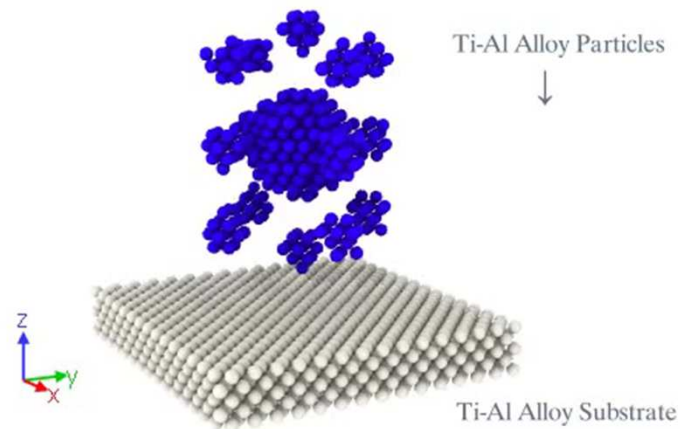
Hardfacing
metalspiping.com


Thermal spray feedstock materials

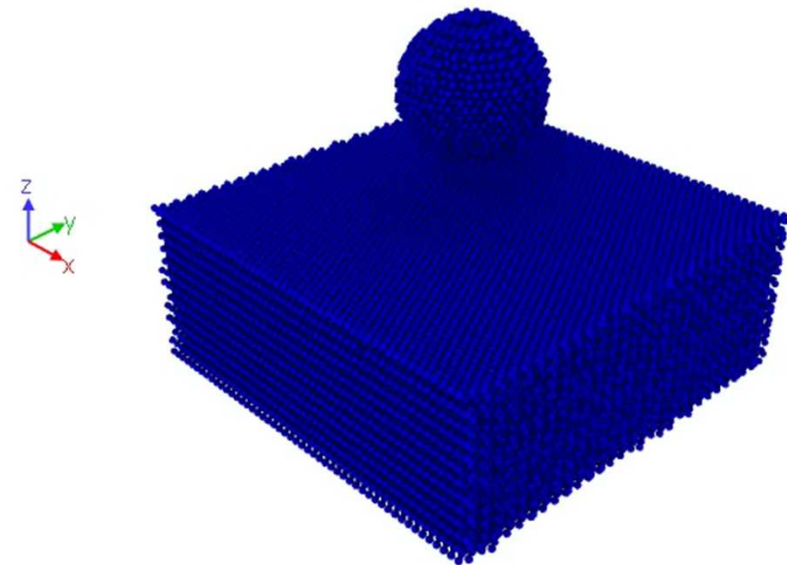
Particle Stream (Gas Dynamic Cold Spray: $v = 1000$ m/s, $T = 500$ K)

Ti Alloy Particle "Cluster" Model

Ti-Al Interatomic Potential from R.R. Zope and Y. Mishin, "Interatomic potentials for atomistic simulations of the Ti-Al system," Phys. Rev. B 68, 024102 (2003). DOI: 10.1103/PhysRevB.68.024102



Particle Atomic Shear Strain (von Mises)
0  1



von Mises Atomic Shear Strain
0  1

Group 1

H

Hydrogen

1

1.008

Hydrogen

Scottish Government plans

5 GW of low carbon hydrogen production in Scotland by 2030 –

Scottish Government Hydrogen Policy, 2020

- **Forecasted demand** for low carbon hydrogen is in the range of **250-460TWh by 2050** (re. UK Hydrogen Strategy)
- UK has announced an aim of **24 GW capacity of new nuclear by 2050** (re. Powering up Britain The net zero growth plan).

About H₂ (some numbers)

- H₂ is a colourless, odourless, tasteless and non-toxic gas.
- H₂ disperses **3.8 times** as fast as natural gas.
- H₂ has highest energy per mass of any comparable fuel with **143 MJ/kg** (~3 times greater than that of liquid hydrocarbon fuels).
- 1 kg of H₂ has the same energy content as 1 gallon (3.2 kg) of gasoline.
- Higher heating value of H₂ = 3.54 kWh/Nm³ = **39.41 kWh/kg**
- H₂ gas costs around £10/kg in the UK

Re. Rodl, Wulf and Kaltschmitt, Hydrogen Supply Chains, 2018, 81-109
<https://www.drivingelectric.com/electric/1363/where-can-i-buy-hydrogen-and-where-is-my-nearest-hydrogen-filling-station>

<https://www.gov.uk/government/news/uk-government-launches-plan-for-a-world-leading-hydrogen-economy>

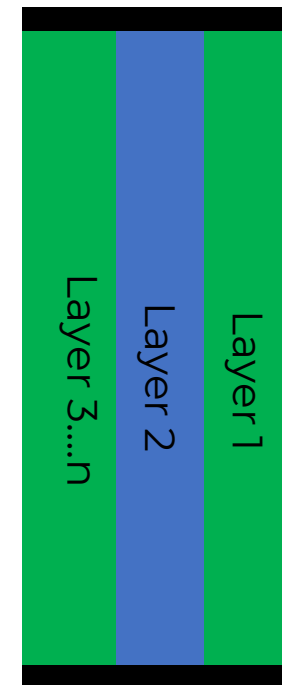
Faraday's laws of electrolysis

(English scientist Michael Faraday in 1833)

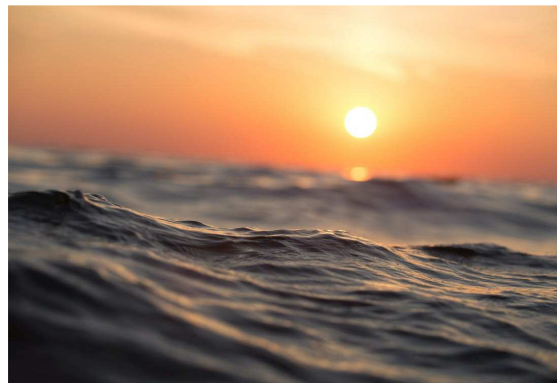
- Faraday's laws of electrolysis – **chemical change/current at electrode-electrolyte/electricity/equivalent weight**
- **Splitting a mole of liquid water** to produce a mole of hydrogen at 25°C requires **285.8 kJ** of energy (237.2 kJ as electricity + 48.6 kJ as heat)
- Faraday constant = 96,485 C/mole
- $z = 2$ (**electrons needed to create a molecule of H₂**)
- Electrochemical potential = **1.481 V is required for splitting liquid water**
- Voltage efficiency = Thermal neutral voltage (E)/Cell operating voltage (V)

$$E_o = \frac{\Delta_f H^\circ}{zF} = \frac{285,840 \frac{\text{J}}{\text{mol}}}{2 * 96,485 \frac{\text{C}}{\text{mol}}} = 1.481 \frac{\text{Volts}}{\text{cell}}$$

Membrane Electrode Assembly (functional layers)



Materials + Feedstock



Sources of high temperature heat energy

- Non-fossil fuel sources of heat (**concentrating solar, nuclear, geothermal, waste heat**) can be used in conjunction with non-fossil fuel sources of electricity (such as **solar, wind, ocean, nuclear**).
- Possible supplies of cheap high-temperature heat for high temperature electrolysis (HTE) are all nonchemical, including **nuclear reactors, concentrating solar thermal collectors, and geothermal sources**.

Note: heat is cheaper than electricity but difficult to hold

Sites of existing and proposed nuclear power stations in the UK



Source: DECC

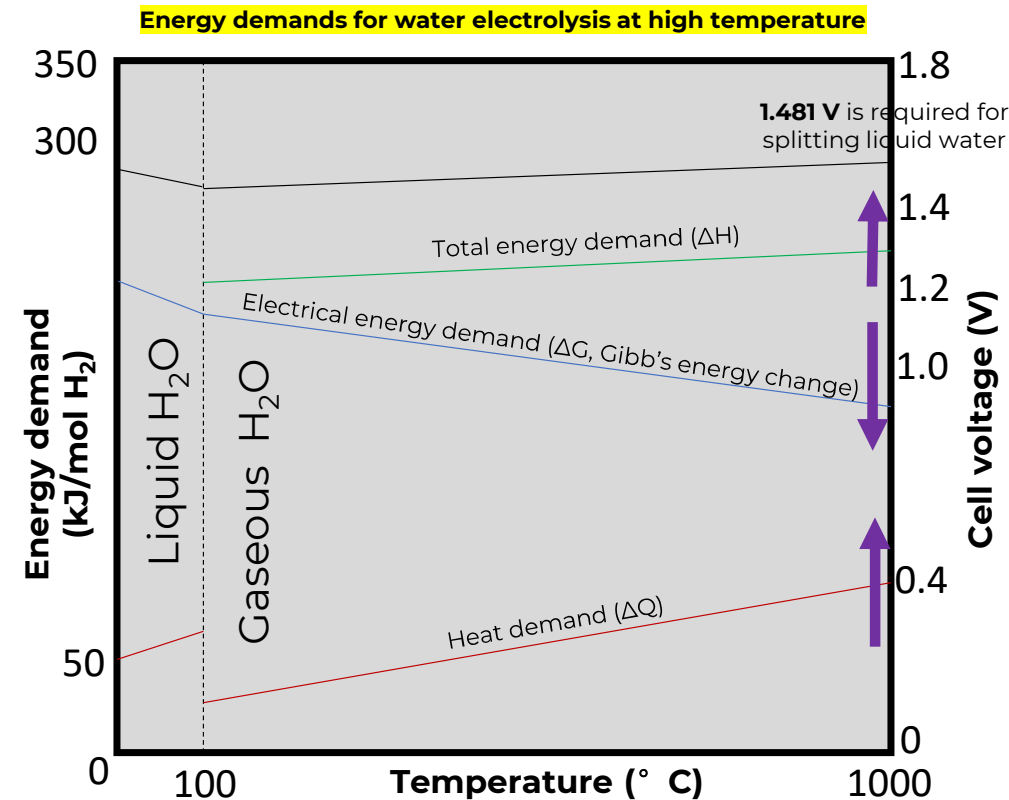
Nuclear reactor power plants usually have a generation end efficiency of 33–35% and about **60% of waste heat**

(Obara & Tanaka, Applied Energy, 292, 2021, 116667)

Why high temperature?

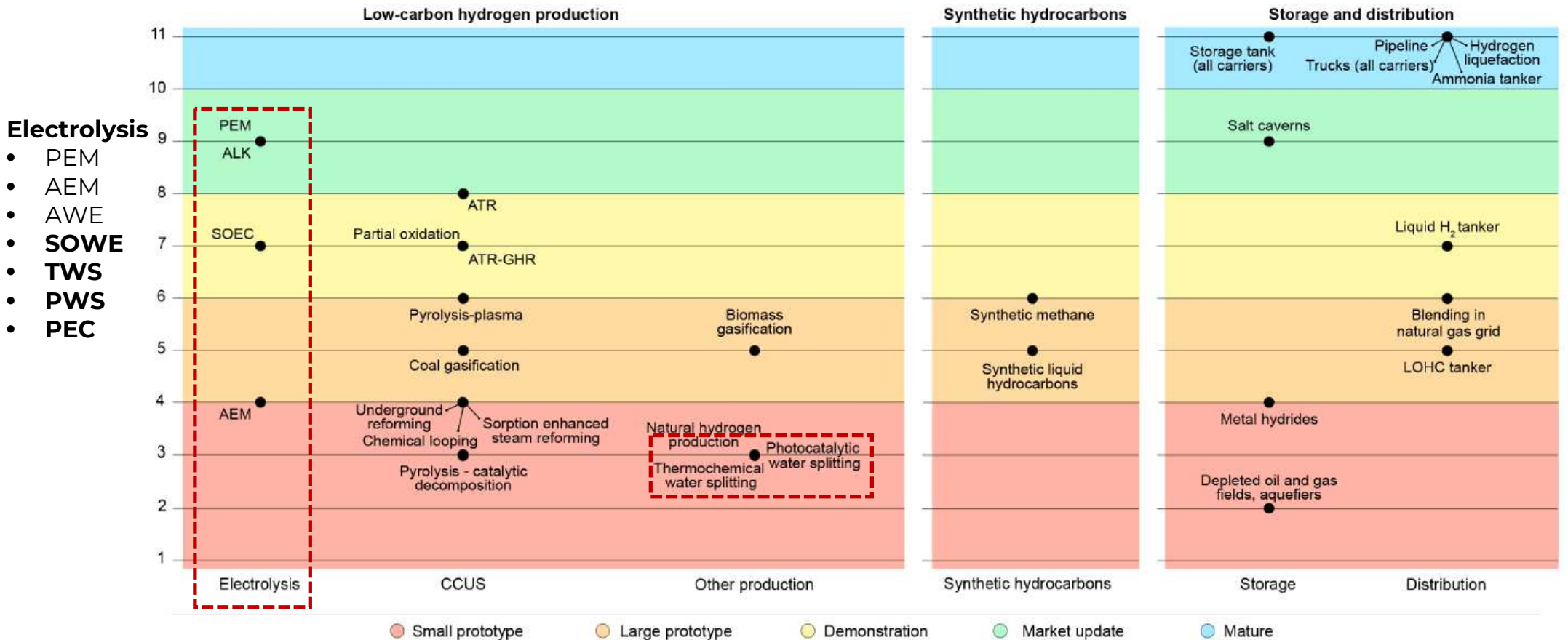
Temperature, energy demand, cell voltage

- The increase in **temperature can eliminate the need for expensive catalysts**, which may be required for some low temperature water electrolyzers.
- High temperature systems operate **between 100 °C and 850 °C**.
- Above 850 °C, the capacity of standard **chromium steels to resist corrosion decreases**.
- At 2500 °C, electrical input is unnecessary because **water breaks down** to hydrogen and oxygen through thermolysis.
- With the increase in temperature (0–1000 ° C), the overall energy demand (ΔH) varies slightly (i.e., between 283.5 and 291.6 kJ/mol H₂).
- The **heat share (ΔQ) rises with temperature, reducing the minimum electrical energy demand (ΔG)**.
- Beside **improved kinetics**, the high heat utilisation of internal losses is a major motivation of high-temperature electrolysis (e.g., 700–900 ° C).



Plot schematically adapted
(from Buttler and Spliethoff, 2018)

Technology readiness levels of key hydrogen production, storage and distribution technologies



IEA. All rights reserved.

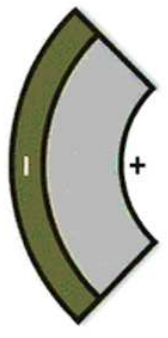
Notes: AEM = anion exchange membrane. ALK = alkaline. ATR = autothermal reformer. CCUS = carbon capture, utilisation and storage. GHR = gas-heated reformer. LOHC = liquid organic hydrogen carrier. PEM = polymer electrolyte membrane. SOEC = solid oxide electrolyser cell. Biomass refers to both biomass and waste. For technologies in the CCUS category, the technology readiness level (TRL) refers to the overall concept of coupling these technologies with CCUS. TRL classification based on [Clean Energy Innovation \(2020\)](#), p. 67.

Source: IEA (2020), [ETP Clean Energy Technology Guide](#).

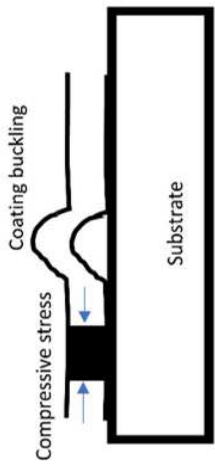
Multimode material degradation
(Corrosion, erosion, radioactive contamination, retention, loads, ageing)



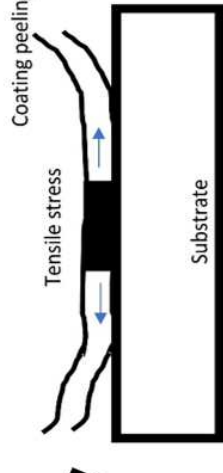
Thermo-mechanical deformation



High residual compressive stress in coating

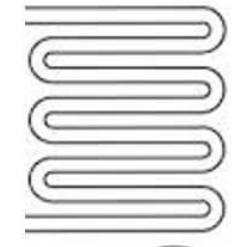


High residual tensile stress in coating



Molten salt, water/steam channel (structural parts)

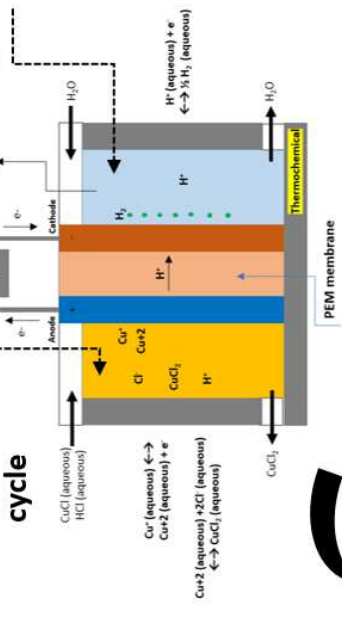
Structural parts: vessels, sheet, plate, strip, billet, rod, bar, heat exchangers, pipes, pumps, flanges, bellows, seals, valves, thermal shields, radiator, tank, fans, and fittings, etc.



Molten salt nuclear power plant

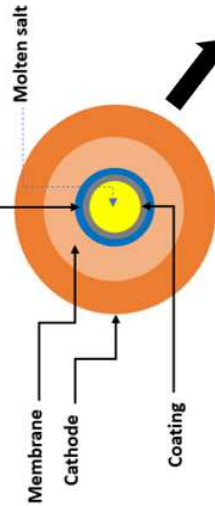


Thermochemical cycle



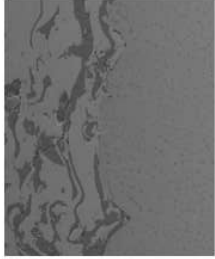
Molten salt

High temperature, abrasion, erosion, corrosion, contamination, retention, mechanical loads, ageing etc.



Flow channel (e.g. tubular)

Interaction of molten salt with flow channel or structural part



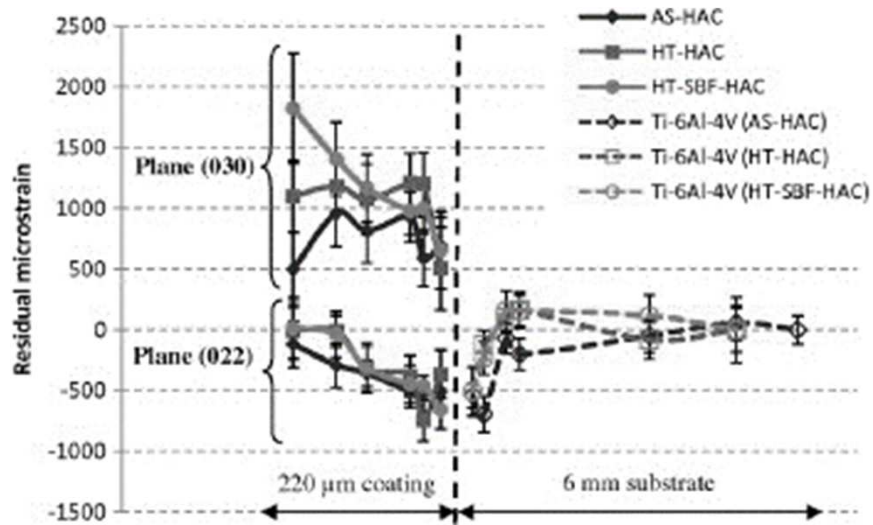
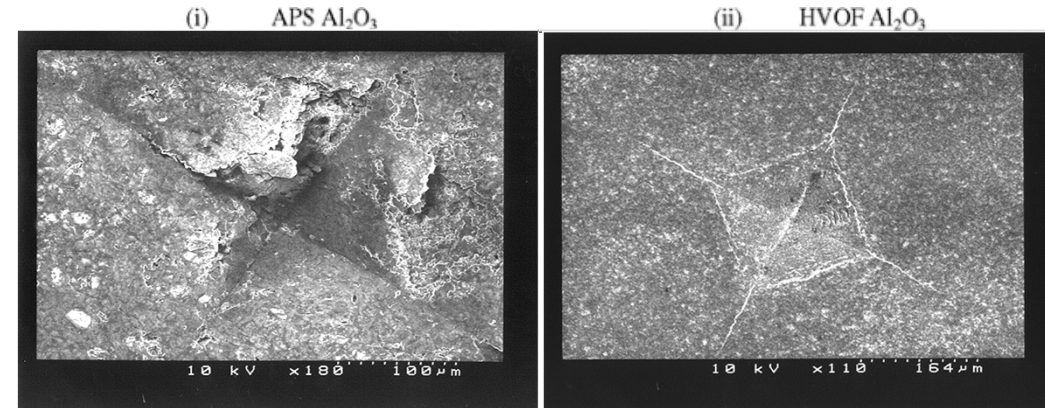
Coating ($\alpha_A, E_A, \nu_A, d_A$)

Substrate ($\alpha_B, E_B, \nu_B, d_B$)

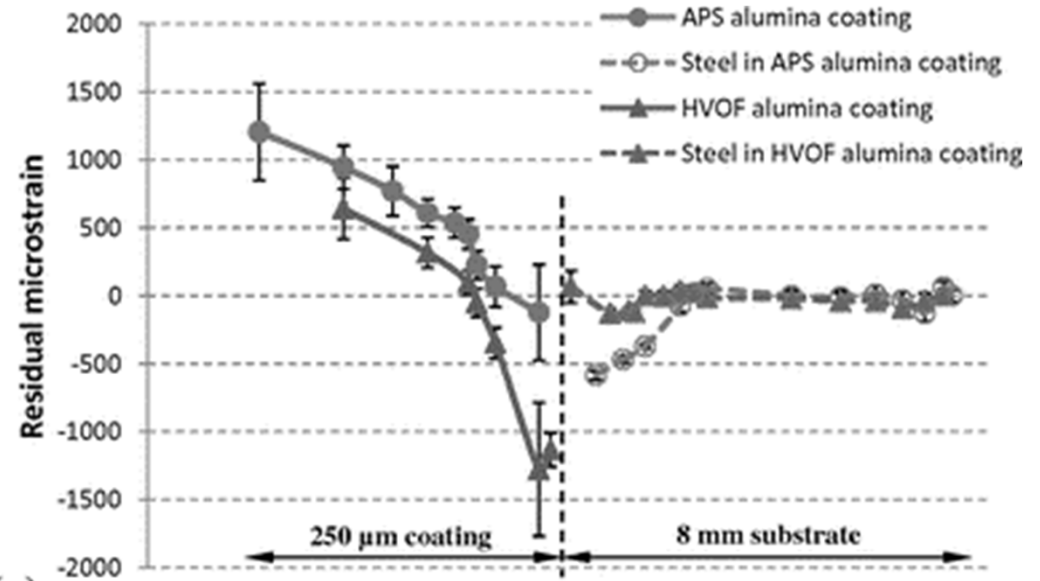
Coating-substrate system

Examples

Al₂O₃

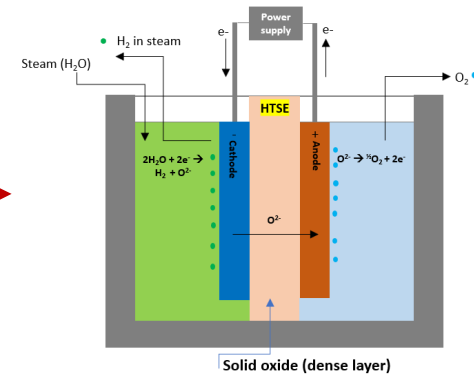
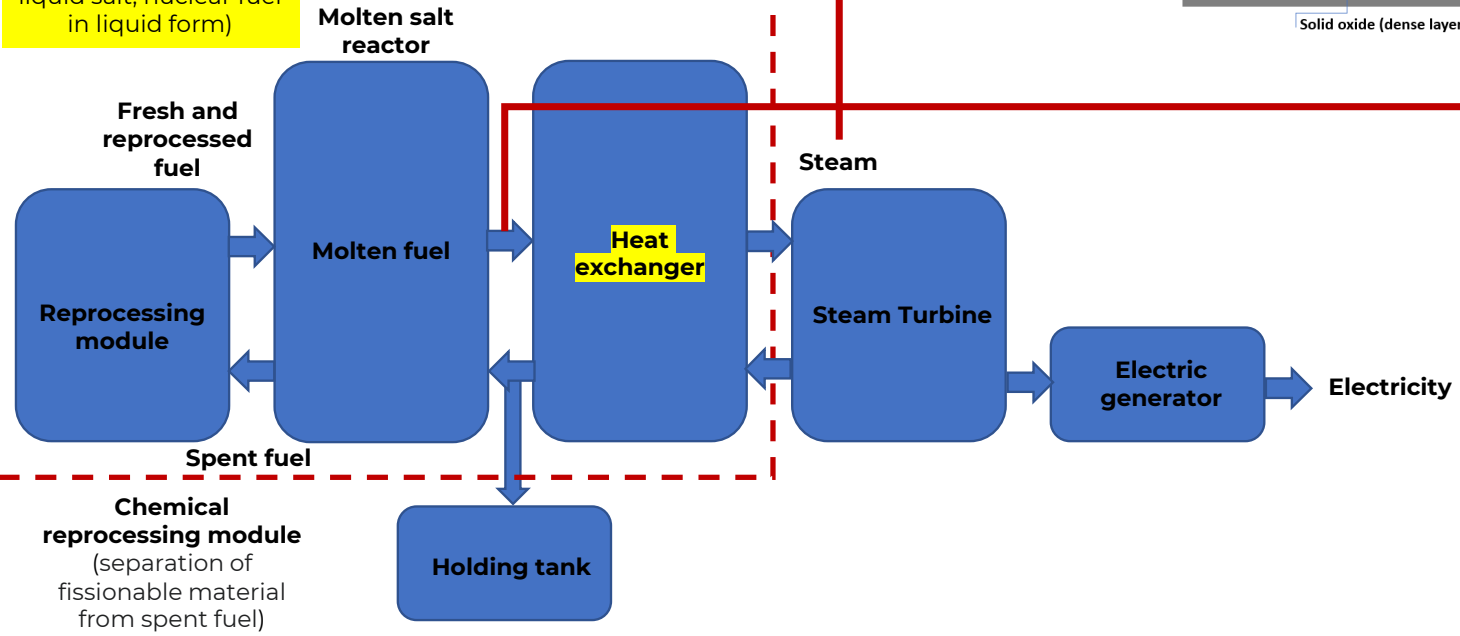


- Residual stress around Vickers indentations is a non-equal biaxial field.
- Both tensile and compressive stresses exist around a sharp indentation and decrease as the distance from the centre of indentation increases.



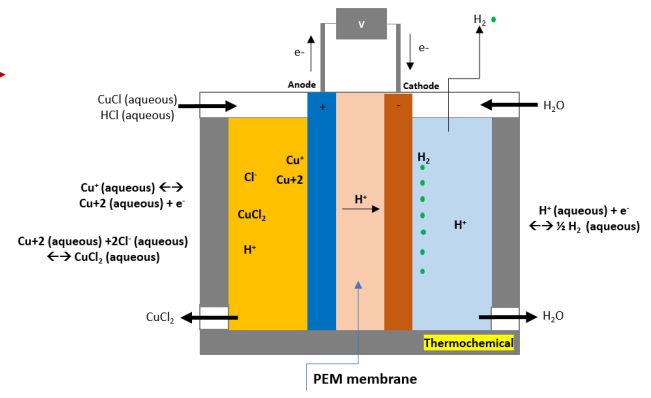
Molten salt reactor

Molten salt nuclear power plant (based on molten salt, fissile material dissolved in liquid salt, nuclear fuel in liquid form)



High temperature steam electrolysis (HTSE)

Thermochemical water splitting (TWS)



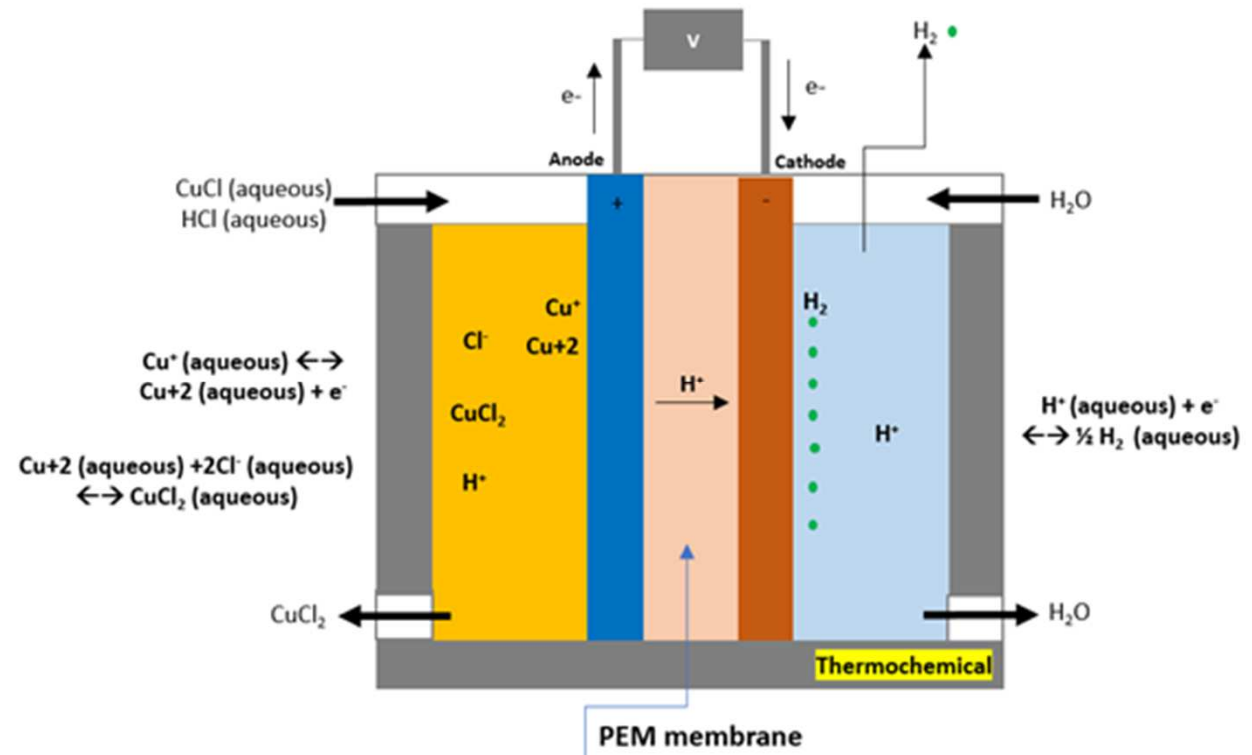
$2\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + \text{O}_2$
 $\text{O}^{2-} \rightarrow \frac{1}{2}\text{O}_2 + 2\text{e}^-$
 $\text{Cu}^+ (\text{aqueous}) \leftrightarrow \text{Cu}^{+2} (\text{aqueous}) + \text{e}^-$
 $\text{H}^+ (\text{aqueous}) + \text{e}^- \leftrightarrow \frac{1}{2} \text{H}_2 (\text{aqueous})$
 $\text{Cu}^{+2} (\text{aqueous}) + 2\text{Cl}^- (\text{aqueous}) \leftrightarrow \text{CuCl}_2 (\text{aqueous})$

Challenges

- Thermochemical cycles typically involve extreme corrosive environment which impacts the lifetime of a hydrogen generation plant.
- As an example, the Cu-Cl cycle produces corrosive hydrochloric (HCl) acid as a by-product.
- Hydrochloric (HCl) acid presents materials challenges in developing corrosion-resistant materials.

Four-step thermochemical Cu-Cl cycle:

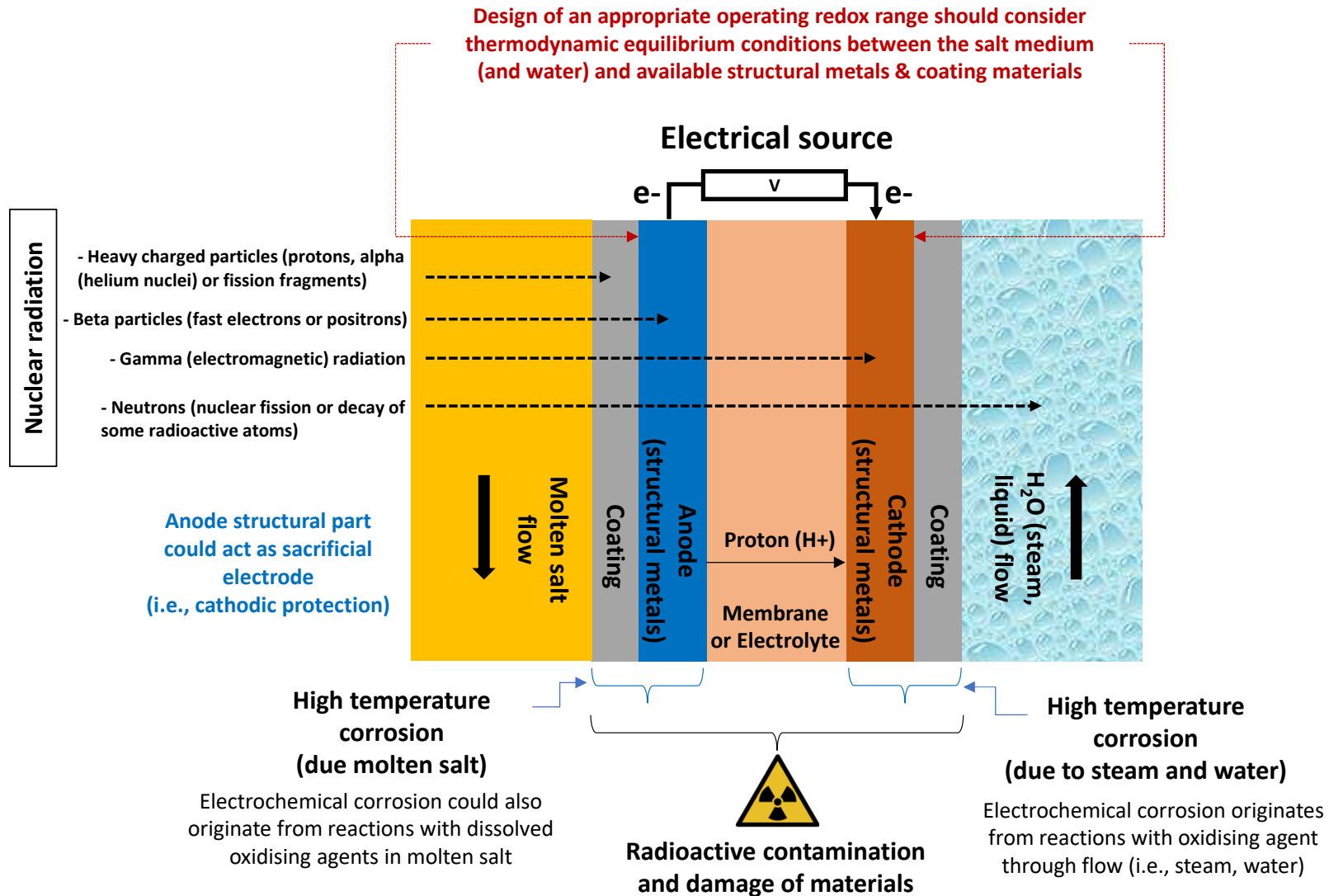
- $2 \text{Cu} + 2 \text{HCl}(\text{g}) \rightarrow 2 \text{CuCl}(\text{l}) + \text{H}_2(\text{g})$ (430-475 C)
- $2 \text{CuCl}_2 + \text{H}_2\text{O}(\text{g}) \rightarrow \text{Cu}_2\text{OCl}_2 + 2 \text{HCl}(\text{g})$ (400 C)
- $2 \text{Cu}_2\text{OCl}_2 \rightarrow 4 \text{CuCl} + \text{O}_2(\text{g})$ (500 C)
- $2 \text{CuCl} \rightarrow \text{CuCl}_2(\text{aq}) + \text{Cu}$ (ambient temperature electrolysis)



Examples of corrosive environment

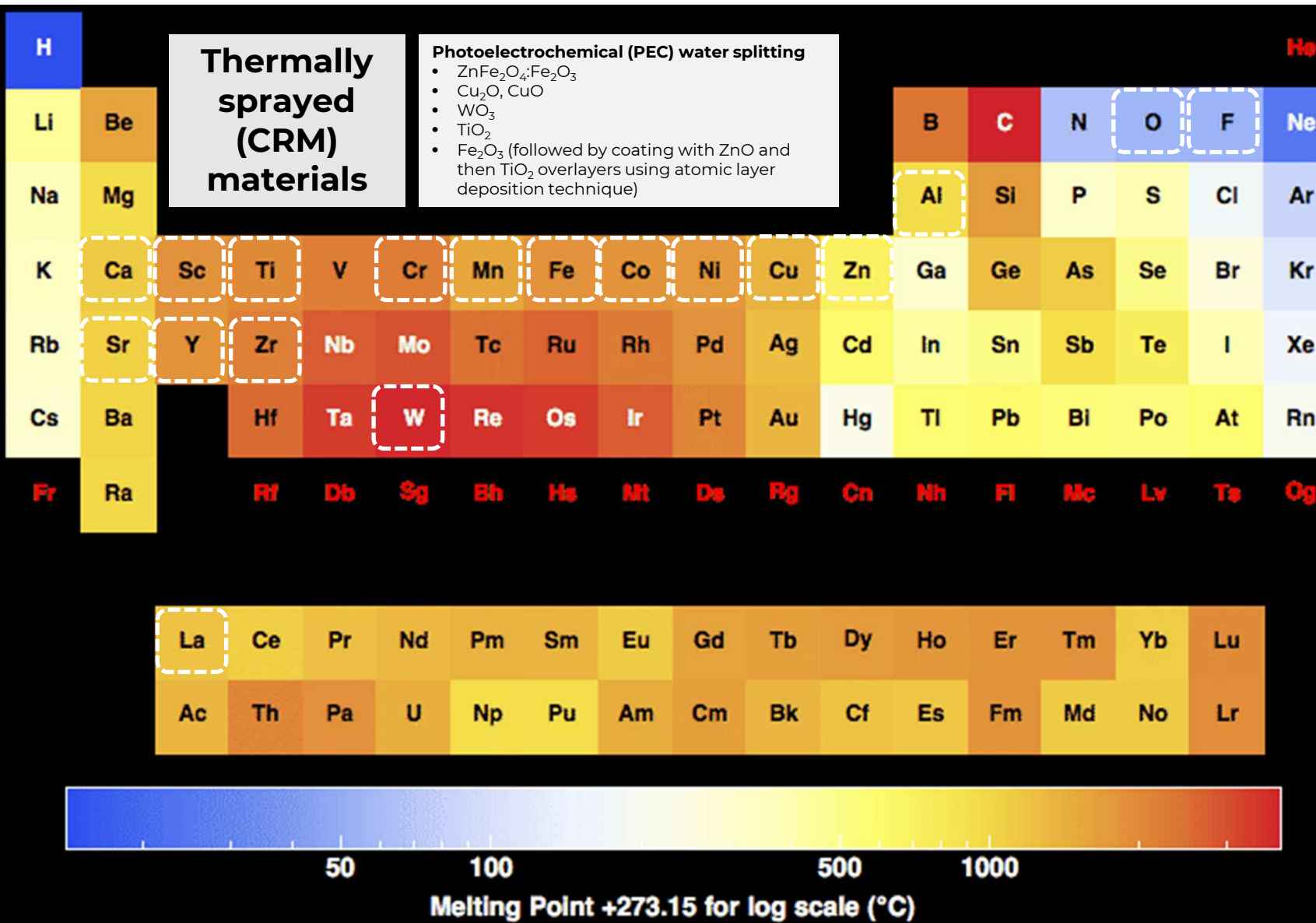
- Molten CuCl
- Molten salt (NaCl, Na₂SO₄, KCl) with gas synthetic air + 10% H₂O
- Molten salt (V₂O₅)
- Molten salt (LiCl-Li₂O)
- Molten LiCl-KCl
- 50wt % Na₂SO₄ and 50wt % V₂O₅ mixture on the substrate
- Calcia-magnesia-alumino-silicate (CMAS) (molten)
- Molten salt (Na₂SO₄ + V₂O₅)
- Water vapour
- Liquid sulfuric acid
- CuCl and HCl
- Molten salt (95% Na₂SO₄ + 5% NaCl)
- Molten salt (Na₂SO₄-82% Fe₂(SO₄)₃)
- Molten salt (Na₂SO₄-60% V₂O₅)

- Molten salt (45wt% Na₂SO₄ + 55wt % V₂O₅)
- Corrosive salts (50wt% Na₂SO₄+50wt%V₂O₅) coated on the substrate 5-7mg/cm²
- Molten salt (ZnCl₂-KCl)
- Coal (boiler environment)
- Modified geothermal fluid
- Air
- Synthetic salt (40 wt% K₂SO₄, 40 wt% Na₂SO₄, 10 wt% KCl and 10 wt% NaCl)
- Molten salt (Fluoride salt)
- Salt mixture (KCl-K₂SO₄)
- Molten salt (NaCl, Na₂SO₄, KCl) with gas synthetic air + 10% H₂O
- Molten salt (FLiNaK)
- Calcia-magnesia-alumino-silicate (CMAS) (molten)
- 75 wt% Na₂SO₄+25 wt% K₂SO₄

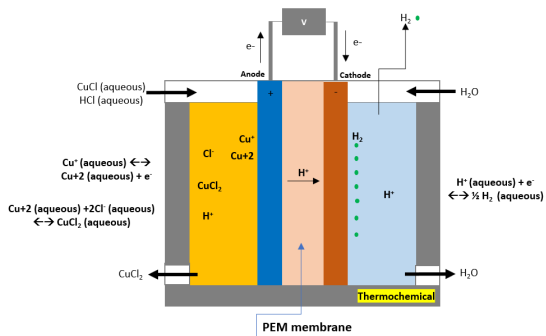


Variables for Data Analytics

- Feedstock materials
- Substrates
- Density
- Melting point
- Thermal expansion coefficient
- Thermal conductivity
- Electrical resistivity
- Proof stress
- Tensile strength
- Manufacturing process
- Corrosive environment (molten salt, geothermal, solar, oxidation)
- Salt
- Testing temperature
- Coating thickness
- Bond thickness
- Powder particle size
- **Corrosion rate**



OTHER MANUFACTURING METHODS AND MATERIALS USED IN HIGH TEMPERATURE ELECTROLYSERS

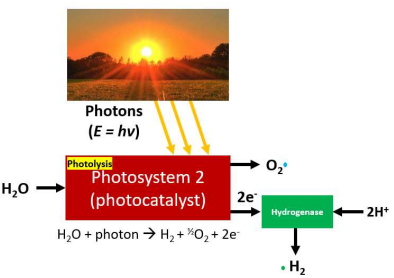


- Manufacturing methods**
- Spin coating method
 - Aerosol spray pyrolysis

- Ferrite
- Ferrite/zirconia

- Manufacturing methods**
- Photo deposition
 - Sol gel method
 - Atomic layer deposition
 - Spray pyrolysis
 - Flame spray pyrolysis
 - Aerosol assisted chemical vapour deposition (AACVD)
 - Wet impregnation method
 - Electrodeposition
 - Radio frequency magnetron sputtering
 - Ultrasonic spray pyrolysis
 - Atmospheric pressure chemical vapour deposition

- Rh/Cr₂O₃
- NiFe₂O₄
- NiFe₂O₄@TiO₂
- CoO_x/TiO₂/Pt
- TiO₂
- ZnO
- Au/TiO₂
- Pt/TiO₂
- NaTaO₃
- Nitrogen modified TiO₂
- CUO and WO₃ loaded on TiO₂ anatase
- CdS/TiO₂
- Cu₂O/TiO₂
- Ag/TiO₂
- NaTaO₃-C
- TiO₂-ZnO
- Ag₂O-TiO₂
- Yttrium and aluminium co-doped ZnO
- Bare TiO₂, Ag₂O-TiO₂, Bi₂O₃-TiO₂, ZnO-TiO₂
- RuO₄/NaTaO₃, RuO₂/La:NaTaO₃
- B-TiO₂
- Cu-TiO₂



Solid oxide water electrolysis (SOWE)

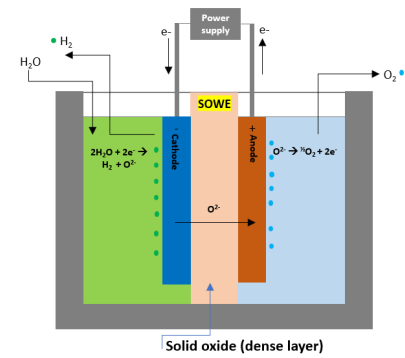
Thermochemical water splitting (TWS)

Photolysis water splitting (PWS)

Photoelectrochemical (PEC) water splitting

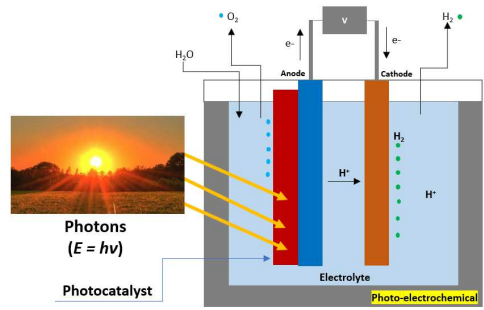
- Anode**
- LSM-YSZ
 - LSM
 - YSZ
 - LSCN-GDC
 - LNO
 - SSC-SDC73
 - BCFN
 - BSCF
 - PdO/ZrO₂ - LSM-YSZ
- Cathode**
- LSCM-YSZ
 - Ni-1Ce10ScSZ
 - Ni-YSZ
 - NiO-YSZ
 - Ni-YSZ
 - NiO-GDC

- Manuf. methods**
- Sol gel method
 - Screen printing
 - Ion plating process
 - Electrodeposition
 - Dry processing
 - Spin coating
 - Impregnation process
 - Slurry coating
 - Physical vapour deposition



- TiO₂
- ZnO
- Cds-TiO₂-WO₃
- Nickel oxide hematite
- C60/hematite, eRGO/hematite, eRGO/C60/Hematite
- α-Fe₂O₃
- Nanostructured WO₃ thin film
- ZnIn₂S₄
- Pt nanoparticles
- Molybdenum disulfide (MoS₂)
- Mn₂O₃-4TiO₂
- Fe-TiO₂/Zn-Fe₂O₃
- WO₃/TiO₂ nanotube array
- TiO₂ nanoparticles
- WO₃-Fe₂O₃
- CuBi₂O₄
- BiVO₄, WO₃

- Manufacturing methods**
- Pulsed laser deposition
 - Spin coating
 - Photo reduction method
 - Sol gel method
 - Electrodeposition
 - Hydrolysis
 - Pulse reverse electrodeposition
 - Spray pyrolysis
 - Atomic layer deposition
 - Aerosol assisted chemical vapour deposition (AACVD)
 - Chemical vapour deposition (CVD)
 - Wet impregnation method
 - Atmospheric pressure CVD
 - Inkjet printing
 - Dip coating



Opportunity: Materials data analytics

Examples of coating materials used (high temperature corrosive applications)

- SHS9172 (Cr, Mo, W, Nb)
- Diamalloy 4006 (Ni 20.5Cr 10W 9Mo 4Cu 0.75C 0.75B)
- YSZ
- Al₂O₃
- Zinc Ferrite
- CuO
- Tantalum
- Lu₂Si₂O₇ + Lu₂SiO₅
- Cr₃C₂-NiCr powder blend with 75% LA - 6304 and 25% LA - 7319
- Cr₂O₃
- NiCrBSi
- Stellite-6 (27%-32% Cr, 4%-6% W, 1%-2% C, 3%-4% Ni, 1%-2% Si, 3%-4% Fe)
- Ni₂₀Cr

- Ni₅₀Cr
- Ni₅₃Cr
- Ni₅₇Cr
- Ni₂₁Cr₉Mo
- MCrAlY
- Ni-5Al
- Fe₃Al
- SYSZ (with NiCrAlY bond coat)
- SiO₂
- CoNiCrAlY
- Cr₃C₂-WC-NiCoCrMo

For thermally sprayed (coating) materials

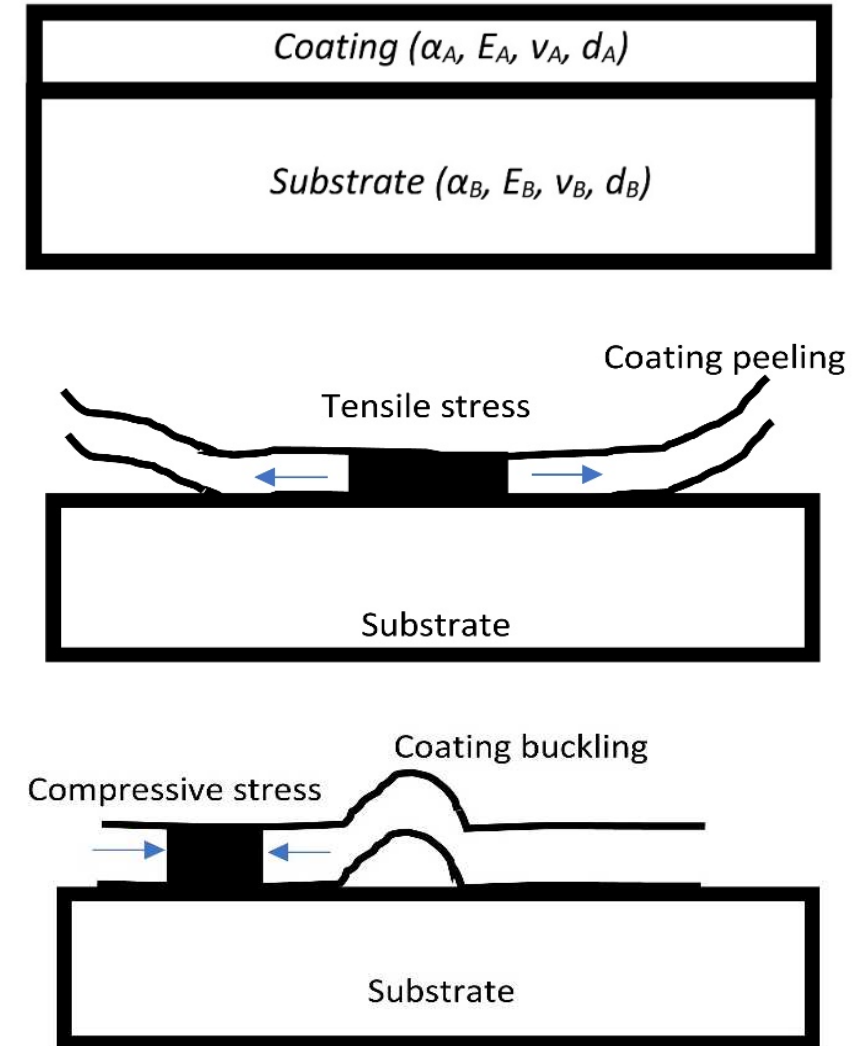
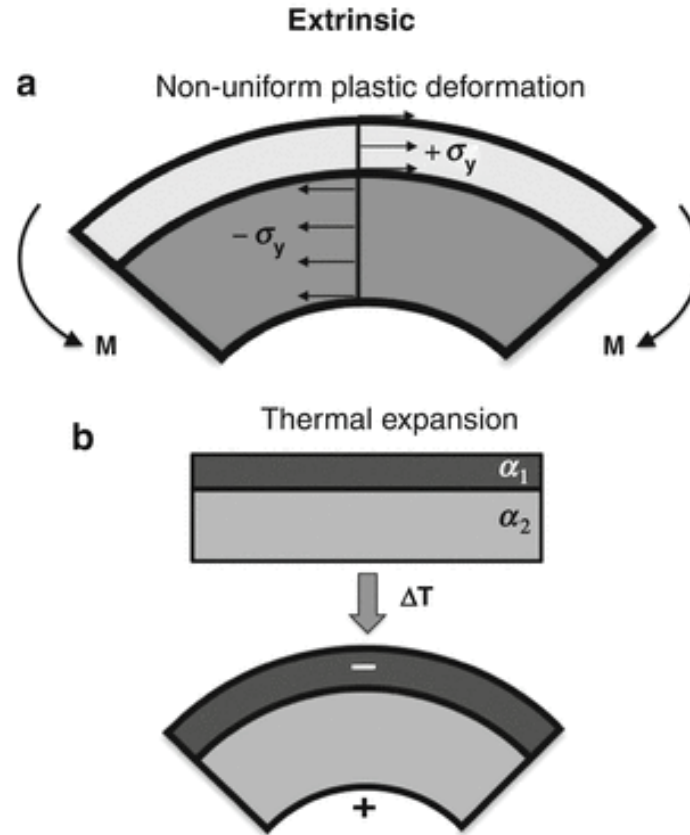
- Temperature range tested: 500 to 1320 C
- Testing duration (molten salt): 20-300 hours
- Testing duration (corrosion test): 30-360 hours
- Coating thicknesses: 100-4000 microns
- Feedstock powder size range: 45-90 microns
- Corrosion rates: 14-31 mm/year

Substrate materials for high temp. application

- Mild carbon steel
- Stainless steel (SS) 316L
- Stainless steel 310
- Ferritic stainless steel/Nimonic alloy 263/iron based alloy (SAN25)
- Stainless steel AL6XN
- Stainless steel 304
- Boiler steel SAE 431
- T24 steel pipes
- SA516 steel
- SA213-T91 (ferritic and austenitic alloy steel)
- AISI P21 is a General Mold Steel grade Tool Steel

- Inconel 625/AL6XN
- Inconel 738
- Inconel 713LC
- Superni 75
- Superni 76
- Superni 718
- Superni 750
- Superfer 800H
- Nickel superalloy (C263)
- Nickel superalloy (IN100)

- Grey cast iron
- Siliconized silicon carbide (SiSiC)
- Alumina
- Mullite ($3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$ or $2\text{Al}_2\text{O}_3 \cdot \text{SiO}_2$)
- Isotropic graphite (9G540)
- Aluminium 6061



Selection of reliable and sustainable materials (MEA's) with reduced potential needed to split water during electrolysis

Greater use of abundant feedstocks for electrolysis (e.g., water, sunlight, heat, electricity)

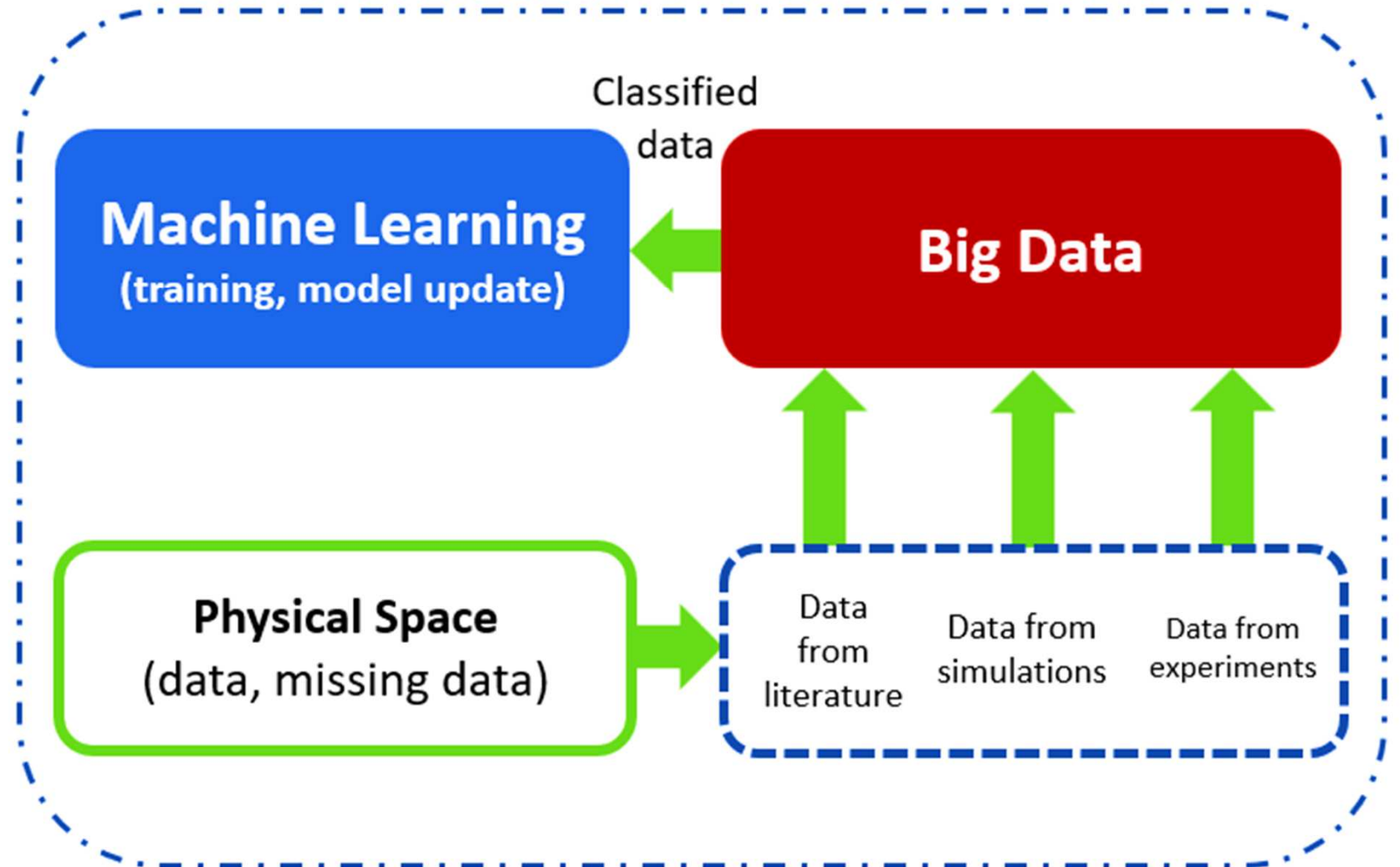
Data driven decisions (performance, materials & durability)

Optimal design of catalysts, transport layer, sealing, bipolar plates, stacks for enhanced electrolysis (e.g., metamaterials). **Reducing cell mass** which do not actively contribute to the electrolyser capacity

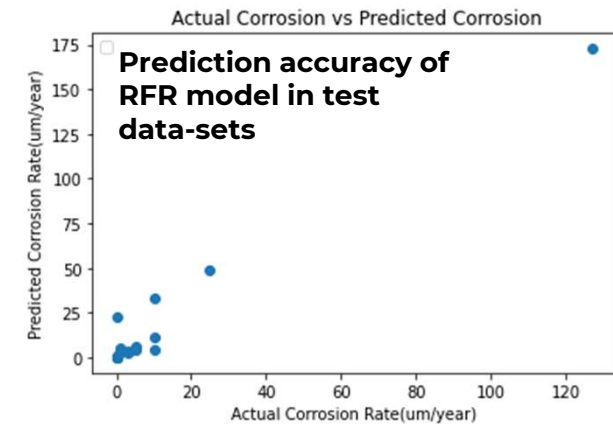
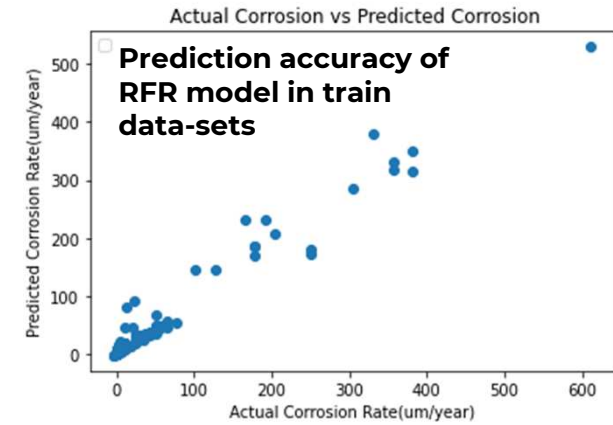
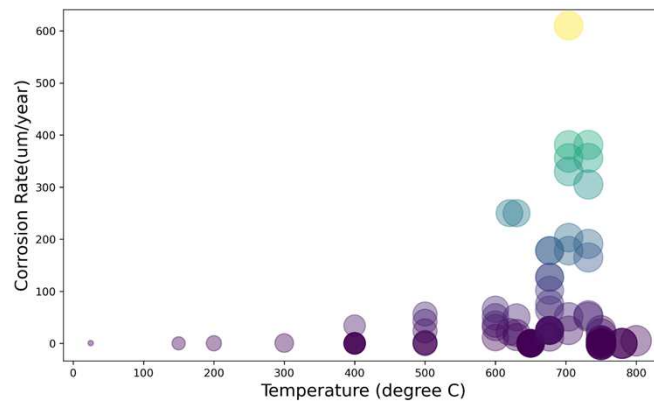
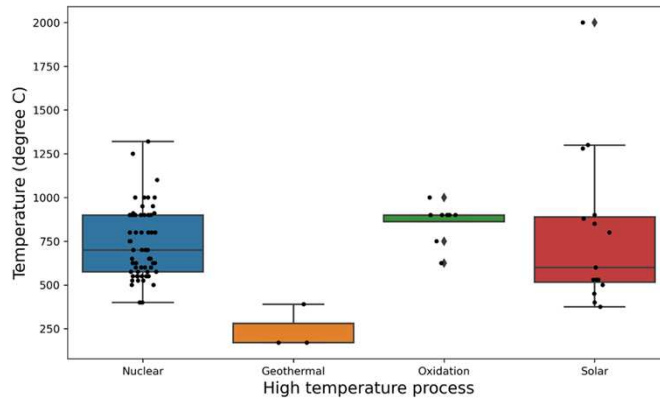
Lowering the cost of manufacturing of catalysts & transport layer (by selecting scalable manufacturing methods, automation)

Enhanced working life of MEA's (efficiency, life cycle assessment, self-healing, functional properties, structural health monitoring)

Ethical, legal, geo-political & other global issues, supply chain (materials access, environment, recycling)



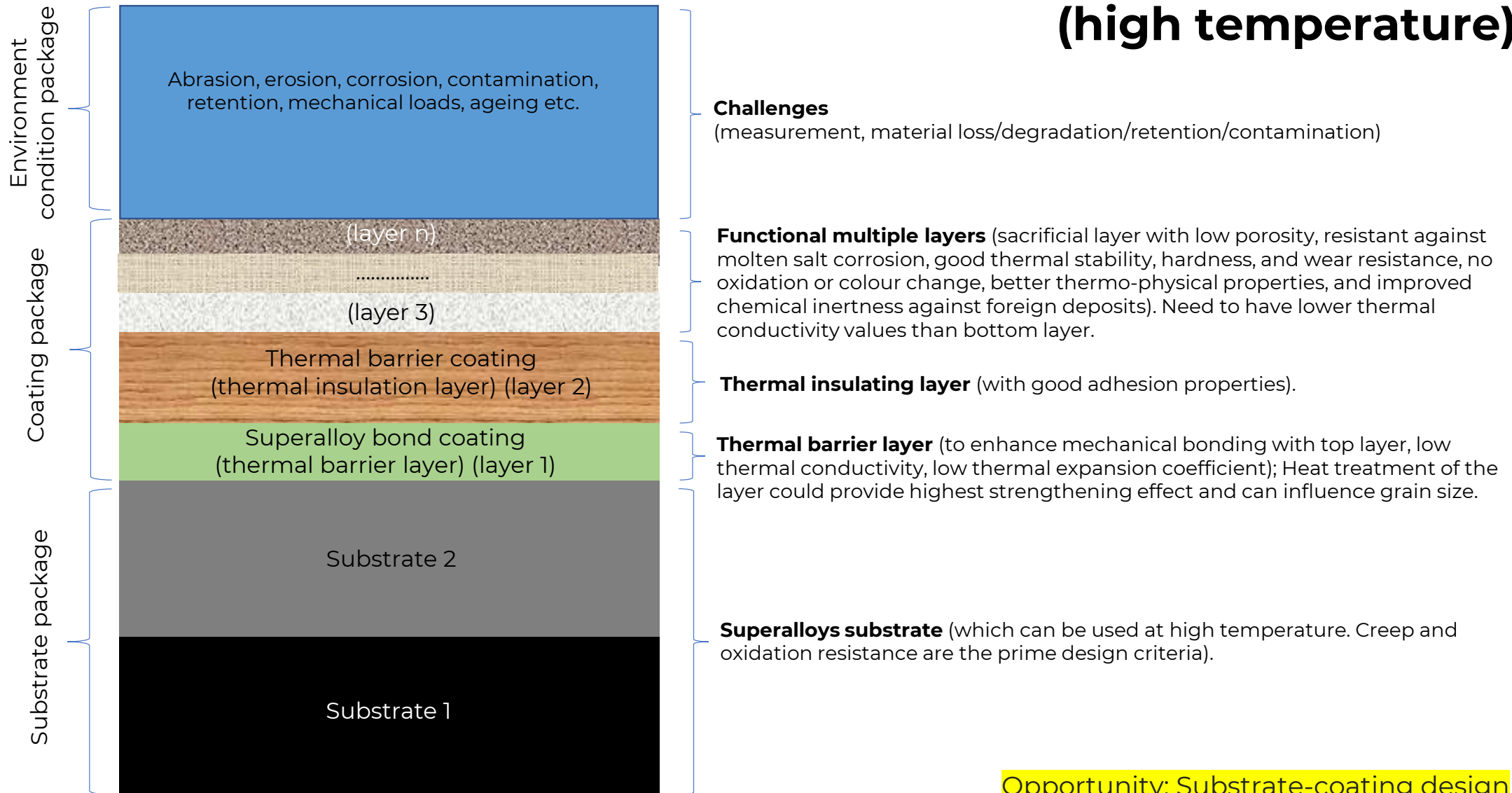
Data Analytics Approach



Regression Model	R^2 value for train data-sets	R^2 value for test data-sets
Linear Regression	0.001	-0.972
SVR	-0.150	-0.063
RR	0.240	-3.425
Lasso Regression	0.239	-3.421
ABR	0.929	0.309
GBR	0.986	0.298
RFR	0.961	0.740

R^2 accuracy validation of each model between train and test data-sets.

Surface and interface issues (high temperature)



Modelling – Example (SOEC)

Thermodynamics & Heat Transfer

Modelling scope

- **Geometry, materials, component integration** (stack structure, steady-state/transient, finite volume model, cathode/anode-supported, cell area, boundary conditions, heat losses assumptions, cell operation – ambient pressure & pressure losses within anode/cathode flow channels, physical properties assumed constant, gas properties calculated, gas streams on the cathode/anode assumed to be in co-current flow)
- **Electrochemical** (related to cell voltage, current density, cell temperature, and cathode/anode species concentration; from this electrical energy consumption and heat balance of the cell can be derived)
- **Mass transfer** (e.g., at the anode oxygen ions are converted to molecular oxygen, thus the oxygen mass flow is increasing along the cell)
- **Thermal balance** (heat sources/sinks due to electrochemical reactions, heat transfer between solid structures and gas streams, gas enthalpy changes and heat conduction)

Analysis

- Reduction in temperature gradient
- Temperature control (no control can lead to degradation problems in transient operation, i.e., in coupling with fluctuating energy sources)
- Transient load regime analysis

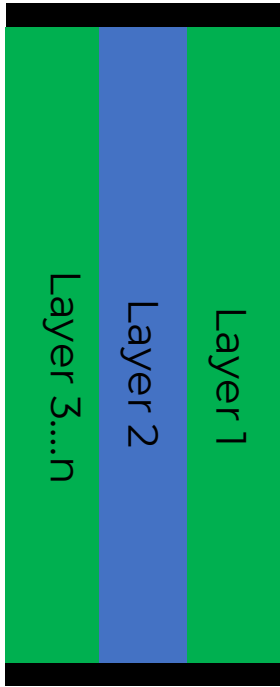
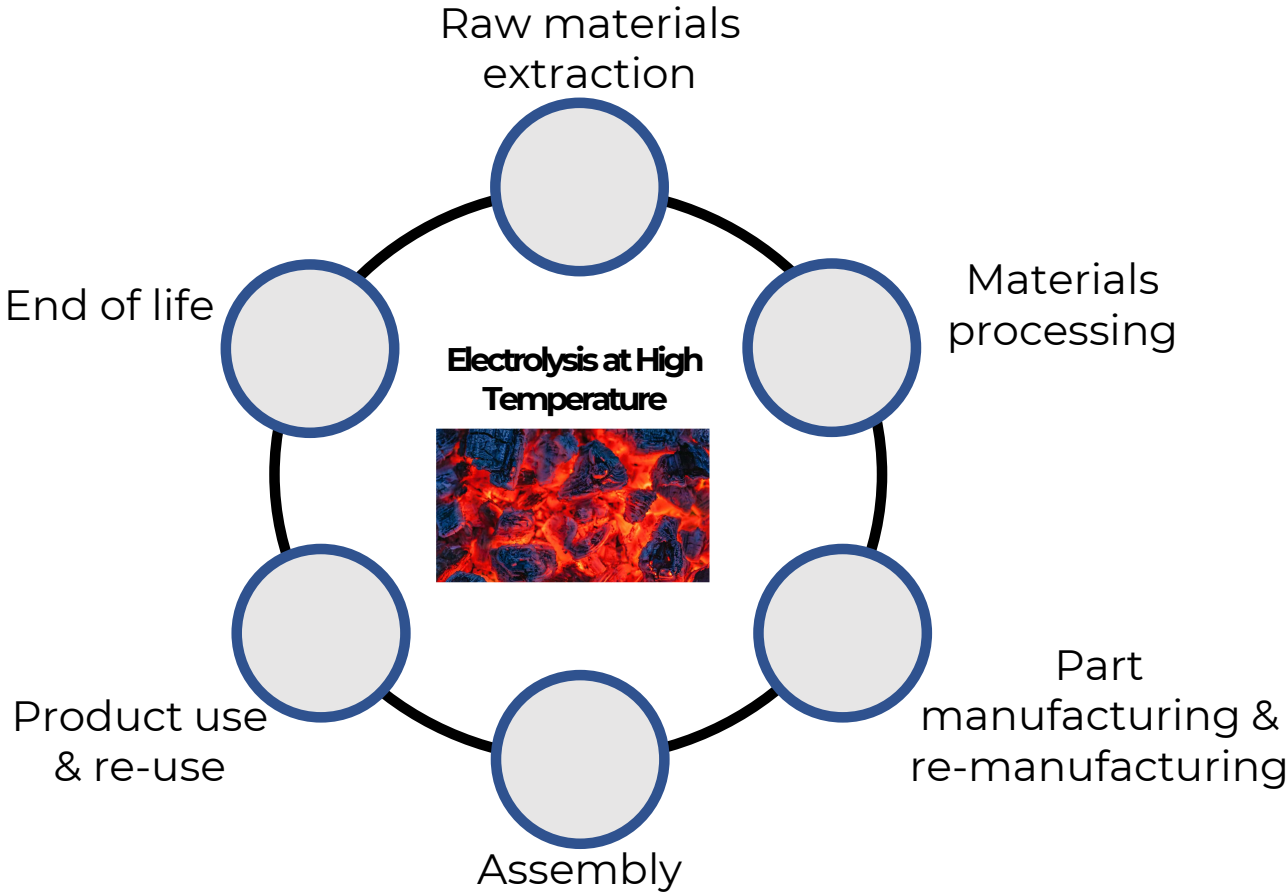
Model input parameters (example)

- Cathode channel height
- Anode channel height
- Solid structure thickness
- Interconnect thickness
- Cell length
- Cell width
- Cathode thickness
- Electrolyte thickness
- Anode thickness
- Cathode electric conductivity
- Electrolyte ionic conductivity
- Anode electric conductivity
- Cathode average effective diffusivity
- Solid structure emissivity
- Interconnect emissivity
- Solid structure heat capacity
- Interconnect heat capacity
- Solid structure thermal conductivity
- Interconnect thermal conductivity
- Solid structure density
- Interconnect density
- Cathode stream Nusselt number
- Anode stream Nusselt number
- Transfer coefficient
- Cathode stream inlet temperature
- Cathode stream inlet composition
- Anode stream composition
- Operating pressure
- Average current density
- Steam utilisation factor

Udagawa et al., Journal of Power Sources 166 (2007) 127–136

Opportunity: Develop modelling methods (Multiphysics)

Life Cycle Assessment (LCA)



Understand the contribution of individual components for electrolysis at high temperature

Opportunity: Life cycle assessment



**ROBERT GORDON
UNIVERSITY ABERDEEN**

Thank You

@nh_faisal