SECA Core Program: Recent Development of Modeling Activities at PNNL

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8th Annual SECA Workshop
San Antonio, TX
August 8, 2007

R&D Objectives & Approach

- **Objectives**:
  - Develop integrated modeling tools to:
    - Evaluate the tightly coupled multi-physical phenomena in SOFCs
    - Aid SOFC manufacturers with materials development
    - Allow SOFC manufacturers to numerically test changes in stack design to meet DOE technical targets
  - Provide technical basis for stack design
- **Approach**: Finite element-based analysis tools coupled with experimental validation:
  - SOFC-MP: A multi-physics solver for computing the coupled flow-thermal-electrochemical response of multi-cell SOFC stacks
  - Targeted evaluation tools for cell design challenges:
    - Interface and coating durability
    - Reliable sealing
    - Time dependent material performance
  - Collaborate with ORNL and ASME to establish and document the stack design approach.

Accomplishments

- Distributed the SOFC-MP and Mentat-FC software packages to multiple industry teams and CTP university researchers for modeling and development of SOFC stacks.
- Established a methodology to assess glass-ceramic seal failure. The damage model was implemented in MSC MARC and used for SOFC stack stress analysis to predict accumulated damage and failure of the seals under thermal-mechanical loading. The methodology was extended to predict seal damage accumulation in stacks due to thermal cycling processes.
- Developed an integrated modeling/experimental framework to predict the life of SOFC interconnect materials. Oxide scale properties were evaluated experimentally and the effects of interconnect oxide growth on interfacial structural integrity during isothermal cooling was studied.
- Initiated a design basis document in collaboration with ASME and ORNL to provide industry teams with technical guidance on materials characterization, constitutive models, modeling techniques, failure analyses, and software usage to support SOFC design and development efforts.

Accomplishments

- Developed modeling methodologies and constitutive models based on experimental characterizations to evaluate the time-dependent mechanical response of stack components. The models can quantify the effect of creep in metallic components and glass-ceramic seals on stack deformations and cell component stresses during operation and shutdown. A homogenization model to predict glass-ceramic seal properties as a function of composition was developed and implemented.
- Established a methodology to assess interconnect scale growth and effect of the associated electrical resistance increase on stack performance. The capability enables evaluation of the long term behavior of prospective interconnect materials with respect to thermal and electrical stack performance.
- Supported development of a standardized SOFC cell geometry for use in the SECA program to evaluate materials and technologies within a common testing platform.

Selected Publications

- Nguyen BN, BJ Koeppel, S Ahzi, MA Khaleel, and P Singh. 2006. “Crack Growth in Solid Oxide Fuel Cell Materials: From Discrete to Continuum Damage Modeling.” *J Am Ceram Soc* 89(4):1135-1368.
- MA Khaleel, KP Recknagle, X Sun, BJ Koeppel, EV Stephens, BN Nguyen, KI Johnson, VN Korolev, JS Vetrano, and P Singh, “Recent Development of Modeling Activities at PNNL,” presented at the SECA Core Technology Program Peer Review, Philadelphia, PA, September 12-14, 2006.
- KP Recknagle, BJ Koeppel, X Sun, JS Vetrano, ST Yokuda, DL King, P Singh, and MA Khaleel, “Analysis of Percent On-Cell Reformation of Methane in SOFC Stacks and the Effects on Thermal, Electrical, and Mechanical Performance,” presented at the Fuel Cell Seminar 2006, Honolulu, HI, November 13-17, 2006. Also published in *ECS Trans.* 5, (1) 473 (2007).
- X Sun, W Liu, J Vetrano, G Yang, MA Khaleel and M Cherkaoui, “Life Prediction of Ferritic Stainless Steel Interconnect under Thermal Stress and Oxide Growth Stress,” presented at the Fuel Cell Seminar 2006, Honolulu, HI, November 13-17, 2006. Also published in *ECS Trans*. 5, (1) 357 (2007).
- W Liu, X Sun, and MA Khaleel, “Fracture Failure Criteria of SOFC PEN Structure,” presented at the 31st International Conference on Advanced Ceramics and Composites, Daytona Beach, FL, January 21-26, 2007.
- W Liu, X Sun, MA Khaleel and J Qu, **“**Global Failure Criteria for SOFC PEN Structure,” SAE 2007 World Congress, Detroit, MI, April 16-19, 2007.
- BN Nguyen, BJ Koeppel, and MA Khaleel, “Design of a Glass-Ceramic Seal for Solid Oxide Fuel Cell Applications by Means of a Homogenization Approach,” presented at the ASME Applied Mechanics and Materials Conference, Austin, TX, June 3-7, 2007.
- X Sun, W Liu, and MA Khaleel, “*Effects of Interconnect Creep on Long-Term Performance of a One-Cell Stack*,” PNNL-16342, Pacific Northwest National Laboratory, Richland, WA, 2007.
- X Sun, WN Liu, E Stephens and MA Khaleel, “*Interfacial Strength and IC Life Quantification using an Integrated Experimental/Modeling Approach”*, PNNL-16610, Pacific Northwest National Laboratory, Richland, WA, May 2007.
- X Sun, A Tartakovsky and MA Khaleel, “Probabilistic Based Design Methodology for Solid Oxide Fuel Cell Stacks,” submitted to ASME *Journal of Fuel Cell Science and Technology*, May 2007.

Collaborations

- Industry
  - Modeling and Software Training
    - GE
    - Delphi
    - Acumentrics
    - Siemens
    - FCE

- University & National Labs
  - Modeling
    - U of Illinois, Chicago
    - Georgia Tech
  - Materials
    - ORNL
    - Carnegie Mellon University
    - Penn State
  - Software Training
    - U of Connecticut

- Vendors
  - MSC Software

Results

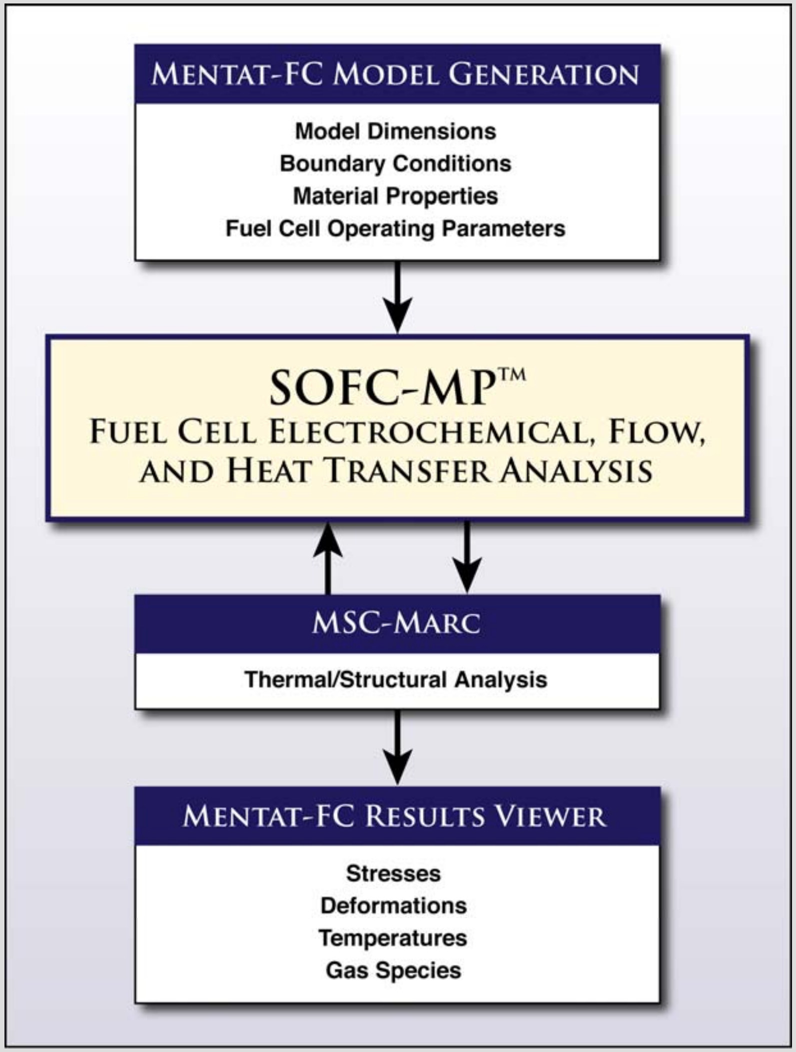
- Support of SECA teams and core program participants
- Advancements for SOFC-MP stack modeling tool
- Metal interconnect
- Glass-ceramic sealants
- SECA Test Cell
- Activities in Progress

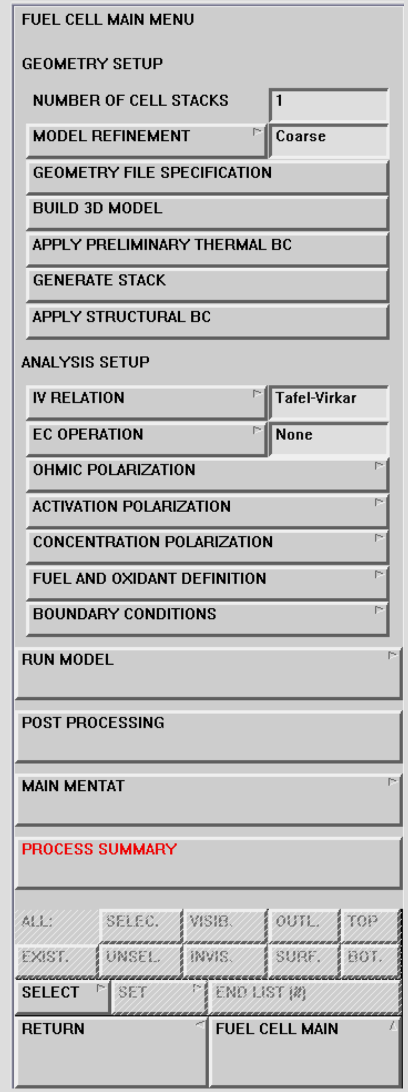
Support of SECA teams and core participants

- Sub-models being added to SOFC-MP
- SOFC-MP used in collaborative efforts for modeling seal creep

SOFC Analysis Overview

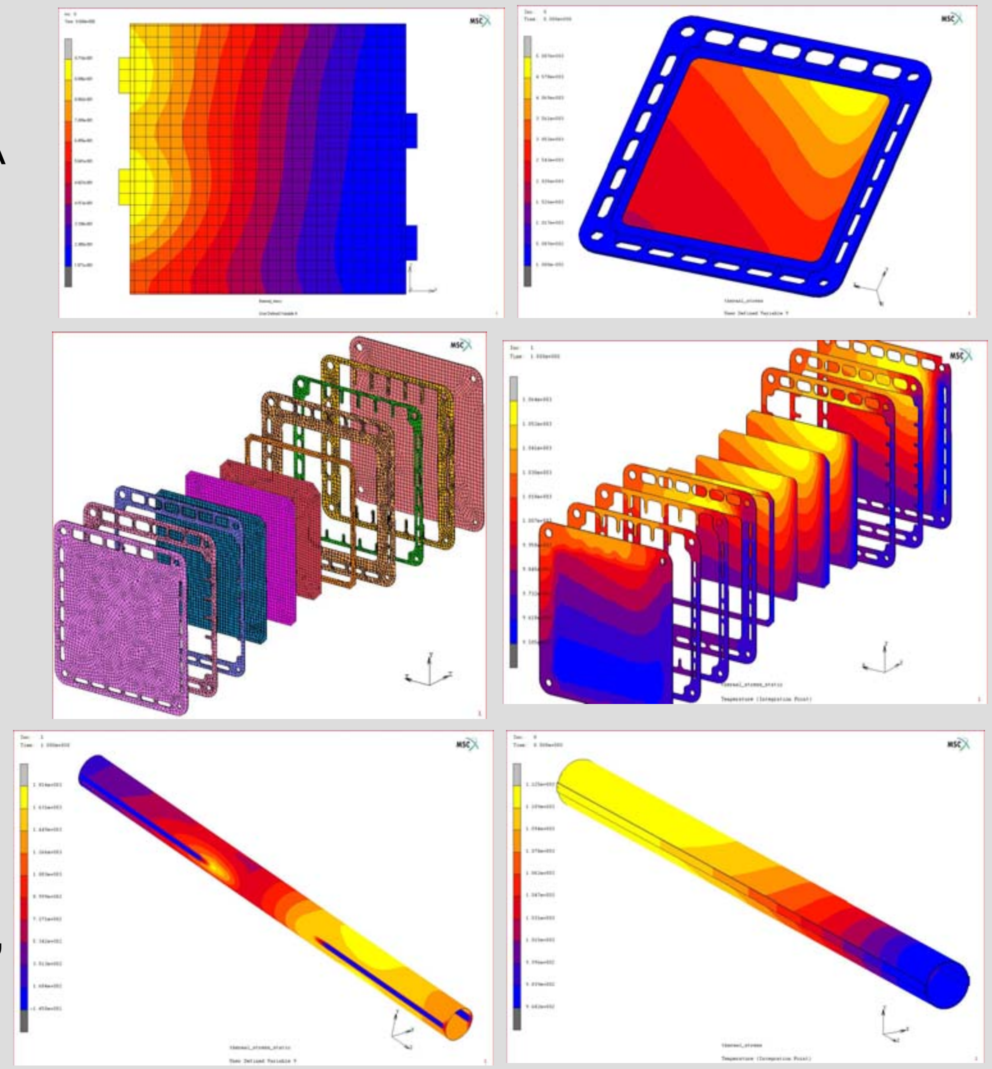
- Developed tools to build/analyze SOFC cells and stacks
  - **Mentat-FC**: GUI to build models from templates, CAD files, or FEA meshes
  - **SOFC-MP**: Coupled thermal, flow, and electrochemistry solver
  - **MSC.Marc**: Structural finite element analysis using SOFC-MP temperatures





SOFC-MP/Mentat-FC

- Mentat-FC GUI
  - Guides user through entire analysis
  - Builds geometry from CAD files, FEA meshes, or templates (planar co-, counter-, cross-flow)
  - SOFC operating parameters (I-V, fuel/oxidant inputs, polarizations)
  - Exterior thermal boundary conditions
  - Material properties database
  - Has tubular capability
- SOFC-MP Solver
  - Finite element based
  - Generic fuel and oxidants (CEA)
  - Efficient reduced order dimensional analyses for electrochemistry and gas flows
  - Contact algorithms treat incompatible meshes
- Post-processing of electrical output, species, thermal distribution, deformations, and stresses



Support of SECA Teams and Core Program Participants

- Model improvements for SOFC-MP:
  - Distributed resistance within active area flow region
    - $\Delta P/L = -\beta u$, β=f(density, channel height, viscosity, temp)
    - Implementation in 3D code in progress
- SOFC-MP used for collaboration with the University of Cincinnati to study the performance of their glass sealant in a realistic SOFC cell.
  - Nirmal Govindaraju
- Other university participants from West Virginia University, Carnegie Mellon University, Georgia Tech, and University of Idaho will participate in summer internships to learn about SOFC modeling.
  - Said Ahzi, Iqbal Gulfam, Emily Ryan, Jackie Milhans, Matt Hinkelman

Advancements for SOFC-MP stack modeling tool

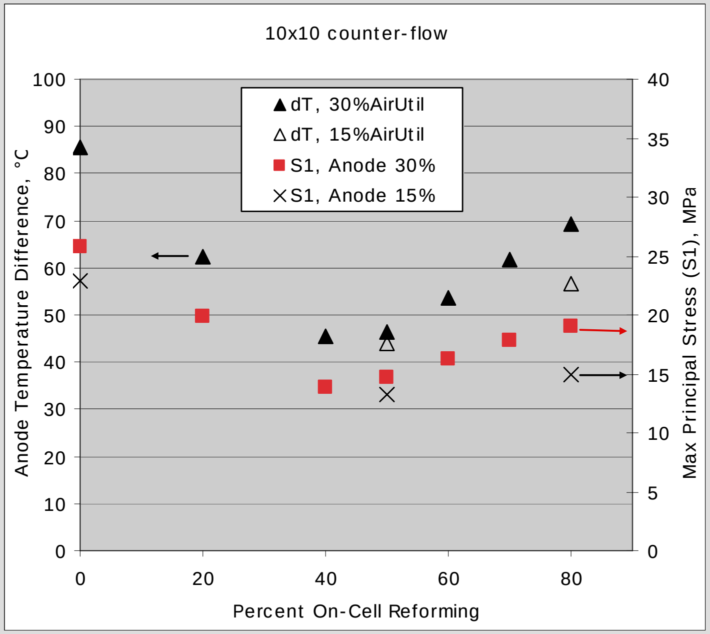
- On-cell reformation
- Pressurized SOFC operation

On-Cell Reformation: Variable Methane Concentration in anode feed

- Objectives:
  - Predict the cooling benefit of on-cell reformation within stacks of various flow configurations and size as the methane concentration of the anode feed is varied
  - Evaluate the thermal and electrical performance of the stacks
  - Optimize the anode feed composition for minimum thermal gradients and anode stress
- Technical Approach:
  - Apply the validated thermal-electrochemistry-reforming calculation methodology within generic models of co-flow, counter-flow, and cross-flow stacks of 10x10 cm and 20x20 cm cell size
  - Anode feed varied to represent the partially pre-reformed compositions
  - Compare results of the simulation matrix for thermal and electrical performance

On-Cell Reformation: Variable Methane Concentration in anode feed - Results

- Temperature difference and anode stress was minimized with 40-50% of reaction occurring on-cell (counter, cross flow 10x10)
- Co-flow benefited most by largest % on-cell reformation (80%) for both 10x10 and 20x20 cell size
- Larger (20x20cm) stacks benefited similarly to the smaller stacks and also benefited from increased air flows



Cell Size / Air Use	Flow Configuration	% OCR	Temperature, °C		Anode Stress S1max, MPa	Power, W/cm[2]
			Maximum	ΔT		
10x10 / 30%	Cross	50	775	74	14.2	0.403
	Co-flow	80	779	74	17.2	0.403
	Counter	40	768	45	13.8	0.405
10x10 / 15%	Cross	50	774	66	14.0	0.405
	Co-flow	80	777	66	14.8	0.403
	Counter	50	768	44	13.3	0.406
20x20 / 30%	Cross	50	866	241	60.2	0.399
	Co-flow	80	844	178	40.0	0.403
	Counter	60	832	196	71.7	0.409
20x20 / 15%	Cross	0	851	191	45.2	0.397
	Co-flow	80	817	124	25.5	0.404
	Counter	0	851	188	45.4	0.415

Pressurized SOFC

- Objective:
  - Predict electrochemical performance in pressurized SOFC systems
- Background:
  - Increased pressure on both anode and cathode sides has three effects:
    - Nernst Potential is increased
    - Activation and concentration polarizations are decreased
    - Increased electrical power results in decreased net heat load

Pressurized SOFC

- Technical Approach:
  - Activation polarization η_{Act}*

$$\eta_{Act} = \frac{RT}{2F}\sinh^{-1}\left(i\frac{4F}{RTS^c}\right)$$

    - Cathode side - dependent upon absolute pressure

$$S^c = P_{\exp}\exp\left(\frac{-E_{act}}{RT}\right)\left(P_{O_2 cath}\right)^{0.5}$$

    - Anode side - independent of absolute pressure

  - Concentration polarization in the cathode:
    - Limiting current is pressure dependent

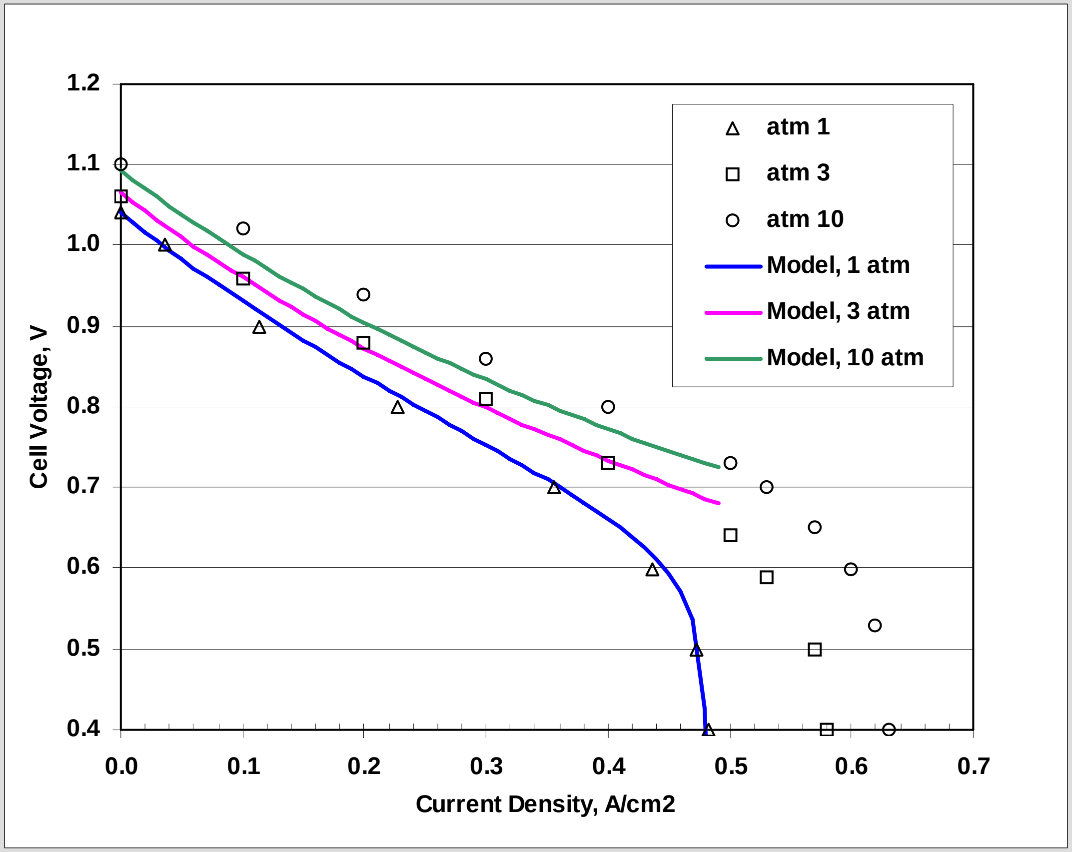
$$V_{ca} = \frac{RT}{4F}\ln\left(\frac{1-i}{i_{cs}}\right)$$

$$i_{cs} = \frac{4FPD_{eff}}{RT\delta}\ln\left(\frac{P}{P-P_{O_2}}\right)$$

*Li, PW, MK Chyu. Transactions of the ASME. Vol. 127, p1344-1362.

Pressurized SOFC

Effect of Pressure on Planar SOFC*



*Nguyen, M. Texas Hybrid Meeting, Galveston TX, Feb. 2002.

Metal Interconnect

- Indentation testing of scale on Crofer and 441
- Numerical analysis of scale/coating strength

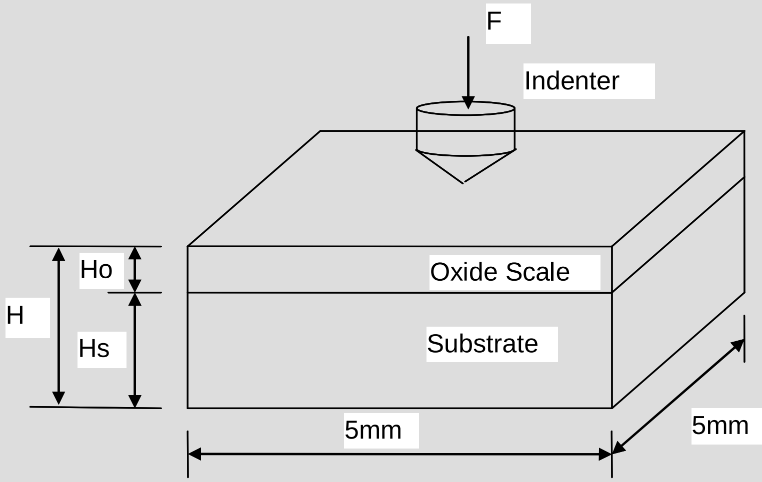
Interfacial Strength Quantification and IC Life Prediction

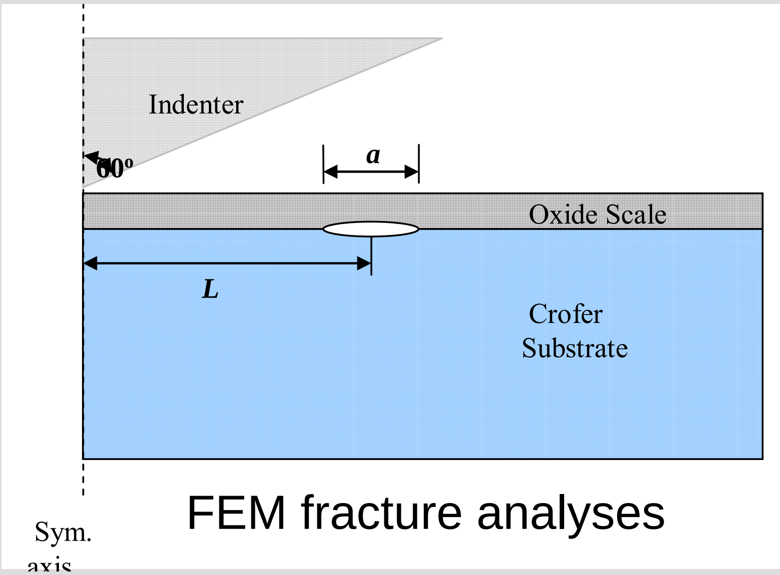
- Overall goal and objective:
  - Predict interconnect life with and without spinel coating under isothermal cooling and thermal cycling
  - Evaluate life of different candidate IC materials by proposed methodology
  - Optimize spinel coating thickness to ensure IC life satisfies SECA life requirement
- Technical approach
  - Quantify interfacial strength by integrated experimental/analytical approach
  - Predict interfacial stress generated during isothermal cooling and thermal cycling
  - Predict interconnect life by comparing stress and strength at the interfaces

Interfacial Strength Quantification and IC Life Prediction

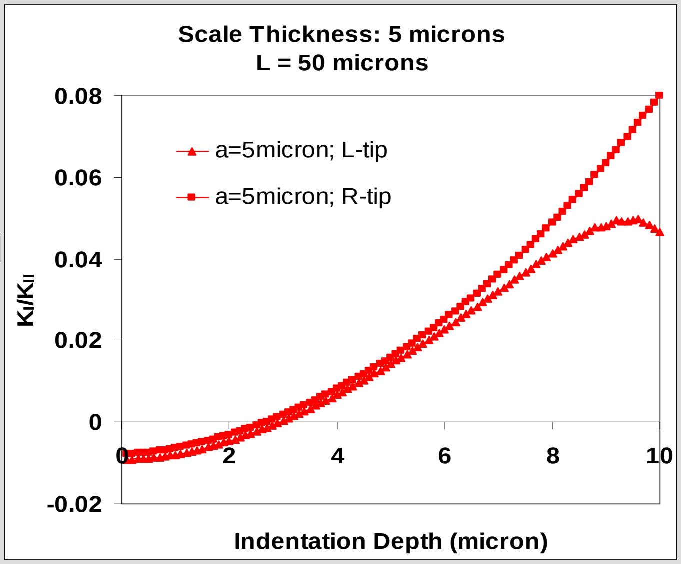
- Accomplishments:
  - Identify the driving force for interfacial delamination – Interfacial shear stress
  - Finished experimental indentation tests on Crofer22 and SS441 with and without spinel coating
  - Quantified the strength of oxide/Crofer22 interface
  - Predicted Crofer22 life under isothermal cooling without spinel coating
  - Quantify the strength of oxide/SS441 interface

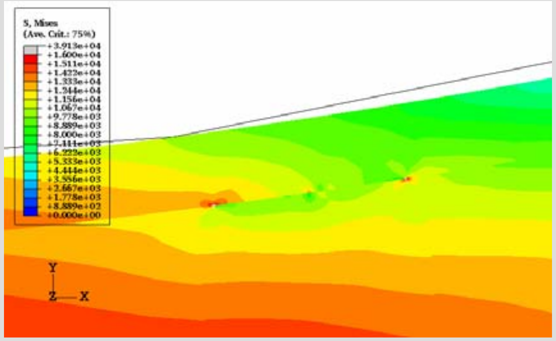
Accomplishment - Identify the driving force for interfacial delamination





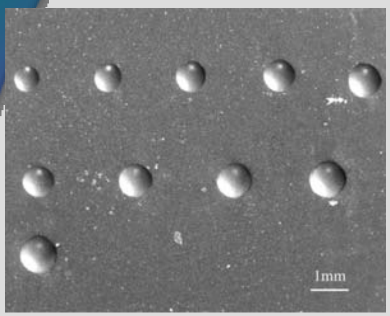
KII dominant interfacial crack growth → Shear stress at the interface identified as the driving force for interfacial delamination

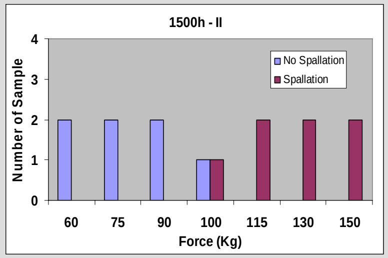




Battelle

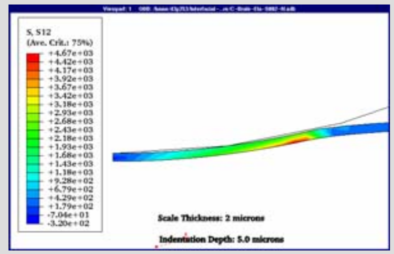
Accomplishment - Interfacial Strength Quantification and Life Prediction for Uncoated Crofer22





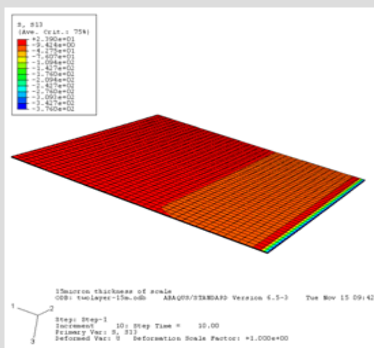
1/16" Rockwell indentor

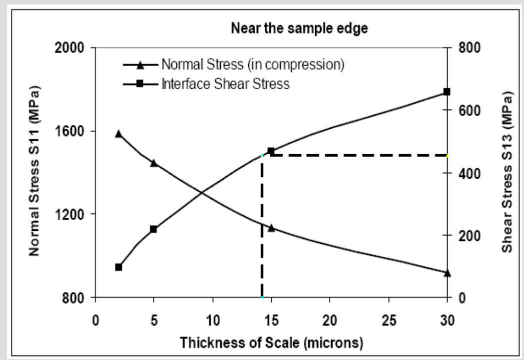
+



=> Determine interfacial strength using critical indentation force and corresponding finite element indentation analysis: 455MPa

=> Determine critical scale thickness at which interfacial shear stress of 455MPa will be created during cooling





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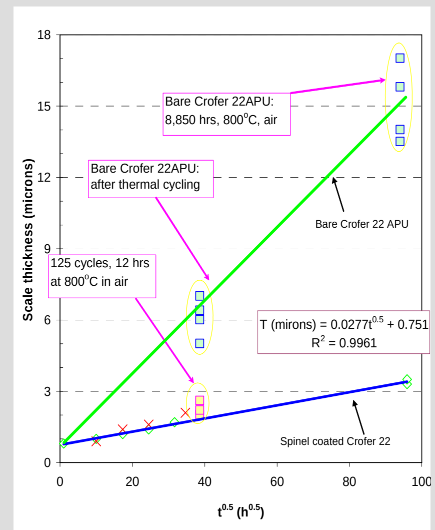
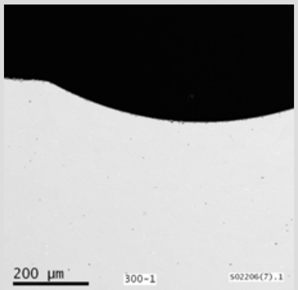
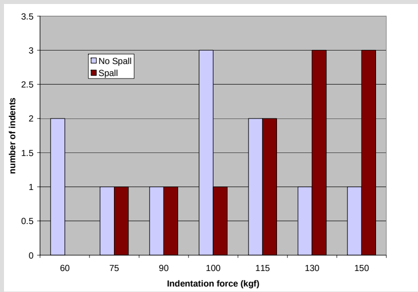


7570 hour <= Determine IC life using the scale growth kinetics results and the critical scale thickness for delamination <=

PNNL report - 16610

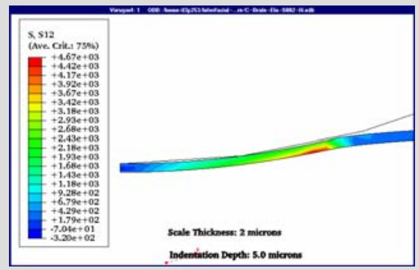
Accomplishment - Interfacial Strength Quantification for Uncoated SS441





1/8” Rockwell indentor

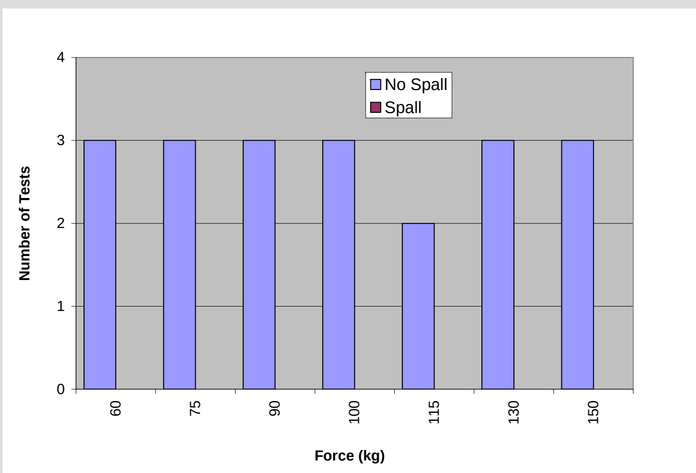
\+



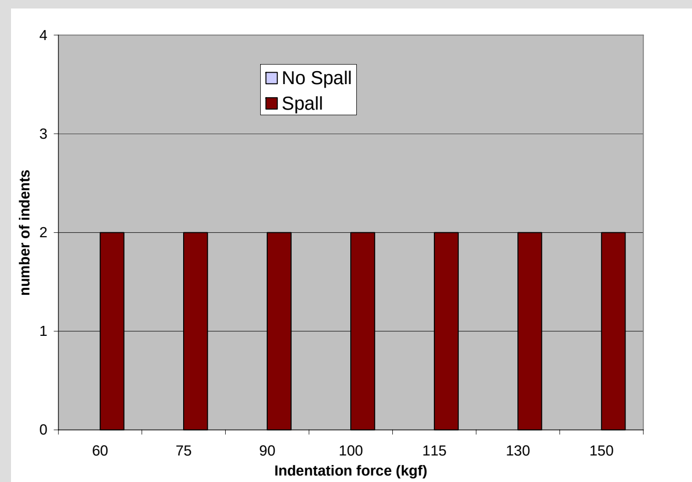
=> Oxide/SS441 interfacial strength: 344MPa

=> strength of oxide/Crofer22 interface > strength of oxide/SS441 interface

=> consistent with observations from experimental indentation tests



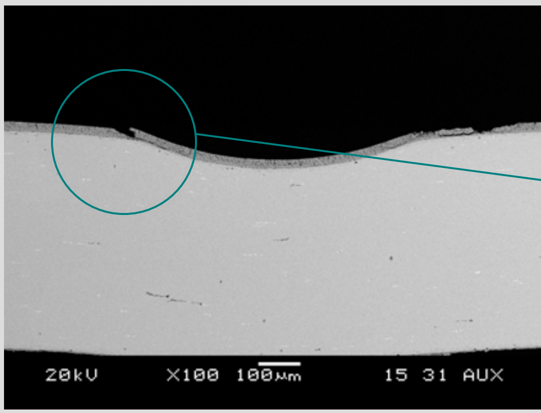
Crofer22: 1.5micron scale thickness, 1/16” indentor

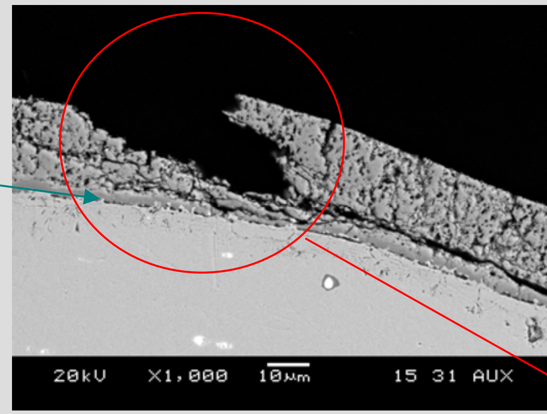


SS441: 1.13micron scale thickness, 1/16” indentor

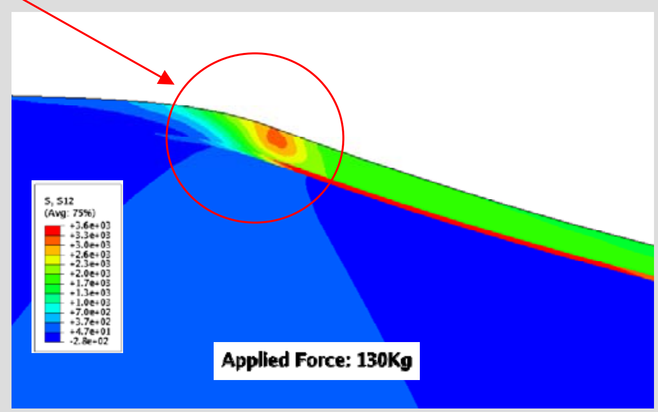
Accomplishment – Experimental Indentation Tests on Coated Crofer22 and SS441 Tri-layer Systems

Spinel-coated Crofer illustrating failure occurring at spinel/oxide interface. Failure load was 60kgf utilizing 1/16” ball indenter.

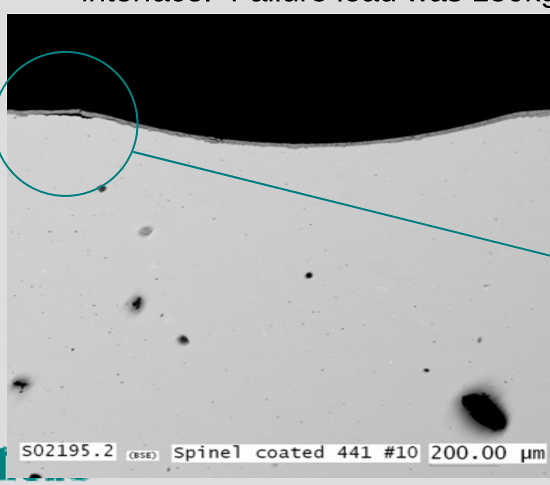


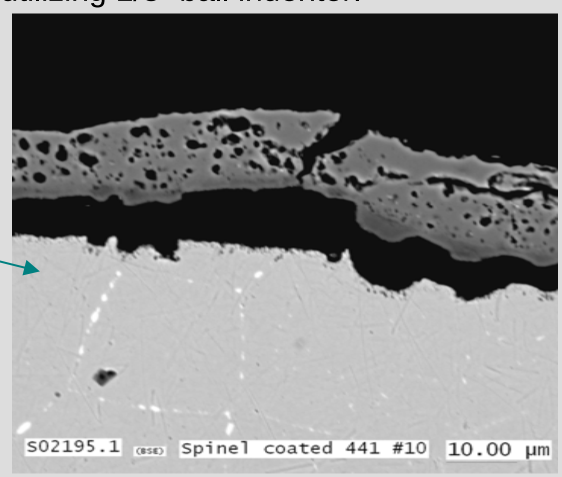


Shear-driven failure in the spinel coating has been observed during indentation tests. Consistent failure zone size and shape have been predicted by finite element indentation simulations.



Spinel-coated SS441 illustrating failure occurring at oxide/substrate interface. Failure load was 150kgf utilizing 1/8” ball indenter.





Current and Future Research Activities on Metallic Interconnect Modeling

- Current activities
  - Identify the weakest interface of spinel/oxide/Crofer22, validate with integrated analytical/experimental approach
  - Identify the weakest interface of spinel/oxide/SS441, validate with integrated analytical/experimental approach
  - Incorporate statistical nature of the interfacial into distribution of interfacial strength
- Future activities
  - Predict life for SS441 without spinel coating
  - Predict life for Crofer22 and SS441 with spinel coating
  - Optimize spinel coating thickness by considering growth stress, thermal stress and interfacial strength
  - Predict reliability of IC at different operating time based on interfacial strength distribution

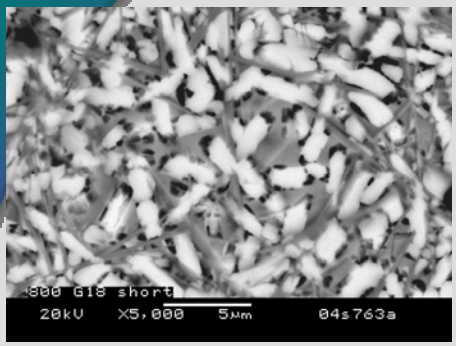
Seals

- Creep testing and initial creep model
- Improved creep model
- Thermal & mechanical property predictions

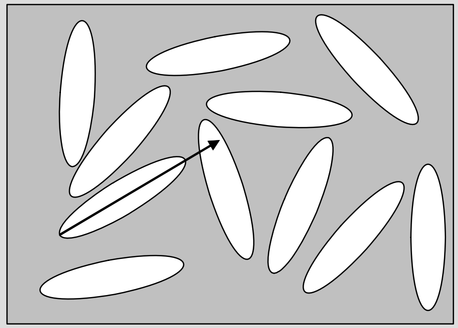
Seal Modeling and Design

- Objectives
  - Derivation of accurate constitutive relations for refractory glass-ceramic
  - Optimization of seal properties for desired stack performance
  - Design of processing methodology for seal material with desired properties
- Methodology
  - Experimental characterization: elastic properties, thermal properties and creep behavior
  - Micromechanical modeling and statistical homogenization
  - Correlation of microstructure to physical/mechanical properties and creep flow behavior
  - Validation

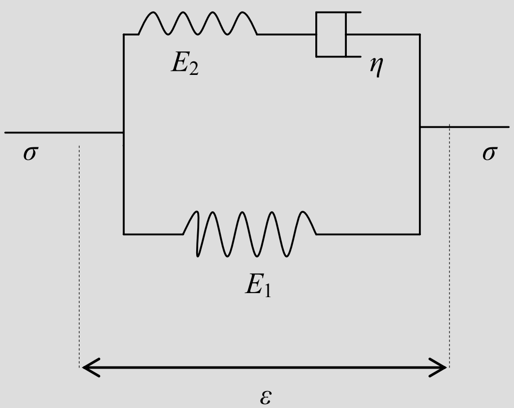
Accomplishment - A Homogenization Approach to Modeling of Glass-Ceramic Seals



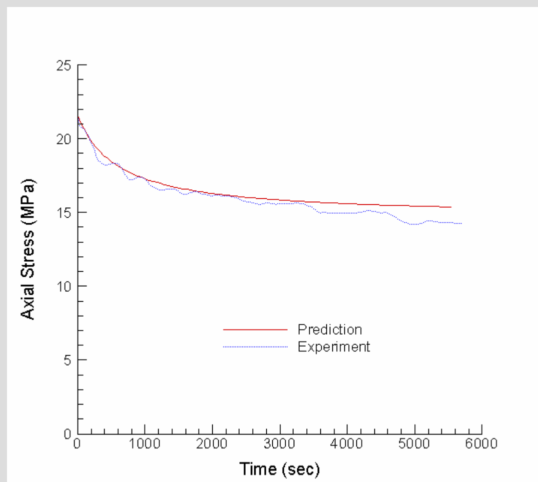
A microstructure of glass-ceramic considered in modeling



Orientation is depicted by means of orientation tensors



A rheological model for glass-ceramic: spring E1 represents the crystallites while spring E2 in series with dashpot η describes the viscoelastic behavior of the glassy phase



Relaxation response of a glass-ceramic seal for 0.5 % uniaxial applied strain at 700ºC

Assumptions

- *Elastic ceramic* crystallites and *viscoelastic glassy* phase
- Glassy matrix obeys Maxwell's model
- Ellipsoidal and 3-D random orientation crystallites
- Perfect crystallite/matrix interface

Approach

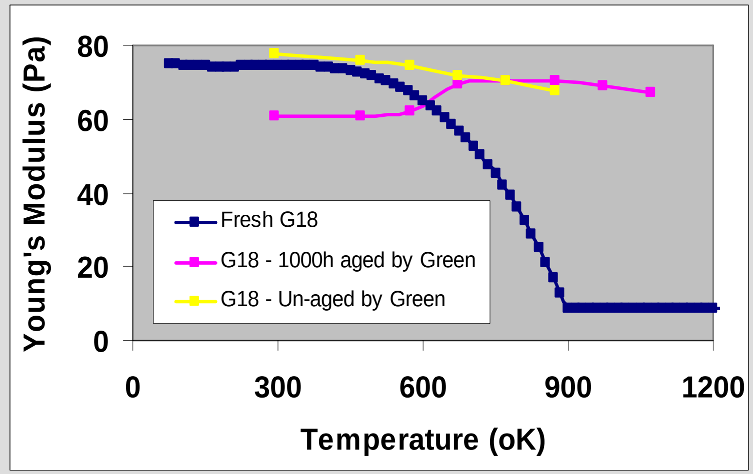
- An incremental homogenization method has been developed to model the viscoelastic response
- This is an incremental procedure that involves the computation of the instantaneous stiffness tensor of the glassy matrix
- Orientation of crystallites is accounted for using the orientation averaging technique developed for random fiber composites

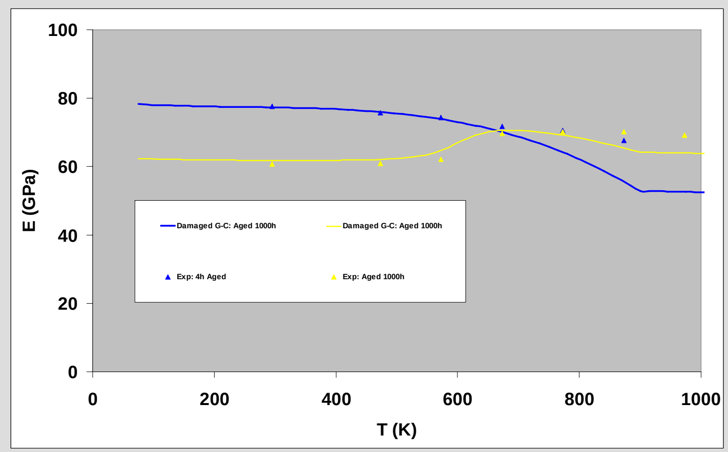
Accomplishment - Mechanical Property of Fresh and Aged G18 Glass/Ceramic

- Dynamic resonance technique (ASTM C1198) was used to measure the elastic moduli of G18

- Fresh Glass
  - Modulus dramatically drops when T is higher than Tg
- Aged Glass/Ceramic:
  - Presence of crystals
  - No Tg
  - Modulus varies slightly with temperature
  - Ageing induced micro-damage

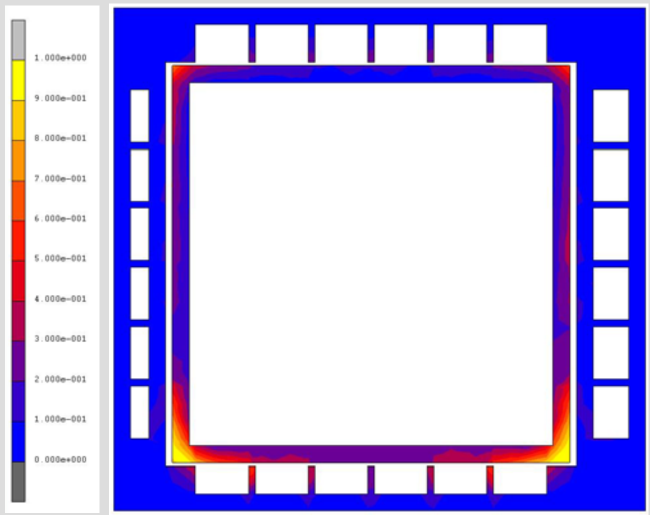
- Modeling using continuum damage mechanics

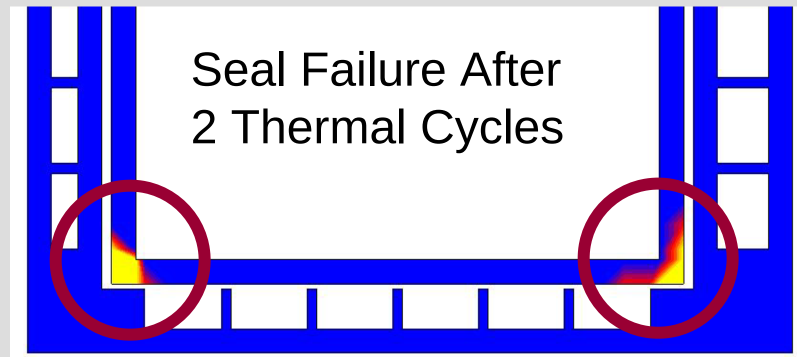




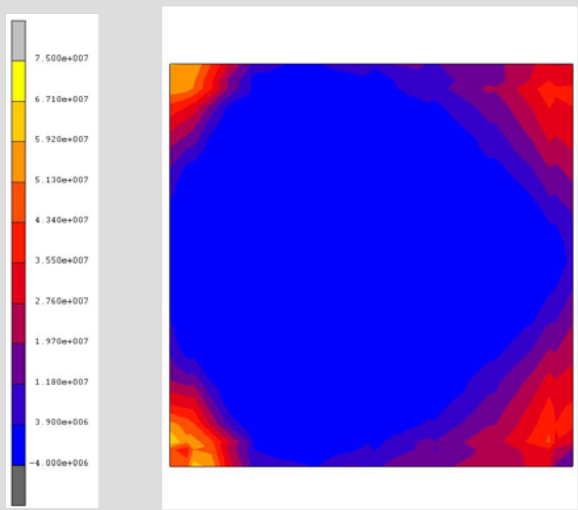
Seal Property & Time Dependent Behavior: Stack Modeling Results

Seal Damage Distribution





Anode Principal Stress Distribution



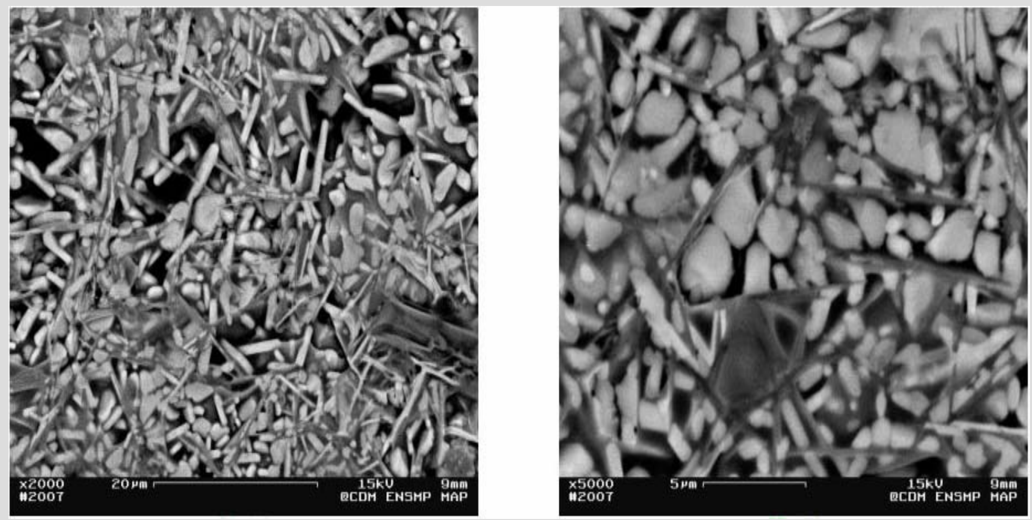
Temperature (C)	Elastic Model: Anode Maximum Principal Stress (MPa)	Viscoelastic Model: Anode Maximum Principal Stress (MPa)	Change
Cycle 1 Operation	38.4	36	6.3%
Cycle 1 Shut-Down	65.6	62.7	4.4%
Cycle 2 Operation	40.2	40	0.5%
Cycle 2 Shut-Down	74.4	67.4	9.4%

Accomplishment – Microstructure Characterization for G18

- Multi-phase microstructure of the glass-ceramic seal by SEM
- Preliminary nanoindentation test results

	Modulus, E_r (GPa)	Hardness, H (GPa)
Amorphous Matrix		
Sample 1	119.5996	7.989734
Sample 2	100.0175	7.984434
Sample 3	113.7207	7.727709
Sample 4	95.39279	7.897548
Sample 5	93.50994	7.883003

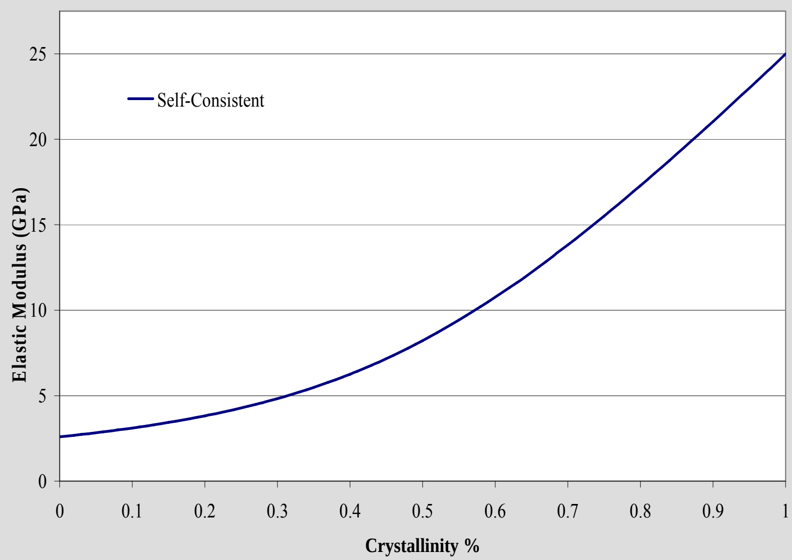
Room Temperature Nanoindentation results for G18 aged for 4 hours at 750°C.

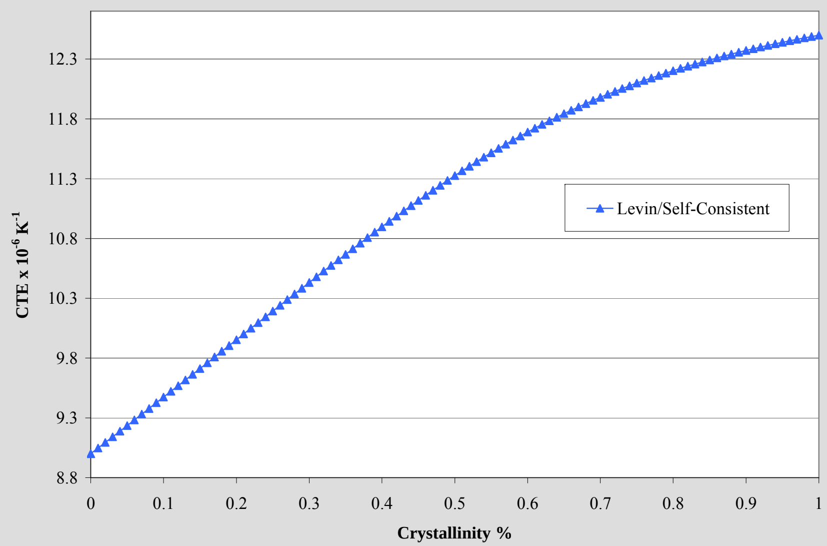


SEM backscatter images of G18 at different magnifications are shown. The white phases represent the barium silicate needles, while the dark phase is the amorphous matrix. The darker needles are hexacelsian

Current Activity – Seal Microstructure/Properties Relationship

- Case Study: modeling results for the effective elastic properties and CTEs for a glass-ceramic seal material with elastic moduli ratio Ec/Ea=10.





Properties at high temperature (500°C)

These results depict how the effective elastic moduli and CTE evolve with the microstructure (such as the volume fraction of the ceramic phase). The modeling accounts for the interaction between the phases

This type of analysis will be used to design the microstructure leading the desired properties.

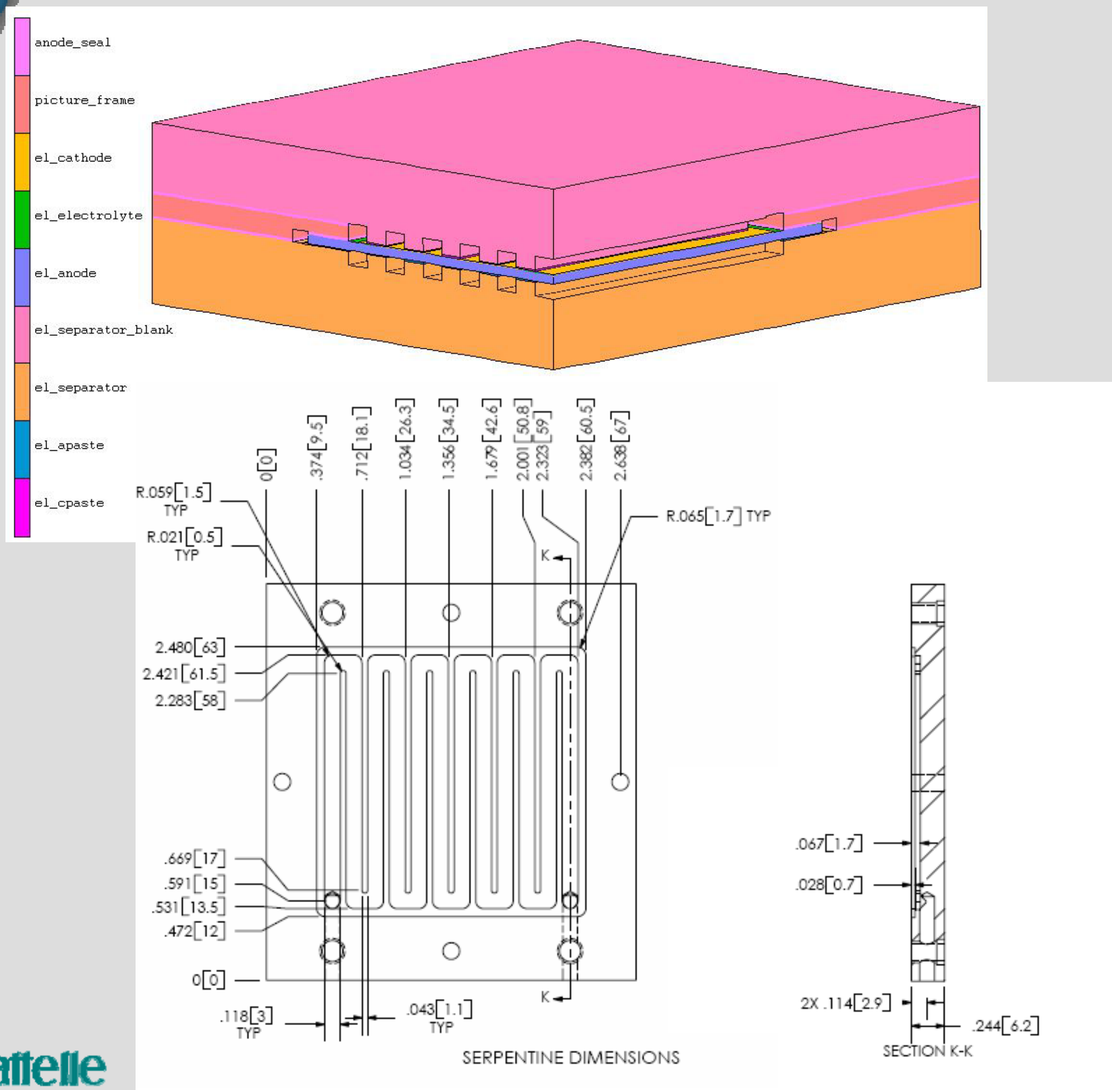
SECA Test Cell

- Thermal and structural modeling
- Design guidance

SECA Test Cell

- Objectives:
  - Examine proposed initial designs for test cell suitability
  - Long-term: Assist in design of next generation test cell
- Technical Approach:
  - Apply modeling tools to evaluate thermal and structural performance of designs
  - Predict the reliability of the proposed designs using elastic-plastic and creep behaviors of the materials
  - Examine influence of geometry, preload, and seal type
  - Evaluate the initial designs for structural performance and reliability

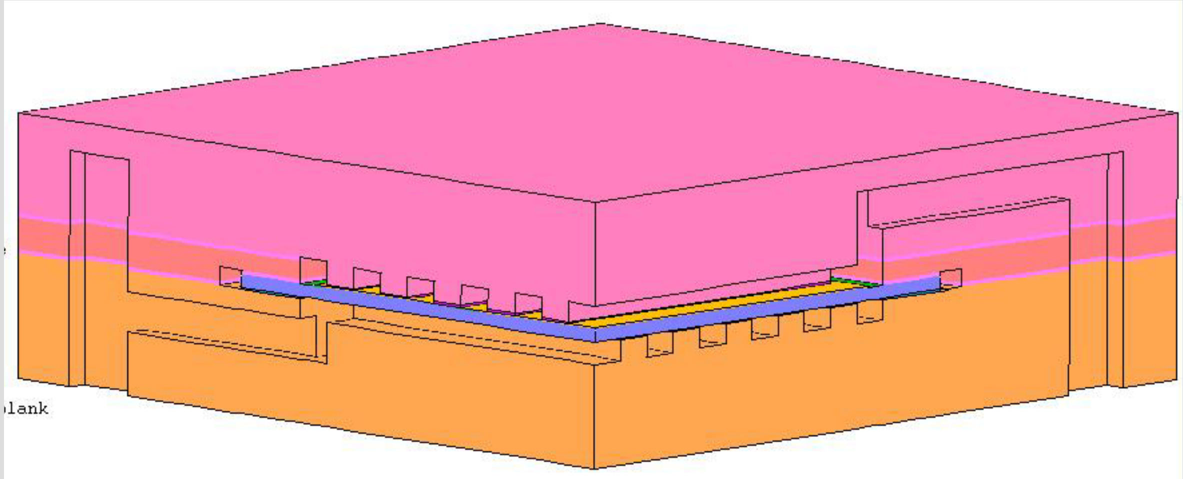
Baseline Test Cell Geometry

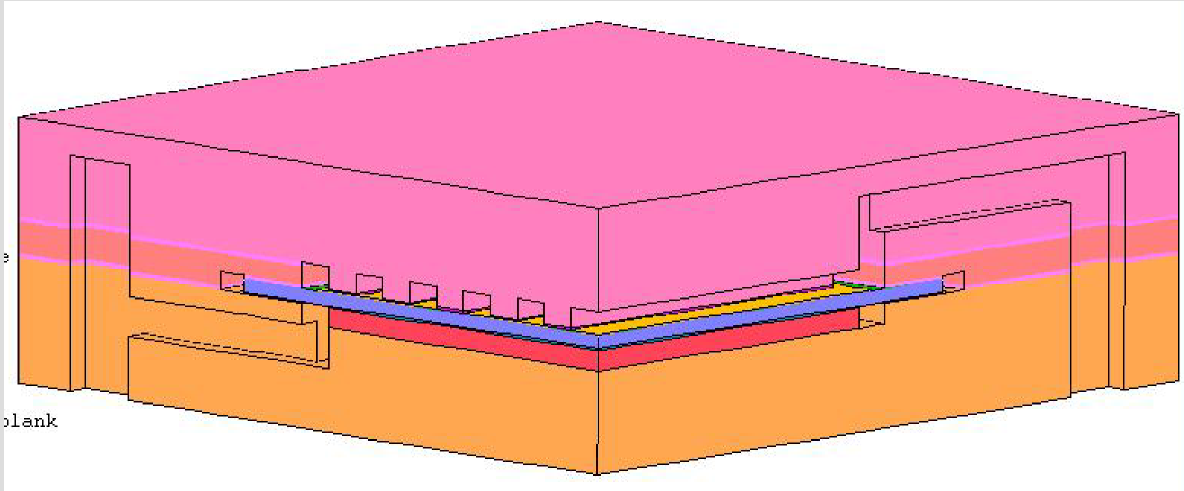


- Serpentine flow channels
- Thick plate construction with integral ribs
- Separator plate added to facilitate glass-ceramic seal fabrication

Alternate Test Cell Geometries

- Same general construction
- Cross-flow ribs
  - Improved pressure drop for large cells
- Hybrid design
  - Fuel: porous mesh
  - Oxidant: rib channels





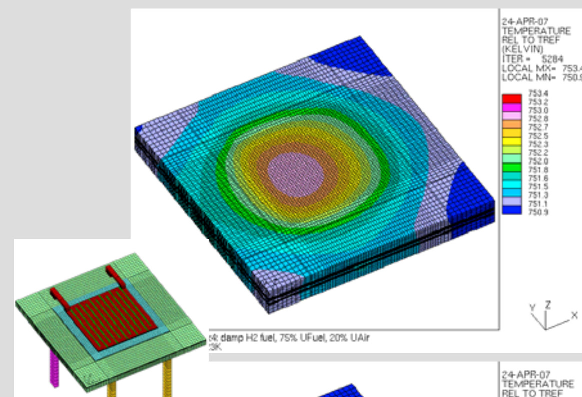
Test Cell Model Description

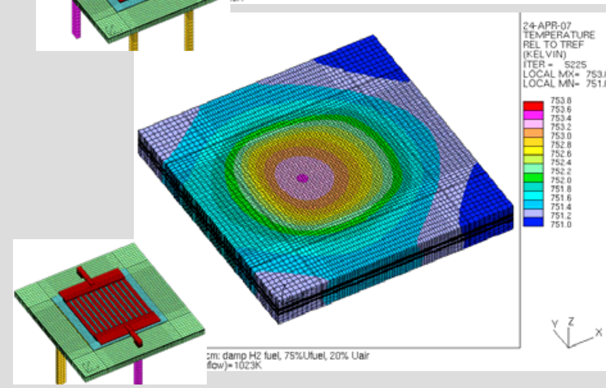
- Stack model
  - 1 cell model
  - Compressive preload
  - Operating and shutdown conditions
- Components
  - Interconnects: SS441
  - Picture frame: SS441
  - Seals: glass-ceramic
  - Anode contact paste: Ni
  - Cathode contact paste: LSM
  - Anode: Ni:8YSZ
  - Cathode: LSM
  - Electrolyte: 8YSZ
- Geometry
  - 50x50 mm cell with edge seal
  - 40x40 mm active area
  - 80x83 mm stack
  - 1.8 mm rib/channel width
  - 1.0 mm channel height
- MSC MARC FE code
- Evaluations
  - Effect of geometry
  - Effect of material models
  - Effect of preload
  - Effect of sealing temperature
  - Effect of sliding seal

Test Cell: Pressure Drop and Thermal-Electrochemical Analysis

- Pressure drop analysis showed:
  - Serpentine geometry cell had small ΔP (< 0.3 psi (10” H_2O)) for 4 cm test cells.
  - Cross-flow channel design had very small ΔP for 4 cm size, and could be used for up to a 30 cm cell with similar ΔP showing promise for use in next generation test cell (< 0.2 psi (6” H_2O)).
- Thermal analyses of both the serpentine and cross-flow design showed that the entire structure was nearly isothermal (within 5°C).
- Structural analysis was subsequently performed assuming isothermal conditions.

$$\Delta p = \frac{1}{2}\frac{fL}{D_h}\rho u^2$$





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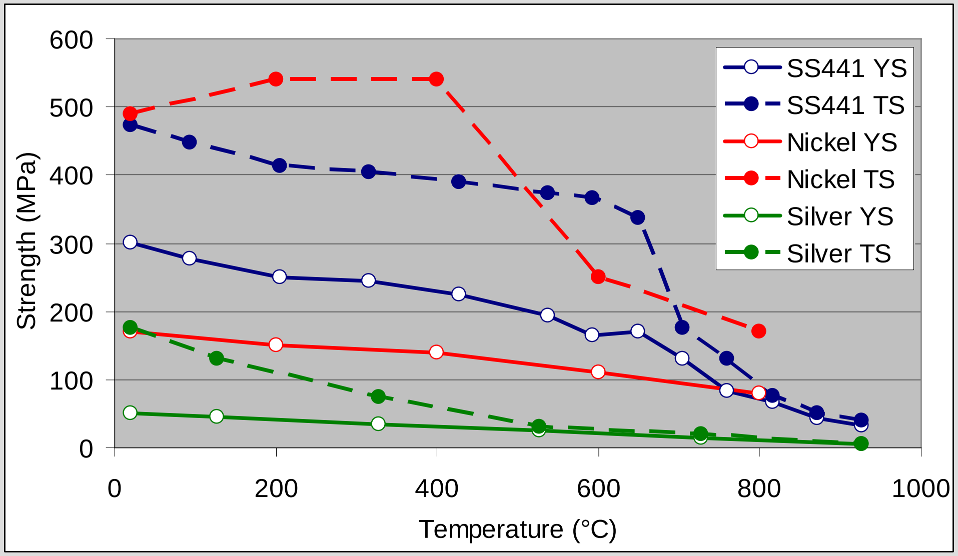
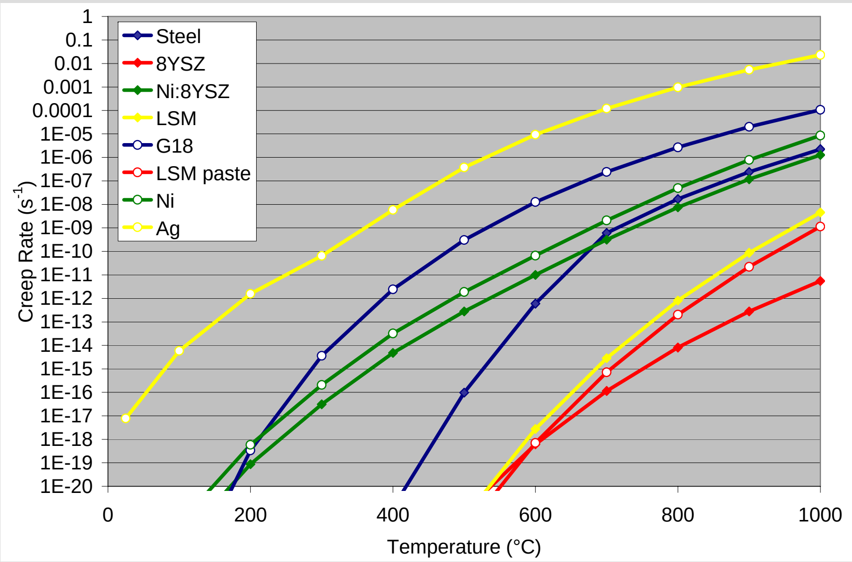
Test Cell Structural Analysis Material Properties

- Plasticity
  - SS441 interconnect
  - Ni anode contact paste
  - Bilinear stress-strain curve
- Creep
  - All materials
  - Experiment & literature data
  - Secondary creep only
  - Temperature & stress dependence included





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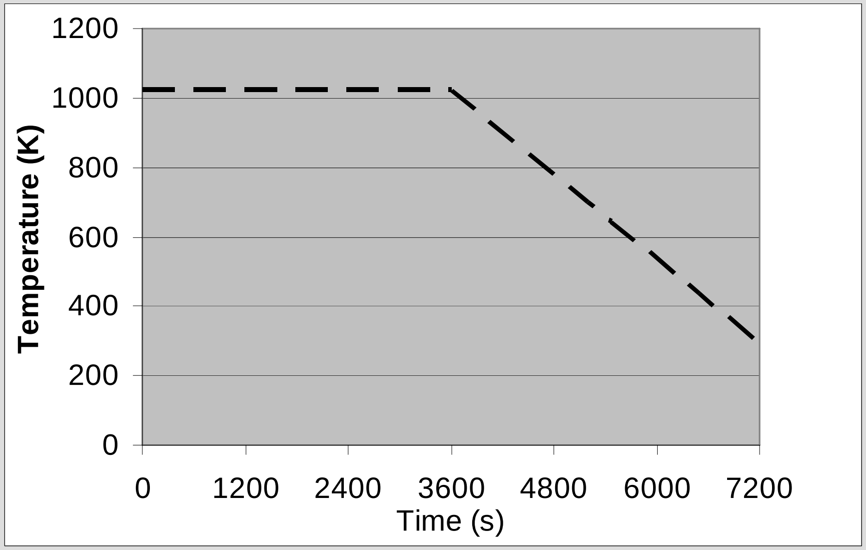
Test Cell Structural Analysis Loading

- Electrochemistry analyses showed less than 5°C variation across the stack for furnace operation
  - Use isothermal temperature loading for analysis
- Evaluate stresses at operation and shutdown
  - Begin at stress-free temperature 800°C
  - 1 hr operation 750°C
  - 1 hr uniform cooling to room temperature
- Assume stack has compressive preload applied uniformly to top
  - 0.2 MPa (~30 psi)
- Bottom of stack allowed to slide on rigid plane



Test Cell Structural Analysis Reliability Post-Processing

- Computed reliablity from Weibull data sources
  - ORNL: 8YSZ, Ni:8YSZ
  - PNNL: G18 bend bar
  - Literature: LSM
- Assumptions
  - 2 parameter Weibull model
  - Weakest link theory
  - Volumetric flaws
  - PIA model for multiaxial stresses

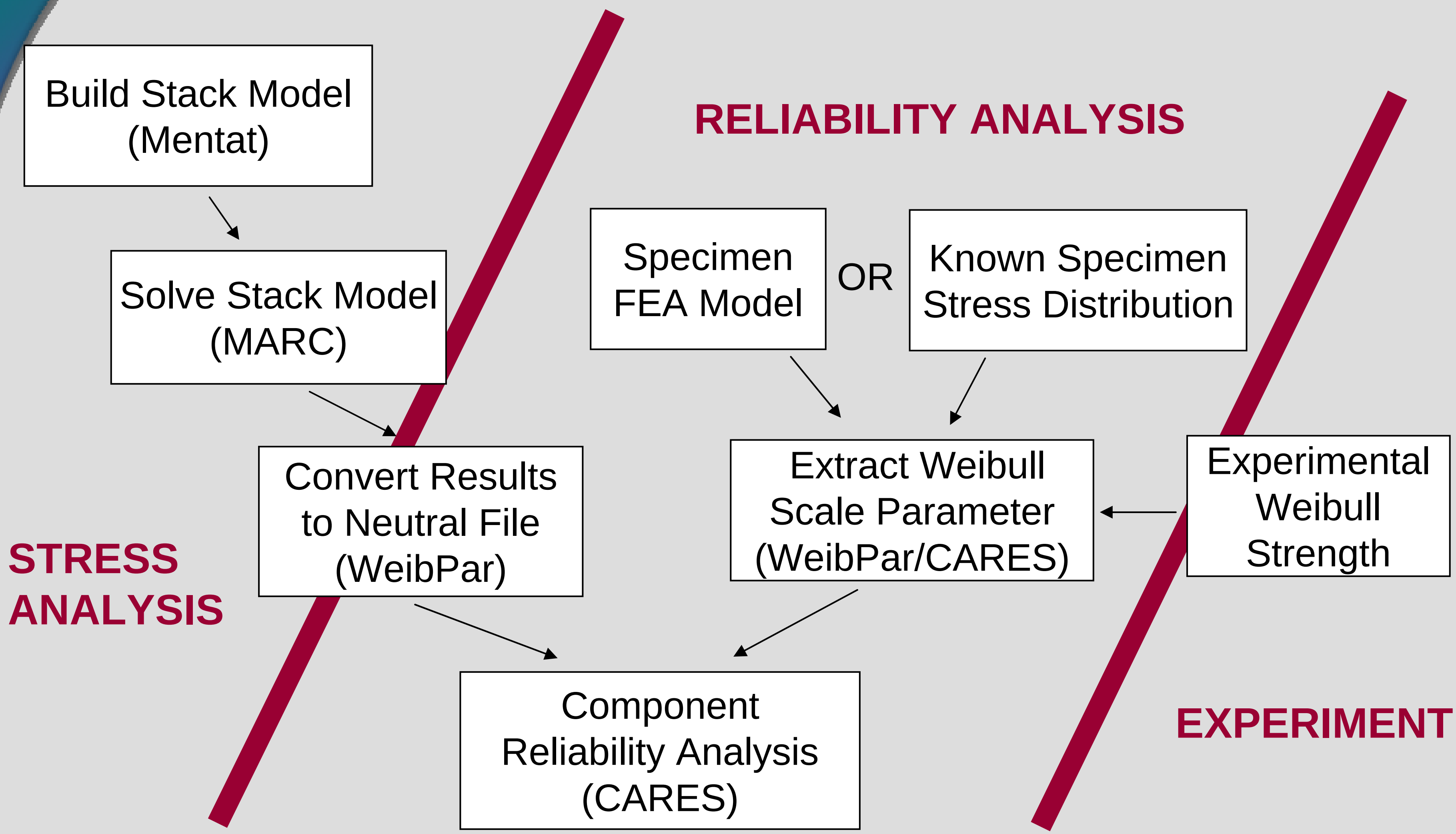
		RT	600C	800C
NiO:YSZ	σ_{oV}	6.16	6.08	11.68
	m_V	6.13	7.17	7.04
	σ_{oS}	22.64	22.00	42.68
	m_S	6.13	7.17	7.04
Ni:YSZ	σ_{oV}	1.16	3.03	11.61
	m_V	4.55	5.63	9.79
	σ_{oS}	11.46	21.68	36.71
	m_S	4.65	6.63	9.79
YSZ	σ_{oV}	2.16	8.92	2.96
	m_V	4.42	7.66	4.97
	σ_{oS}	26.06	26.32	31.27
	m_S	4.42	6.09	4.97

		RT	800C
LSM	σ_{oV}	0.30	0.61
	m_V	3.92	4.68
	σ_{oS}	11.16	6.18
	m_S	6.76	3.16

		25C	600C	700C	750C	800C
G18 4 hr	σ_{oV}	7.68	3.06	3.05	8.98	6.12
	m_V	7.49	6.22	6.73	10.61	9.61
	σ_{oS}	24.22	16.43	13.49	20.96	16.60
	m_S	7.49	6.22	6.73	10.61	9.61

$$\sigma_{oV}\left(MPa \cdot m^{3/m_V}\right) \quad \sigma_{oS}\left(MPa \cdot m^{2/m_S}\right)$$

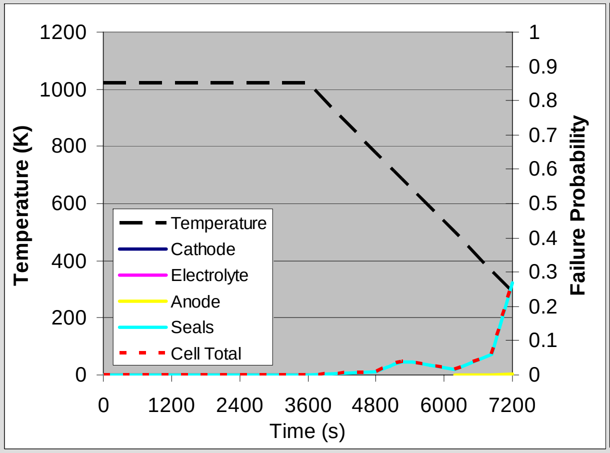
Test Cell Structural Analysis Solution Procedure



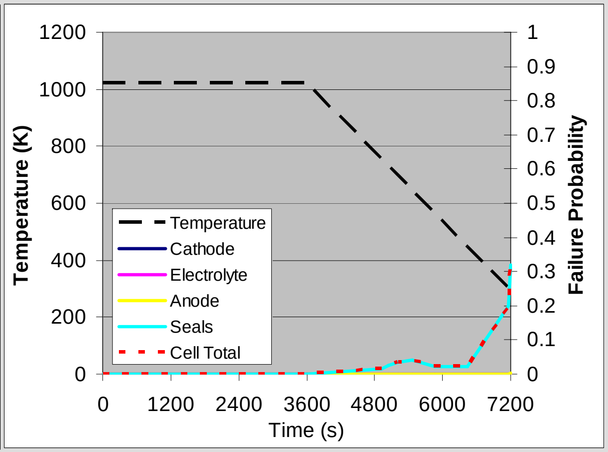
Test Cell Structural Analysis Results: Effect of Geometry

- Serpentine and cross-flow ribbed geometries similar results
  - Reliability good at operating temperature
  - Glass-ceramic seal failure rate of 27-32% at room temperature
  - Remaining components acceptable
- Anode mesh material with low stiffness presents challenges
  - High stresses in anode, cathode, and seals at shutdown
  - Bending of anode due to high preload and low stiffness of mesh
  - Choice of stiffer mesh material can address the challenges

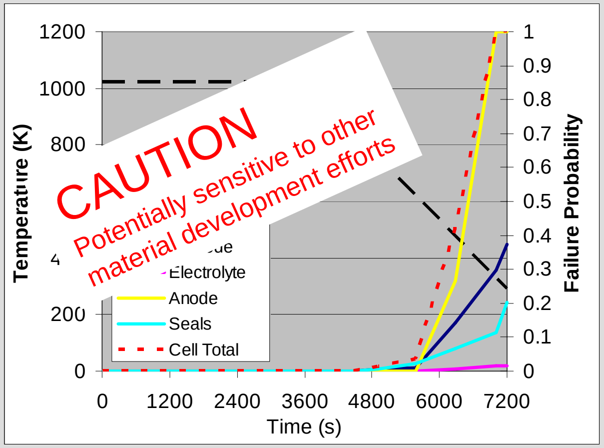
Serpentine



Cross-Flow

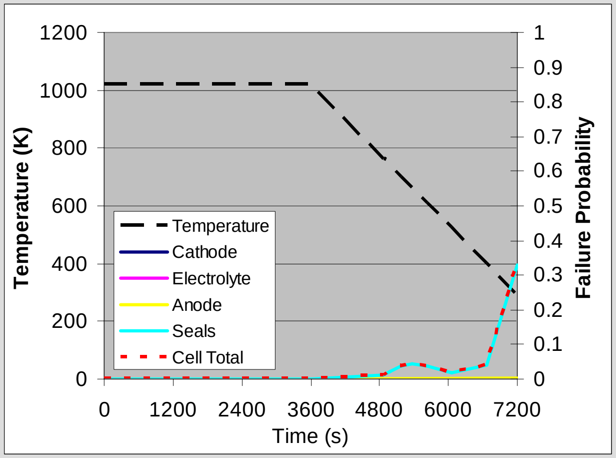


Anode Mesh

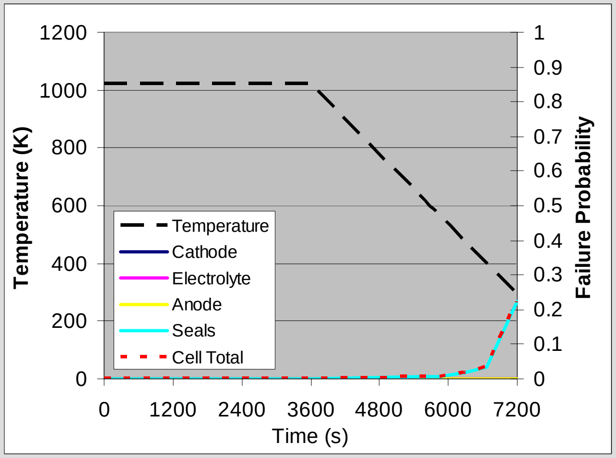


Test Cell Structural Analysis Results: Effect of Preload

- Stack preload had only small effect on reliability
  - Nominal value 0.2 MPa
  - Decrease to 0.083 MPa caused only minor increase in failure rate from 32% to 33%
  - Increase to 2.0 MPa caused moderate reduction in failure rate from 32% to 23%
- Effect of maldistribution of preload on stresses and contact will be of interest
- Initial test cell design fairly insensitive to preload



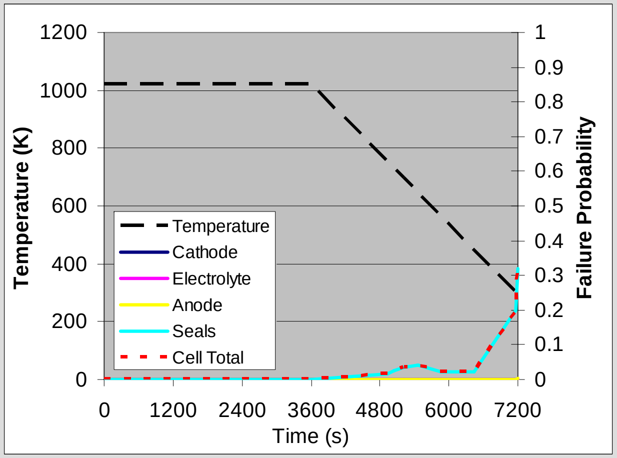
0.083 MPa



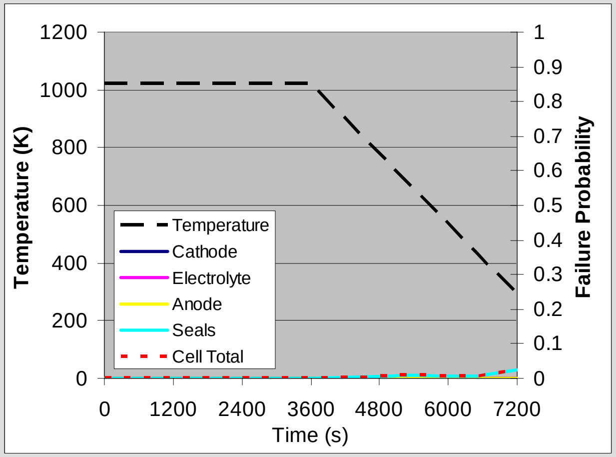
2.0 MPa

Test Cell Structural Analysis Results: Effect of Seal Technology

- Evaluated the influence of having a “sliding” seal surface in stack to mitigate thermal strain mismatches
  - Used same mechanical properties of glass-ceramic, and…
  - Allowed frictional contact between seal and interconnect with Coulomb friction coefficient of 0.1
  - Significantly reduced shutdown seal failure rate from 32% to 2.6%
- “Sliding” seal could benefit the test stack during shutdown



Rigid Seal



“Sliding” Seal

Test Cell Structural Analysis Summary

- Summary
  - Reliability predicted for proposed test cell designs
  - Stack elastic, plastic, and creep behaviors characterized
  - Influence of geometry, preload, and seal type characterized
- Conclusions
  - Reliability issues only on shutdown
  - Dual rib design good with only potential seal problem on shutdown
  - Sliding seal reduces shutdown stresses further
- Next Steps
  - Multi-cell effects
  - Cathode contact sintering stresses
  - Validation with experimental tests

Activities in Progress

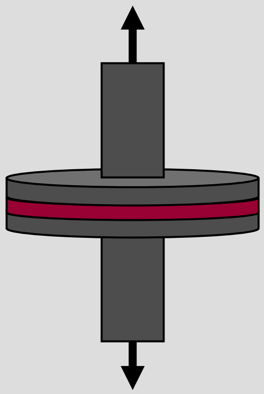
- **Improvements for the SOFC-MP modeling tool**
- **Cathode contact modeling and experiments to determine required strength (collaboration with ORNL)**
- Continued modeling support for test cell development
- Stack performance simulation considering creep of multiple components
- Scale-up modeling for prediction of thermal and electrochemical performance of large stacks
- Coated interconnect life prediction: Crofer and SS441
- Development of methodology for correlating seal microstructure to properties
- Sealant material creep testing

Proposed SOFC-MP Improvements

- Distributed resistance model w/ thermal property effects
- Interface with user-provided electrochemistry subroutine
- Post-processing of all species variables
- Symmetry plane capability
- Coal-based fuels capability
- Stack performance data summary
- Shell element capability
- Compressive preload
- Sliding contact surfaces

Cathode Contact

- Objectives:
  - Provide “target” contact layer strength to material development activities
  - Establish a predictive methodology for stack assembly stresses
  - Develop modeling and analysis tools (aided by material experiments to characterize constitutive and failure behaviors) to evaluate and improve durability of cathode-side mechanical interfaces
- Approach
  - Combined numerical and experimental approach to develop needed models and validate experimentally



Tension test schematic of coated IC/ceramic paste interface

Conclusions and Future Directions

- In the last year, the modeling tools had greater usage and additional capabilities to address durability issues have been developed. Future modeling activities will continue to focus on reliability, degradation, time-dependent response, and scale-up issues:
- Continue to add new capabilities to the modeling tools to meet the needs of the SECA program.
- Continue to increase the usage of the tools by the industry and academic teams.
- Continue to add improved material models and numerical procedures to the modeling tools for simulation of time-dependent response and reliability.
- Continue modeling to improve bond strengths of the oxide and protective coating layers for ferritic stainless steel interconnects.
- Evaluate thermal management needs, influence of high pressure electrochemistry, and reliability of seal/cell structures during cell scale-up

Conclusions and Future Directions … continued

- Continue to support development of a robust test cell design.
- Evaluate the mechanical requirements for successful fabrication using refractory glass sealants and low-temperature sintering of cathode contact materials for reliable interconnection during operation and shutdown.
- Continue to develop seal property predictions via homogenization methods to identify reliable composite seal structures and compositions for stacks.
- Develop analytical methods to evaluate the time-dependent mechanical behavior (creep, thermal fatigue, loss of interconnect contact) of fuel cell stacks/components and corresponding influence on electrochemical performance.

Development of ASME Design Guide for Reliable SOFC

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San Antonio, TX
August 9, 2007

Battelle

Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

R&D Objectives & Approach

- **<u>Objectives of the guidelines are to provide recommended</u>**:
  - Rules and practices for design of SOFCs stacks
  - Associated SOFC modeling and analyses procedures
- Guidelines may serve as a repository for state-of-the-art knowledge and experience gained in SOFC designs
- **<u>Technical approaches</u>**:
  - Documenting design and experimental practices following ASME past and similar experiences.
  - Providing technical basis by:
    - Quantifying the electro-chemistry activities and the associated thermal-mechanical behaviors of various SOFC design configurations
    - Quantifying the variability in material properties and design parameters of all elements in the SOFC structure
    - Evaluating the reliability of various SOFC components
    - Providing methodology for deriving possible design improvements

Status

- NETL Kick-off meeting
- Weekly/Bi-weekly teleconferences
  - PNNL, ORNL, and ASME participation
  - Using C&S Connect online repository
  - Hosted visit by technical consultant Rick Swayne's visit to PNNL
  - Developed document outline
  - Obtained consensus on the document outline
  - Assigned authorship for various sections
- Writing of document
  - Finished first draft version of the document on July 30, 2007
  - Sent to ASME external review committee for first round of review

Collaborations

- Internal collaborators:
  - Jeff Stevenson, Prabhakar Singh
  - Gary Yang
  - Matt Chou
  - Dave King
- External collaborators:
  - Rick Swayne - Reedy Engineering
  - Edgar Lara-Curzio - ORNL
  - Jim Ramirez, Raj Manchanda, Brandy Smith - ASME
  - Travis Shultz - NETL

SOFC Design Basis: Document Organization

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    - 5.1.3. Elastic Constants
    - 5.1.4. Strength – Tensile, Yield, and Shear
    - 5.1.5. Mechanics of Brittle Materials
    - 5.1.6. Elastic-Plastic Behavior
    - 5.1.7. High-temperature Creep Behavior
    - 5.1.8. Fatigue Behavior
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    - 5.1.10. Interfacial Properties
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  - 6.1. Thermal-Fluid-Electrochemical Solution
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    - 6.2.1. Load Cases
- 7.0 Initial Design Scoping Based on Required SOFC Power Output
  - 7.1. Design Philosophy
  - 7.2. Equations and Calculations

Contents of Chapter 8

Contents of Chapter 9

SOFC Design Basis: Next Steps

- Review written sections
  - Complete technical input for section components
  - Ensure technical accuracy and completeness
  - Obtain NETL content approval
- Final document assembly
  - Ensure content and flow sufficient to convey design basis
  - Assemble ancillary information (material properties, examples, references)
- Peer review