Modeling Ni redistribution in the fuel electrode of solid oxide cells

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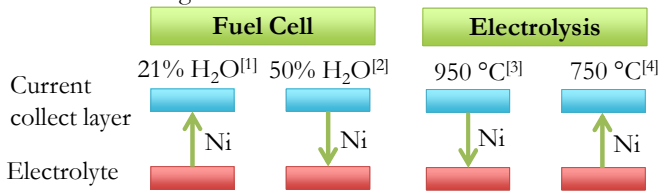
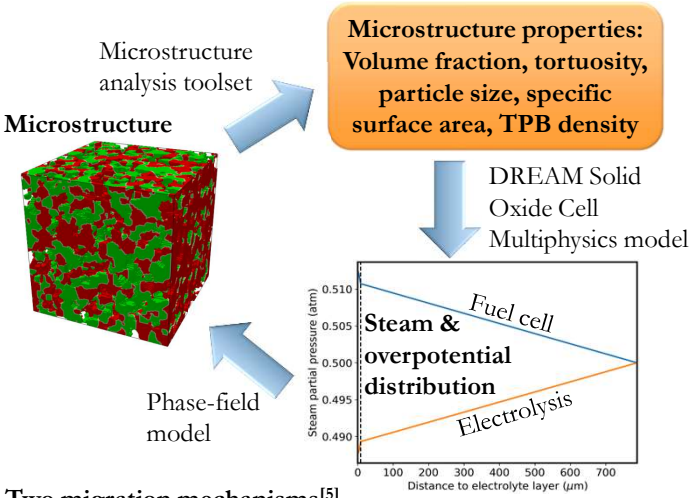
Background

- Ni redistribution: Ni migration from one region in electrode to others.
- Has a strong effect on microstructure properties such as triple phase boundary (TPB) density and Ni surface area, hence the performance.
- Different migration direction under different conditions.



Modeling Framework

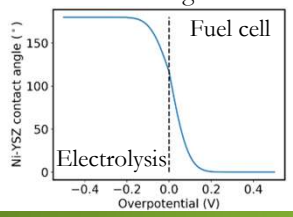


Two migration mechanisms[5]

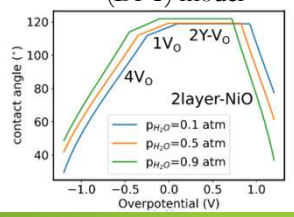
$Ni(OH)_2$ diffusion: $Ni(s)+2H_2O(g)=Ni(OH)_2(g)+H_2(g)$

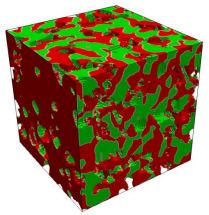
Ni-YSZ contact angle change:

Phenomenological model



Density function theory (DFT) model





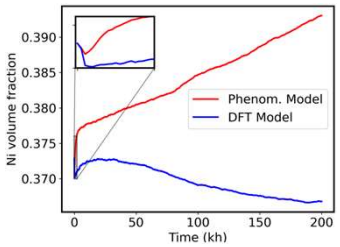
- Reconstructed subvolumes of active layer with the size of 8.32^3 μm^3
- 42% YSZ-39% Ni-19% pore
- A current-collect layer of 780 μm appended when evaluate distribution of steam and overpotential.

Results

Condition I[1]

Fuel cell mode, 700 °C, 0.5 A/cm^2, 21%H_2O-79%H_2

f_v^{Ni} within 1 μm of electrolyte



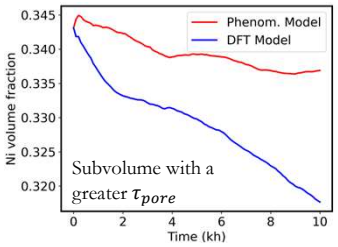
Change in Ni volume fraction near electrolyte

Exp.	Enrichment
Phenom.	Enrichment
DFT	Depletion

Condition II[2]

Fuel cell mode, 850 °C, 0.5 A/cm^2, 50%H_2O-50%H_2

f_v^{Ni} within 1 μm of electrolyte



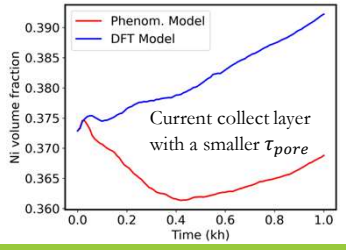
Change in Ni volume fraction near electrolyte

Exp.	Depletion
Phenom.	Depletion
DFT	Depletion

Condition III[3]

Electrolysis mode, 950 °C, 2.0 A/cm^2, 90%H_2O-10%H_2

f_v^{Ni} within 1 μm of electrolyte



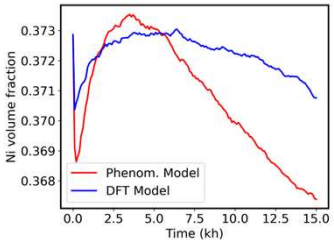
Change in Ni volume fraction near electrolyte

Exp.	Enrichment
Phenom.	Enrichment
DFT	Enrichment

Condition IV[4]

Electrolysis mode, 750 °C, 0.72 A/cm^2, 45%H_2O-55%H_2

f_v^{Ni} within 1 μm of electrolyte



Change in Ni volume fraction near electrolyte

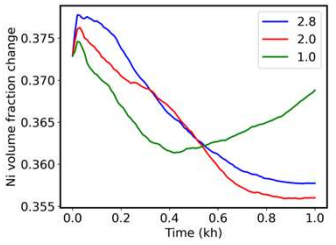
Exp.	Depletion
Phenom.	Depletion
DFT	Depletion

Discussions on Phenomenological model

Effect of τ_{pore} in current-collect layer

Electrolysis mode, 950 °C, 2.0 A/cm^2, 90%H_2O-10%H_2

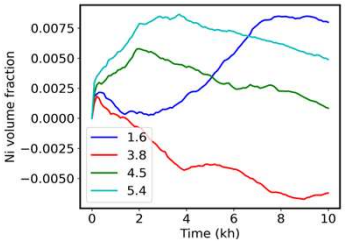
f_v^{Ni} within 1 μm of electrolyte



Effect of initial τ_{pore} in active layer

Fuel cell mode, 850 °C, 0.5 A/cm^2, 50%H_2O-50%H_2

f_v^{Ni} within 1 μm of electrolyte



Ni redistribution can be mitigated by engineering the microstructure properties in both active and current-collect layer.

References:
[1] Menzler *et al.*, J. Power Sources, **478** (2020) 228770
[2] Barfod *et al.*, Proc. Electrochem. Soc. PV **2003-7** (2003) 1158
[3] Hauch *et al.*, J. Electrochem. Soc., **155** (2008) B1194-B1193
[4] Trini *et al.*, J. Electochem. Soc., **166** (2019) F158-F167
[5] Lei *et al.*, J. Power Sources, **545** (2022) 231024.

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