Structural Reliability Considerations for Planar SOFCs:
Cathode Contact, Cell Thermal Gradients & Alternate Geometries

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OVERVIEW

Long term reliability of solid oxide fuel cells (SOFCs) is one of the key requirements for their commercial success. While significant developments have occurred at the materials and component levels of SOFCs, the mechanical reliability of stacks under thermal gradients at normal operating and unexpected shutdown conditions still remains a challenge. Apart from the thermal gradients which can fail nonmetallic SOFC components, contact between electrodes and interconnects (especially the cathode side) was identified as one of the weakest links that can significantly reduce performance in the assembled stacks.

This poster presents the results from the reliability analyses conducted with cathode contact modeling and the alternate geometry configuration simulations for thermal gradient sensitivity evaluations performed to date.

Technical Approach

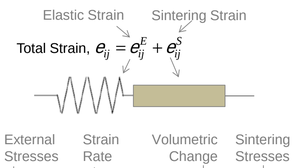
Computational modeling was used to study contact material densification mechanics and to assess the reliability of cathode contact as well as the stack.

- Ø A continuum linear-viscous sintering model for porous materials was considered and incorporated into the commercial Finite Element Analysis code ANSYS® to simulate contact material densification (sintering) behavior that is dependent on time, temperature, constraints, and initial stress state.
- Ø The material property data needed for various cathode contact materials (LSM20, LSC20, LSCF6428) were obtained from the sintering and diametric compression test experiments conducted at PNNL.
- Ø The stack operating thermal distributions are obtained from the in-house SOFC multi physics code SOFC-MP.
- Ø The thermo-mechanical stresses obtained from the FEA are exported to the ceramic reliability assessment software CARES® (based on Weibull statistics).

Skorohod, Olevsky Viscous Sintering Continuum Model for Porous Materials

Ref: E.A. Olevsky, Mater. Sci. Eng. Rep., 23 [2] 40-100 (1998)

- s is stress
- e is strain
- P_L is the sintering stress
- a is surface energy
- r is particle radius
- h_0 is shear modulus of porous skeleton
- h is effective shear modulus
- z is effective bulk modulus
- q is porosity
- $s(W)$ is equivalent stress
- W is equivalent strain rate
- $\dot{\varepsilon}$ is volume change rate
- g is shape change rate
- d_{ij} is Kronecker delta



External Stresses | Strain Rate | Volumetric Change | Sintering Stresses

$$s_{ij} = 2h_0\left(\dot{e}_{ij} + \gamma\dot{e} - \frac{1}{3}j\dot{e}d_{ij}\right) + P_L d_{ij}$$

$$h = j\,h_0 \qquad z = 2\gamma\,h_0 \qquad s(W) = 2h_0 W$$

$$j = (1-q)^2 \qquad \gamma = \frac{2}{3}\frac{(1-q)^3}{q}$$

$$W = \sqrt{\frac{j\,g^2 + \gamma\,\dot{e}^2}{1-q}} \qquad P_L = \frac{3a}{r}(1-q)^2$$

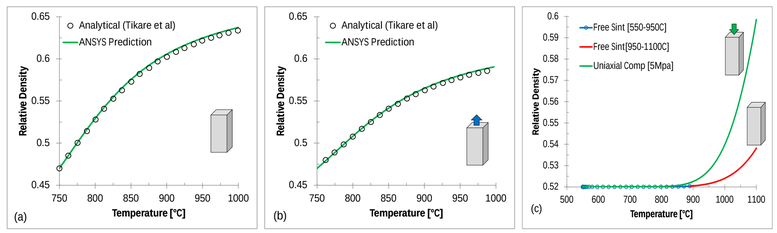
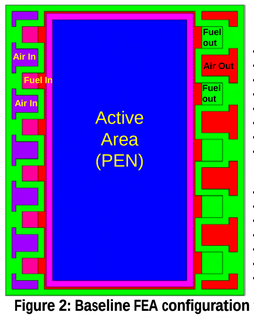


Figure 1: ZnO powder densification results from the FEA model compared to analytical solution (a) Free sintering (b) Forge sintering with 1MPa tensile pressure (c) Densification results with LSM20 under free and forge sintering

Cathode Contact & Cell Reliability Simulations

The reliability of the cathode contact layer as well as the SOFC stack were evaluated using a generic design (inspired by the Delphi Gen-4) that is representative of current generation planar SOFC stacks with large effective cell areas and flexible interconnects as illustrated in Figure 2.



Top to Bottom Materials at Stack Center

- Anode IC(SS441)
- Ni Mesh
- Anode (Ni-YSZ)
- Electrolyte (YSZ)
- Cathode (LSM)
- Contact Material (LSM20)
- SS441 Mesh
- Cathode IC(SS441)

(Near Stack Edges)

- Anode IC (SS441)
- Fuel Seal (Glass)
- Anode Spacer (SS441)
- Picture Frame (SS441)
- Air Seal (Glass)
- Cathode Spacer (SS441)
- Cathode IC(SS441)

Figure 2: Baseline FEA configuration for cathode contact layer and stack reliability evaluations

The cathode contact layer densification depends on the stress state of the stack. Hence, the load contributions from processing and operations are considered in evaluating the reliability of the contact layer. Figure 3 illustrates the thermal profile and load steps used in the FEA simulations.

FEA Model Thermal Load Steps

1. Assumed stress free state (950°C)
2. Pressure load (0.2 MPa compressive)
3. Sintering for 2 hours at 950°C
4. Ramp down to operating condition in 2 hours (operating loads from SOFC-MP)
5. Shutdown to room temperature (30 min)

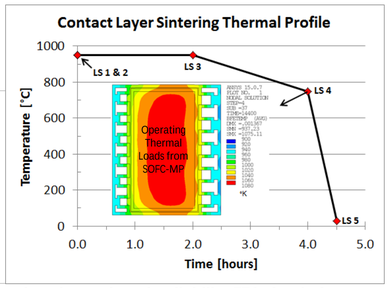


Figure 3: Thermal profile & load steps in contact layer sintering and stack reliability FEA simulations

Component Stress and Stack Reliability Results

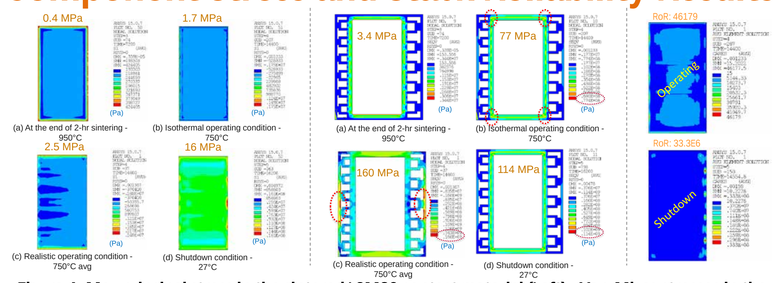


Figure 4: Max principal stress in the sintered LSM20 contact material (Left), Von-Mises stresses in the picture frame (Middle), Risk of Rupture for contact material layer (Right) at various stages

Table 1: CARES reliability analysis summary for baseline stack under realistic operating condition

Loading condition	Anode	Electrolyte	Cathode	Contact Material
Stress Free	100 / 100 / 100	100 / 100 / 100	100 / 100 / 100	100 / 100 / 100
Compression	100 / 100 / 100	100 / 100 / 100	100 / 100 / 100	99.9/99.9/99.9
After Sintering 2hr	99.9/99.9/99.9	99.9/99.9/99.9	98.8/98.8/98.8	99.9/99.9/99.9
Operating state	100 / 100 / 100	96.0/96.0/96.1	99.0/99.9/99.9	99.9/99.8/99.9
Shutdown state	100 / 100 / 100	86.3/86.3/86.3	99.9/99.9/99.9	28.9/88.7/90.5

NOTES: values in xxx / xxx / xxx format indicate the % reliability when evaluated with LSM20 / LSC20 / LSCF6428 Weibull strength data respectively

Cathode Contact and Stack Reliability Analyses Summary

- Ø Significant increase in component stresses due to the thermal gradients in the stack were observed compared to the isothermal state (Figure 4).
- Ø The CARES reliability analysis based on weakest link theory appears to be aggressive for reliability evaluations as localized component stresses could lead to very low stack reliabilities as summarized in Table 1. The Risk of Rupture plots as shown in Figure 4 provide insights on the local effects.

Alternate Stack Geometry Considerations

The structural reliability of SOFCs mainly depend on the component stresses during stack operation/shutdown. Earlier results indicated that operating thermal gradients increase stresses compared to the isothermal state. one of the strategies proposed by Oak Ridge National Laboratory (ORNL) to improve the structural reliability of SOFCs includes identifying alternative geometries that have potential to reduce cell thermal gradients.

- The alternate geometries shall have equal of better electrochemical performance with lower thermal gradients to be considered as viable alternatives.
- Initially, SOFCs with tapered (15°, 30° & 45°) cell configurations (Figure 5) in which flow velocity and convective film coefficient increases in flow direction were studied for their performance and reliability.
- All the tapered models are simulated to have the same active length, area and fuel flow rate as the baseline configuration.
- The performance of alternate configurations was evaluated based on metrics such as fuel utilization and stack current densities compared to a baseline (non-tapered) configuration.

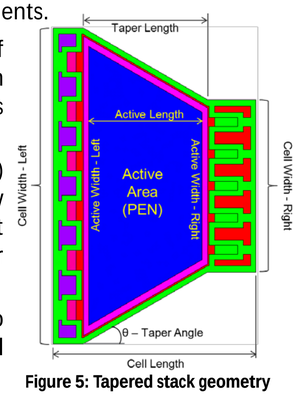


Figure 5: Tapered stack geometry

Table 2: Cell performance from the baseline and sensitivity study models

Tapered Model	Active Area (cm^2)	Stack Current (A)	Cell Voltage (V)	Power (W)	Cell Temp max (°C)	Stack ΔT max (°C)	Cell ΔT max (°C)	% Fuel Utilization
0°	402	152.5	0.8425	128.5	830	146	145	76.5
15°	398	152.5	0.8334	127.1	824	143	138	76.5
30°	395	152.2	0.8383	127.6	826	147	139	76.3
45°	393	152.4	0.8463	129.0	825	146	137	76.4

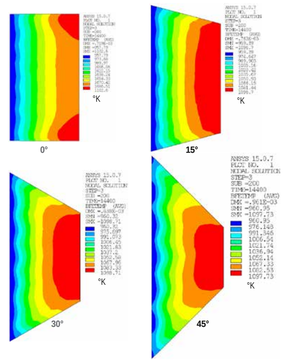


Figure 6: PEN operating thermal gradients from the baseline, 15°, 30° and 45° models

Alternate Geometry Analyses Summary

- Ø No significant differences in the cell performance, the maximum temperatures, and thermal gradients (Figure 6) were observed between the baseline (0°) and the tapered sensitivity models.
- Ø The insignificant effect of the tapered configurations on the cell thermal gradients could be attributed to the reduction in area for heat transfer despite increased velocity and heat transfer coefficient towards the tapered region.
- Ø Other designs are under consideration.

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