SAND2014-20513C

Brittle Materials Assurance Prediction Program ("BritMAPP")

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and
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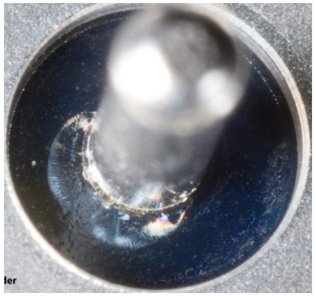
Predicting Performance Margins (PPM) Summit 3.0
Albuquerque, NM
December 8, 2014

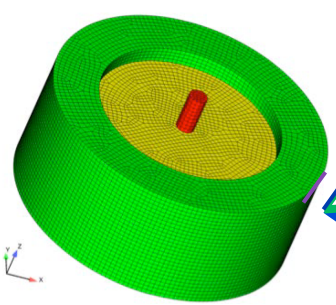
Exceptional service in the national interest

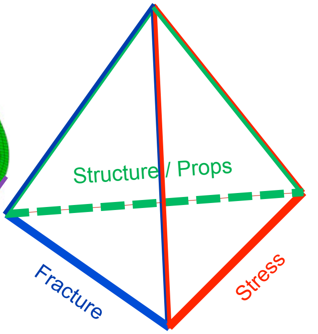
Sandia National Laboratories

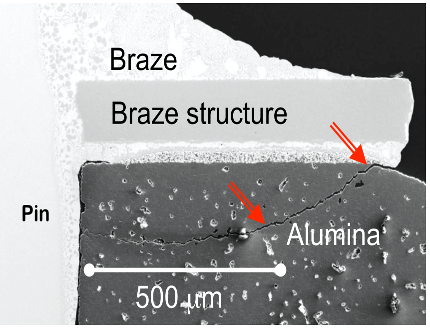
U.S. DEPARTMENT OF ENERGY

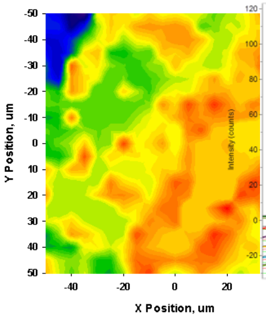
NNSA National Nuclear Security Administration

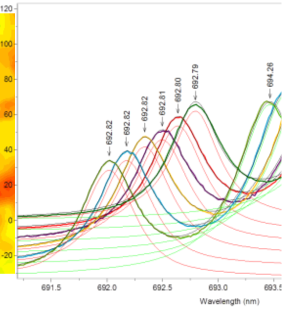












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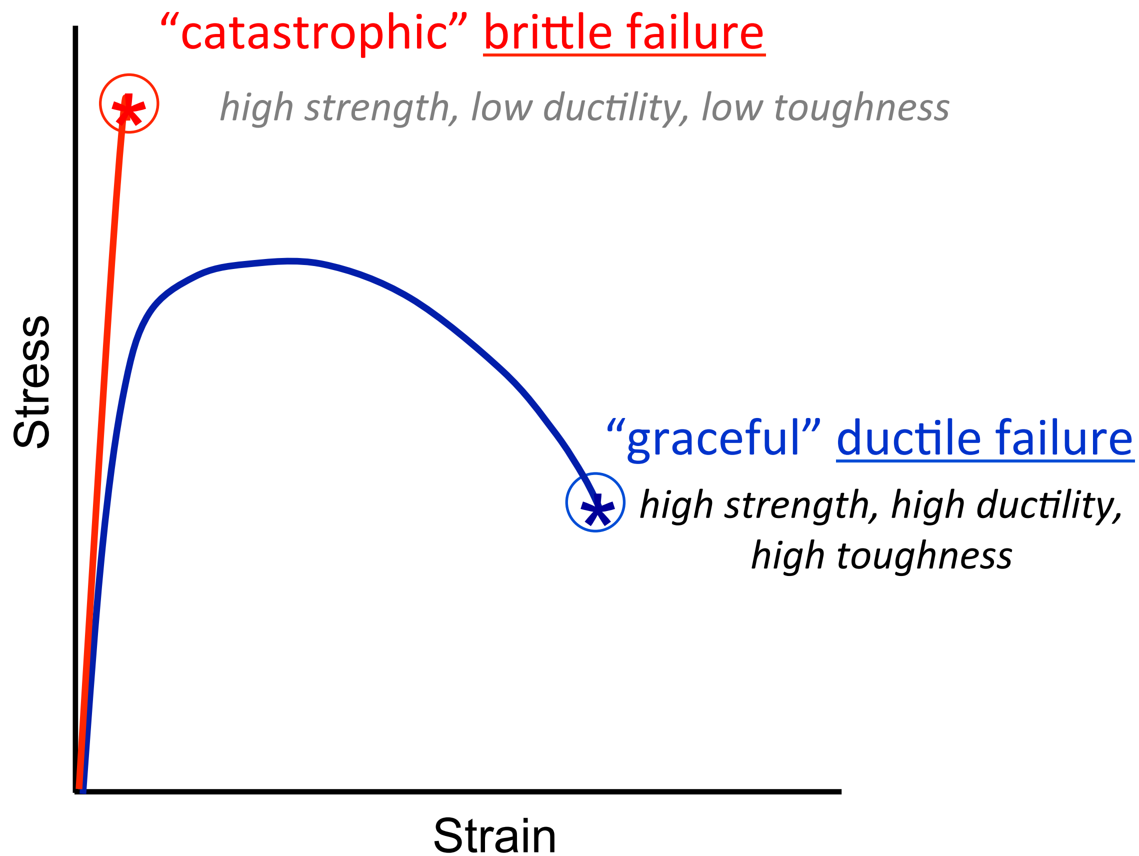
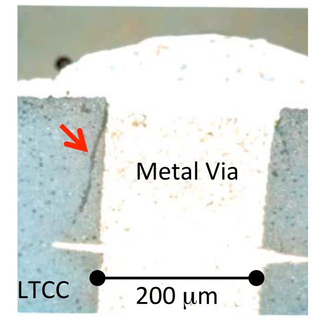
A Crack In A Brittle Material Is A Red Flag

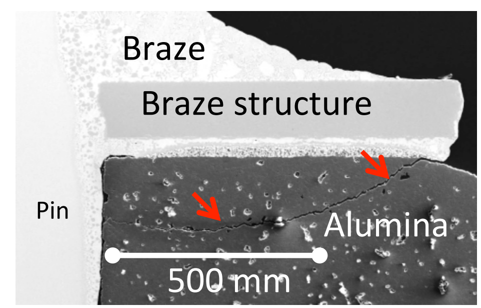
Ceramic Brittle Failure Is Distinctly Different From Metal Ductile Failure



Electronic Substrate



Electrical Feedthru

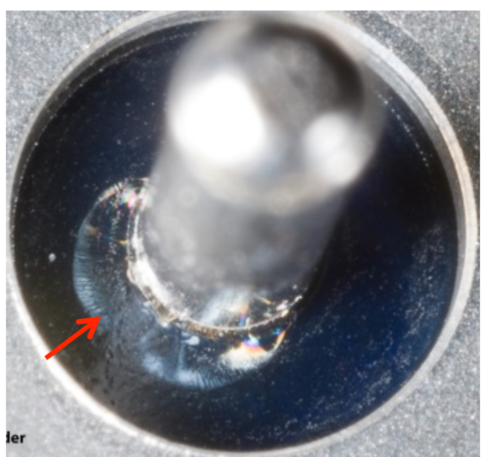


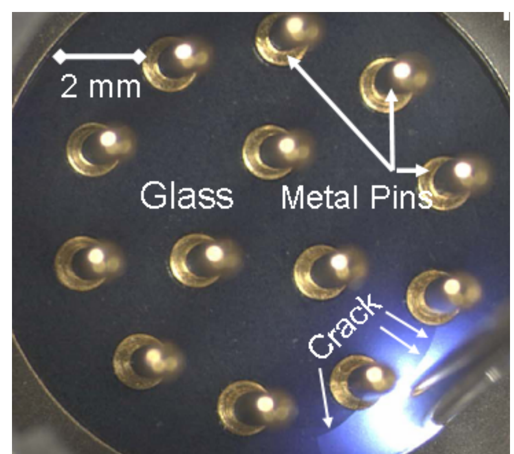
Brittle materials are susceptible to sudden catastrophic failure

Sandia's Interests & Capabilities To Predict Brittle Failure Align With The National Challenge

	Identified In 2012 NSF Workshop	Sandia National Laboratories
The Challenge	Brittle Failure Prediction Is A Ceramic Material Grand Challenge	Brittle Materials Performance & Reliability Are Critical To Mission Success
Critical Capabilities	3D Microstructure Characterization & Multi-Scale Modeling/ Simulation	Core Capabilities In Materials Characterization And Modeling/Simulation

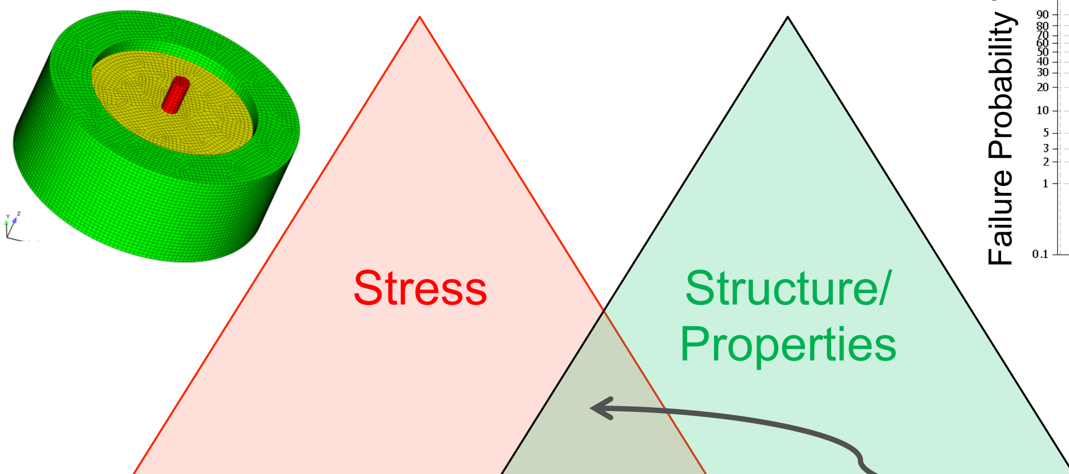
Glass-to-Metal Seals

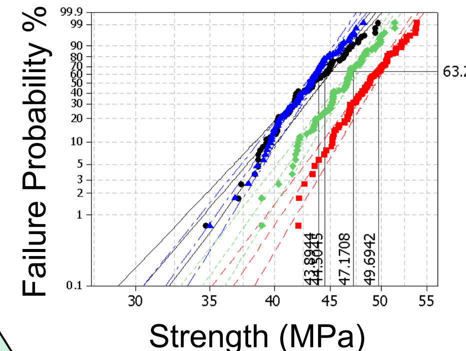




Current State: <u>Qualitative</u> Stress-Based Predictions (*We Design To Avoid High Stress*)

$$\sigma \sim \sigma_{crit}$$



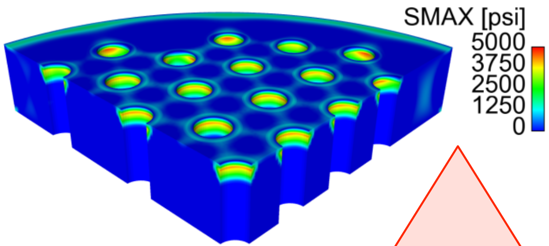


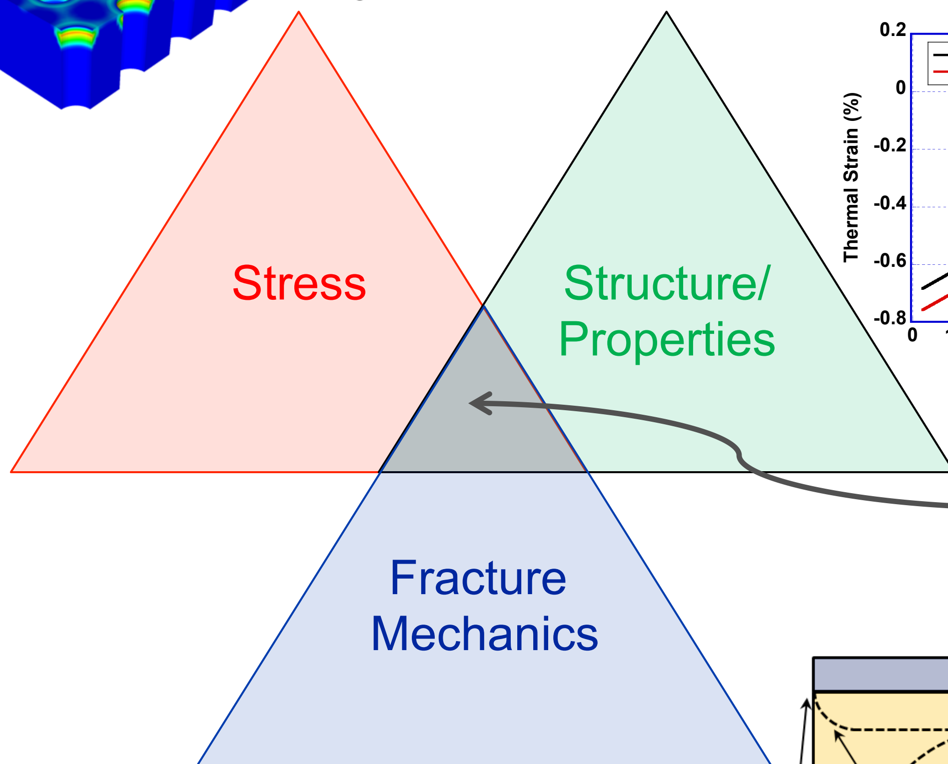
<u>Qualitative prediction</u> of brittle failure based on engineering judgment/experience

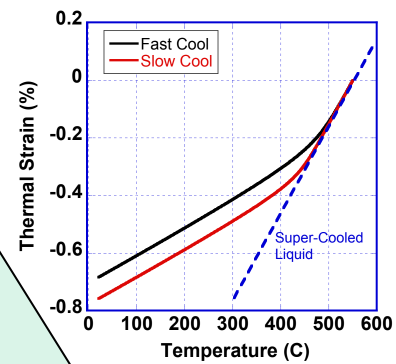
- A <u>qualitative</u> failure metric
  - "Insight" based on practical experience
- Engineering judgment has deficiencies
  - Neglects flaw populations, heterogeneities, & interfaces
  - Does not incorporate fracture mechanics
  - Ignores process history and handling effects

Future State: Quantitative Mechanics-Based Prediction of Brittle Failure & Reliability

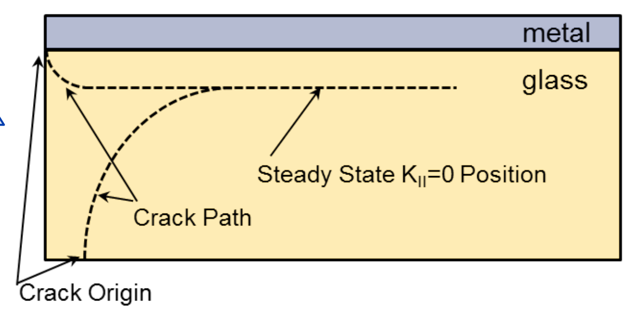
$$K \sim \sigma a^{1/2} \sim K_{IC}$$







Quantitative mechanics-based brittle failure prediction



Engineering & Materials Research Foundations Will Develop New Capability To Predict Brittle Failure

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- **Vision**
  - Transition from **Qualitative** stress-based engineering judgment to **Quantitative** mechanics-based failure prediction.
    - Create a science-basis for materials performance & lifetime reliability.

- **Goal**
  - Develop the capability to predict & control the performance & lifetime reliability of brittle materials in high-consequence applications.
    - Understand & control design, materials, and process variability & margins.

- **Approach**
  - Develop foundational materials characterization & modeling S&T comprising **stress/loading**, **fracture mechanics**, & **structure/properties** to quantify performance & reliability. *(the S&T "highway")*
    - Leverage & enhance SNL core capabilities in characterization & modeling.
  - Develop S&T enabled engineering solutions. *(the "off ramps")*
    - Materials qualification & specifications.
    - Crack acceptance criteria.

Coupled Experiment & Modeling Are Advancing Three Key Areas To Predict Brittle Failure & Reliability

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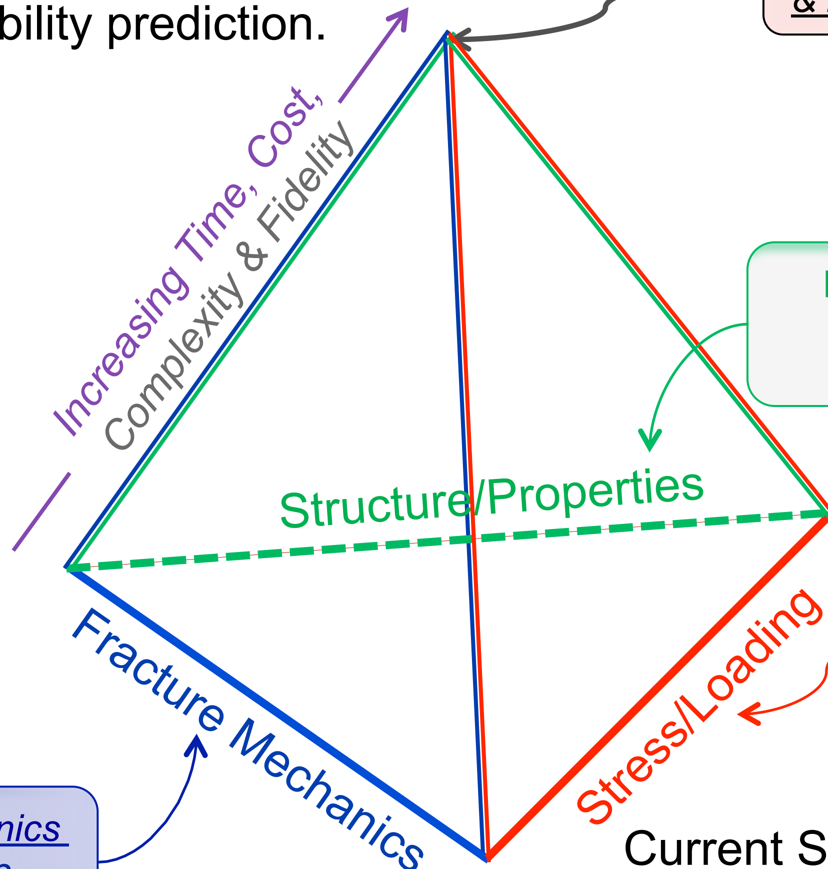
Future State (2020): **Quantitative** mechanics-based failure & reliability prediction.

Quantitative brittle failure & lifetime reliability prediction



Determine & model process-*structure-property* relations.

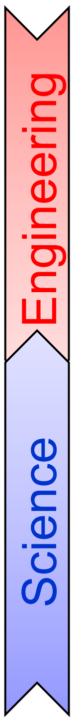
Stress determination considering materials, processing & *loading* history.

Fracture mechanics
Crack initiation, stability, & growth

Current State (2013): **Qualitative** stress-based failure analysis (i.e., engineering judgment).

Stress/Loading Tasks & Timeline Of Major S&T Advances To Address Key Engineering Questions

Short-Term, Fast Answer, Specific Application, Existing S&T



Slower Developing, Advanced S&T, Broad Application

0-3 Yrs

What affects the residual stress in my part? What is critical?

- *Incorporate design & physically-based materials behavior & variability into stress modeling.*
- *Determine the sensitivity of model input parameters & assumptions.*

Quantify design, materials behavior, and sensitivity in FE stress modeling.

1-5 Yrs

What is the residual stress in my part? Is it acceptable?

- *Develop new methodology to determine stress.*
- *Determine the effects of assembly, handling, testing, & use on residual stress.*
- *Couple analyses to better predict additive stress.*

Quantify stress prediction margins & uncertainty.

3-7 Yrs

How can I improve performance & reliability?

- *Determine the effects of processing & assembly on structure, properties & residual stress.*
- *Determine if & how micro structure & stress change with time.*

Quantify process-structure-property-stress relationships.

BritMAPP Goals Will Be Realized Via Integrated Advances In Fracture, Stress, & Structure/Properties

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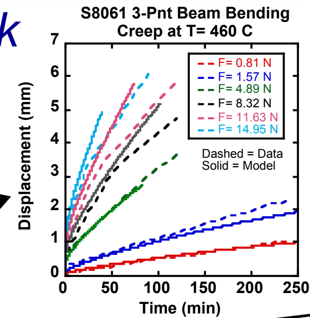
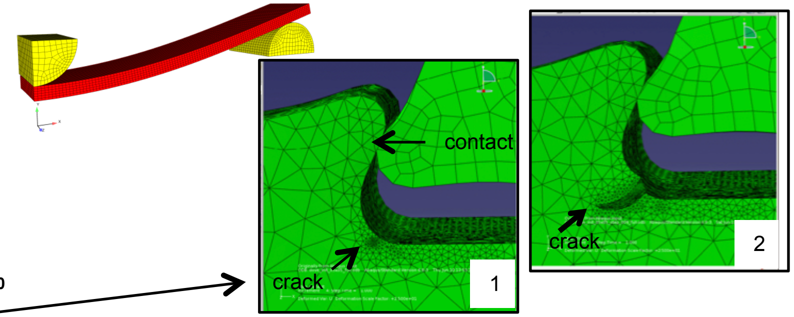
1. Understand and predict crack growth in brittle materials.

- Develop and validate improved constitutive property models to better predict residual stress.
- Develop and verify FE-based modeling for crack propagation.
- Identify, implement, & validate a fracture criterion.





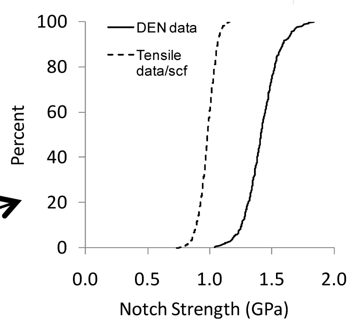
Cooled SS/borosilicate beams generate crack growth

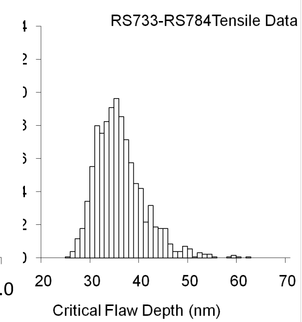
Initial crack 5 mm below interface

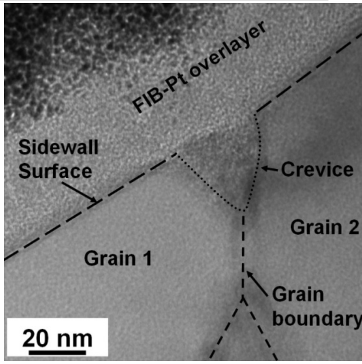
Initial crack normal to bottom edge

2. Understand and predict strength variability in brittle materials.

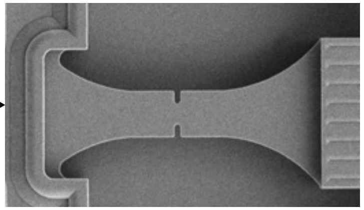
- Strength/variability depends on:
  - ✧ Flaw size/distribution (depends on processing, forming, handling)
  - ✧ Toughness and toughening mechanisms (depends on scale; meso/micro/nano-structure)
  - ✧ Stress (depends on material properties/behavior, component geometry and extrinsic loading)







Plane	K_{IC} (MPa-m$^{1/2}$)	source
(111)	0.82±0.07	Chen
(110)	0.90±0.11 0.91±0.09	Chen Yasutake
(100)	0.95±0.05 0.95±0.10	Chen Yasutake



SUMMiT V^{TM} polycrystalline silicon

Technical Work

Focus Area: Stress/Loading

Enabling S&T:

Stress Determination (Modeling & Characterization)

Property/Behavior Characterization

Engineering Applications:

Glass-Ceramic and Glass-to-Metal (GC/GtM) Seals

Brazed Alumina Connectors

S&T Advances Are Required To Quantify Uncertainty & Margins For Brittle Failure in GtM Seals

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FE Stress Modeling for Glass-to-Metal (GtM) Seals

Routinely used
Newly Implemented
Missing/Incomplete

viscoelastic glass

shell plasticity $s_y(T)$, $E_H(T)$

material property data

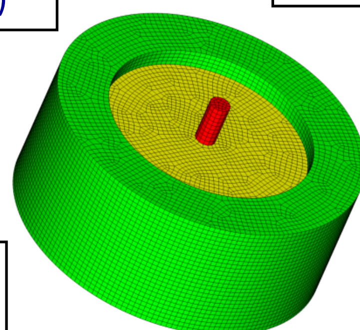
interface mechanics bonding, friction, properties, voids, inhomogeneity

elastic glass perhaps E(T)

pin plasticity $s_y(T)$, $E_H(T)$

structural relaxation glass strain history

bonded interfaces



CTE prescribed $e_{th}(T)$

viscoelastic solidification

surface wetting glass meniscus

idealized geometry

assumed stress-free temperature, T_{set}

crack initiation

thermal history

neglect processing history (spatially uniform temps)

estimate crack initiation rule of thumb ~ 5 ksi

experimental validation

crack propagation

coupled thermal-mechanical analysis, T(<u>x</u>, t)

next level assembly weld distortion, heating

linear elastic fracture mechanics

Metal Constitutive Behavior Is Being Characterized And Modeled To Support FE Stress Modeling

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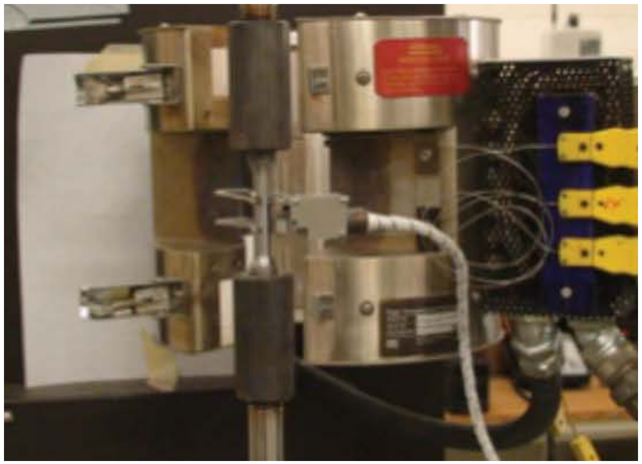
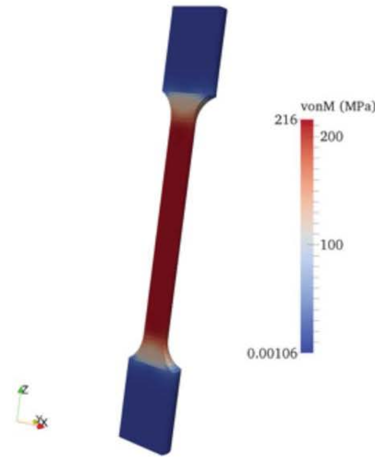
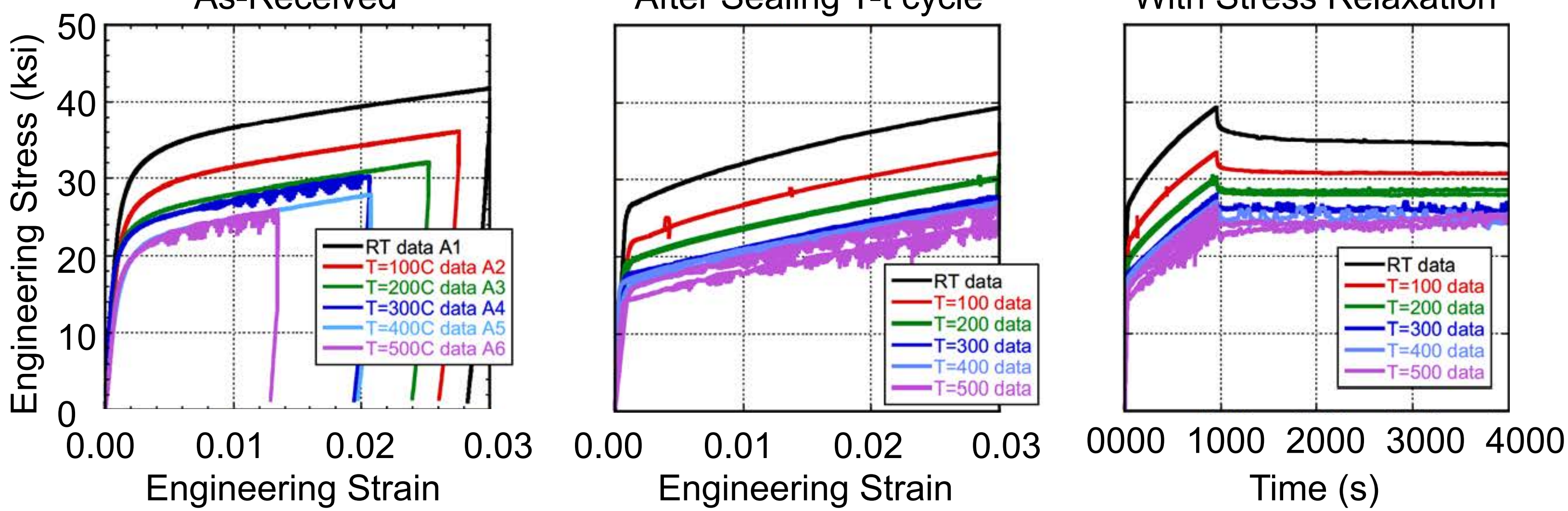
Elevated Temperature Small Strain Measurements





FE Stress Model
of 300°C Tensile Test

Stainless Steel Tensile Tests @ 3x10^{-5} Strain Rate



Glass Constitutive Behavior Is Being Characterized And Modeled To Support FE Stress Modeling

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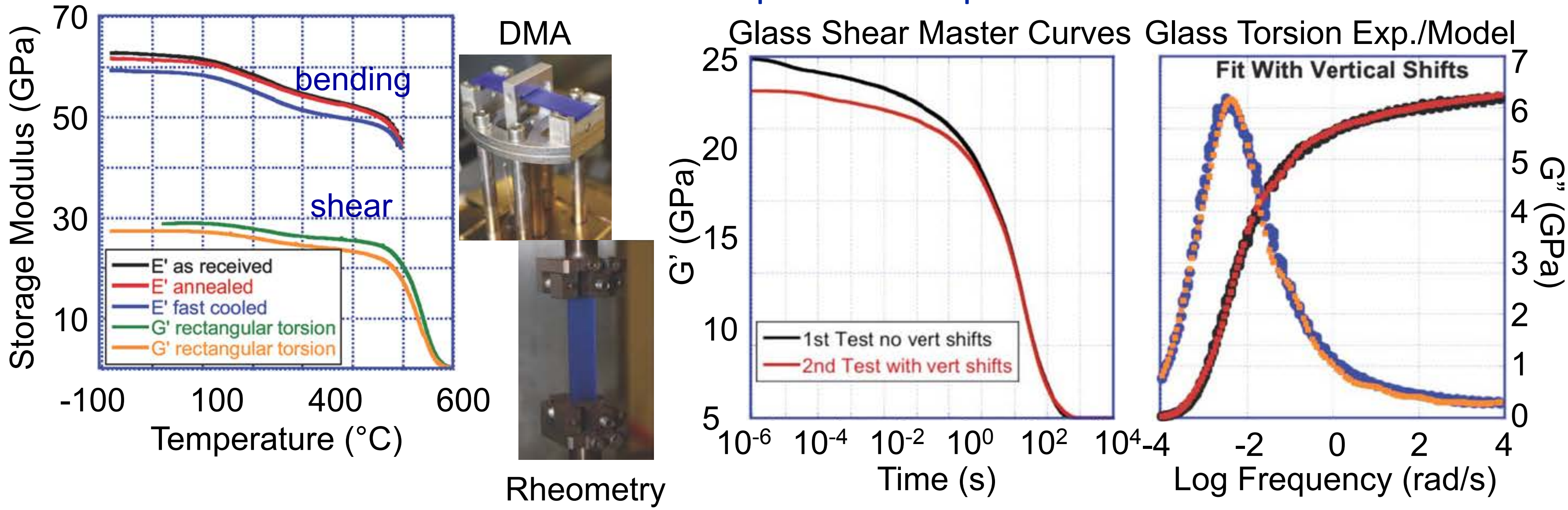
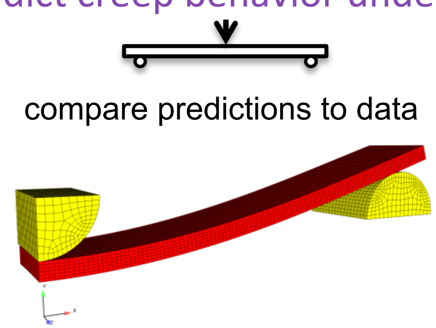
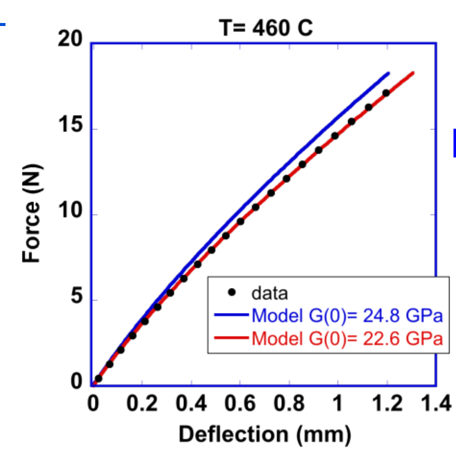
Stress Relaxation & Temperature Dependent Moduli



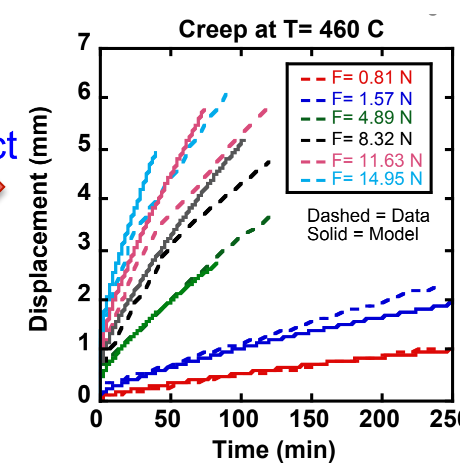
3-Point Bending @ Ref. Temperature

- Calibrate viscoelastic model
- Predict creep behavior under loads



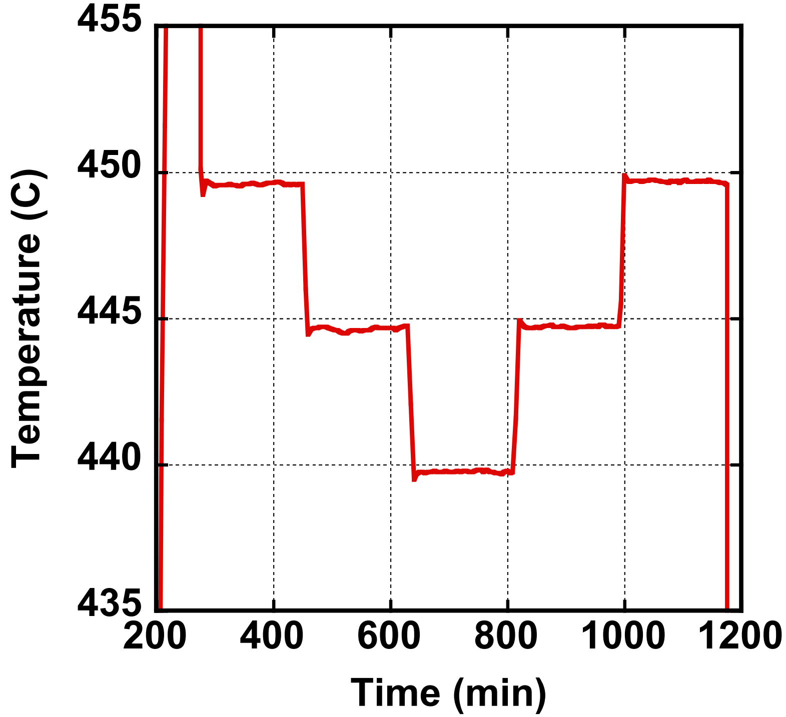


predict

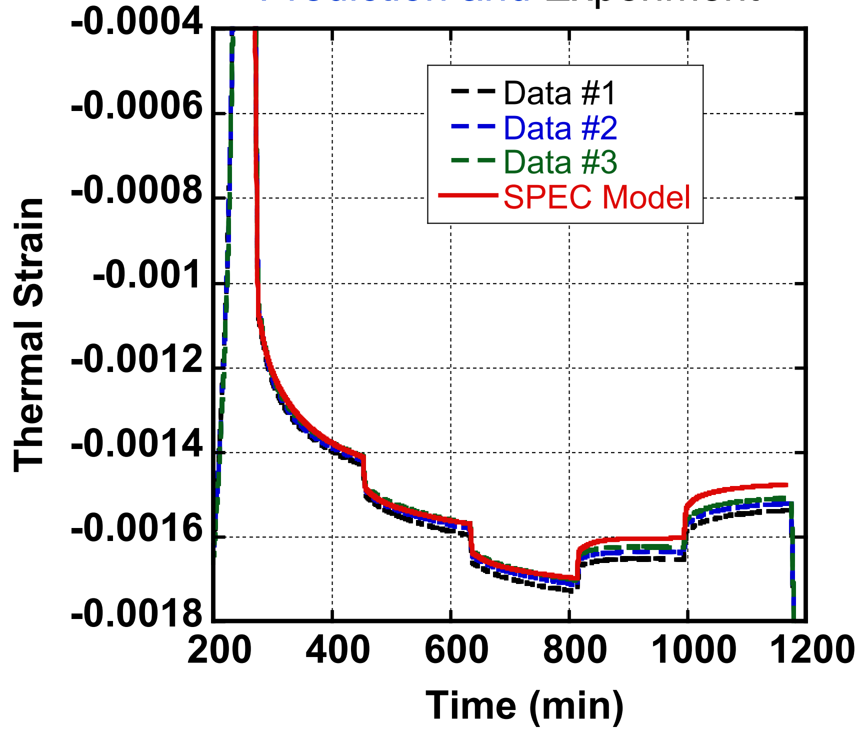


SPEC Viscoelastic Model Predictions Of Strain Are Consistent With Experimental Measurements

Step Temperature Experiment



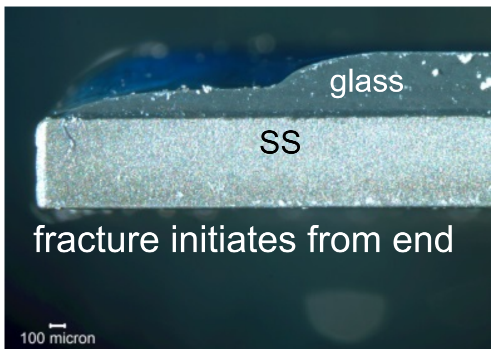
Comparison of Model Prediction and Experiment

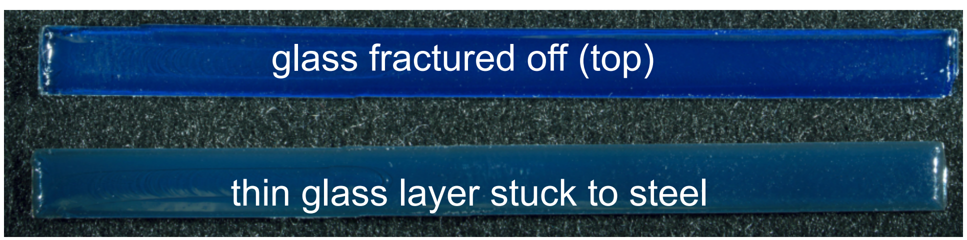


Stress & Fracture In Model Bi-Material GtM Seals Are Being Characterized To Test/Refine Modeling

Bi-Material Beams

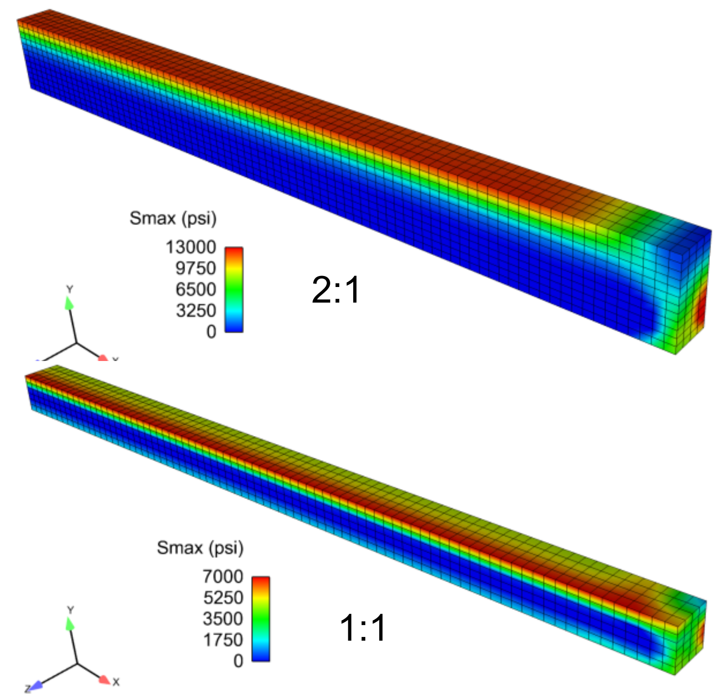
- Bond glass to stainless steel (SS)
- Measure beam curvature on cooling
- Compare measured deflection to predictions



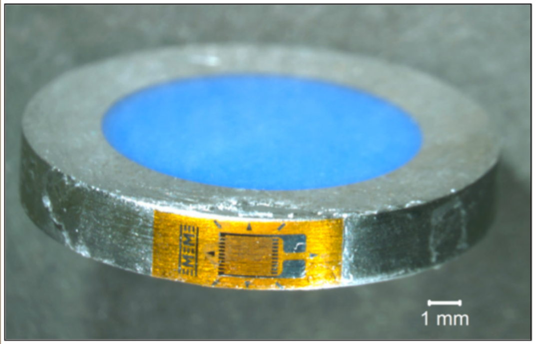


**Simulations explain cracking observed with a 2:1 ratio glass:metal thickness - recommends a 1:1 ratio.

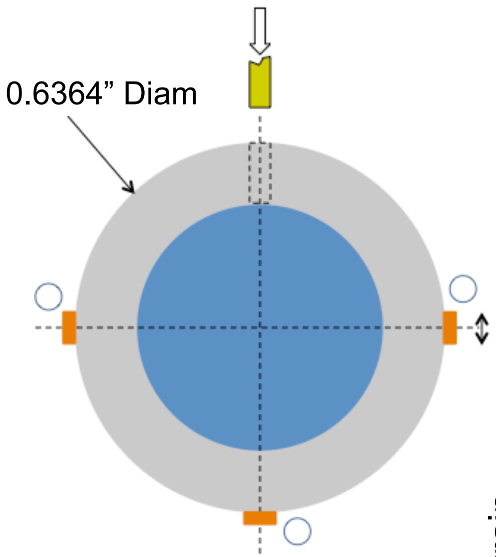
Residual Stress Predictions



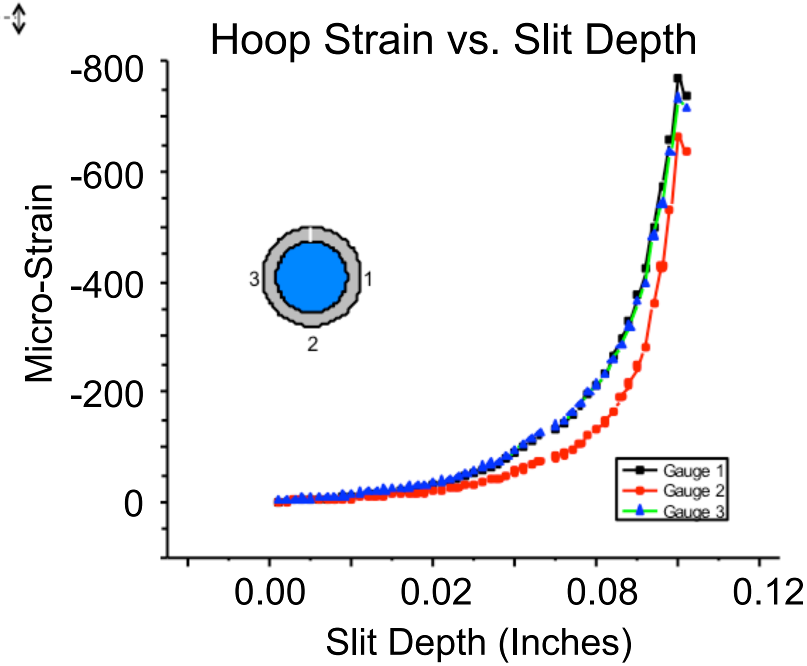
Model Stress/Strain Experiments Provide Insight Into Design Sensitivity And Changes With Machining



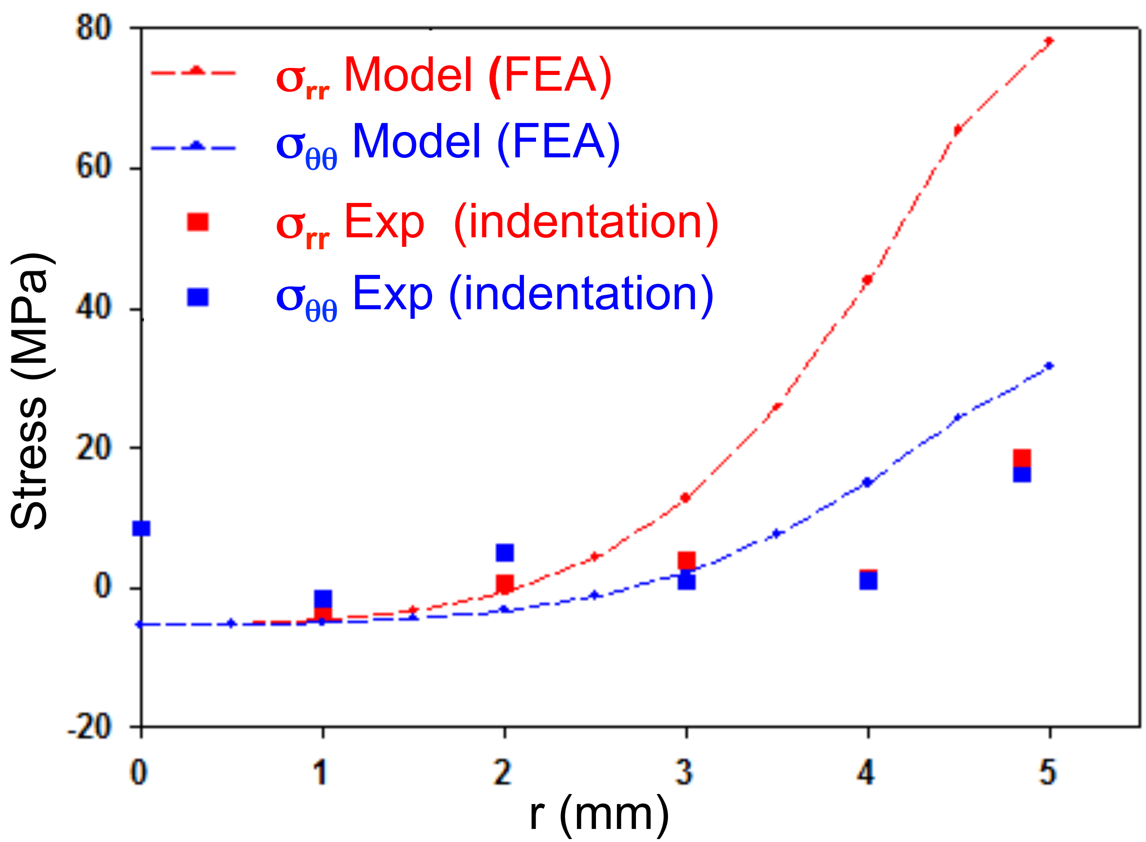
Concentric GTM seal with strain gauges on shell

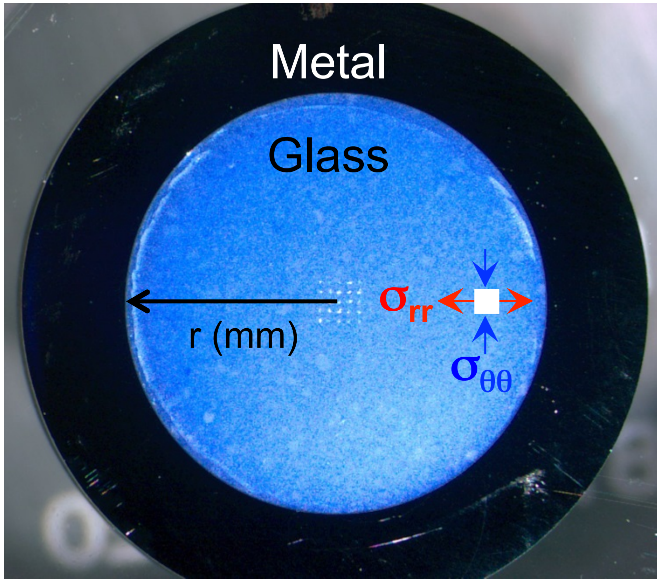


Cut through shell & measure change in strain



Coupled Experiments & Modeling Enable Better Stress Determination





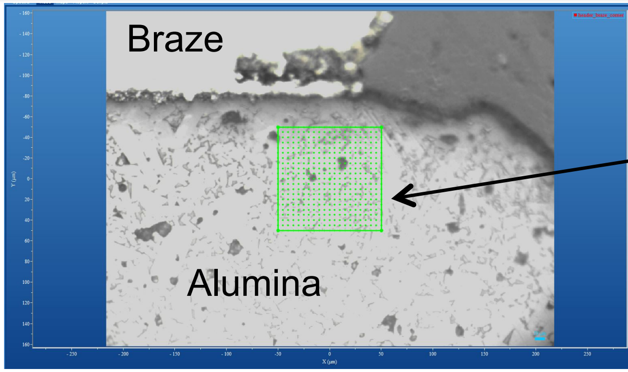
Experimental assumptions

- do not measure stress directly
- complicated gradients & tensorial nature of stress

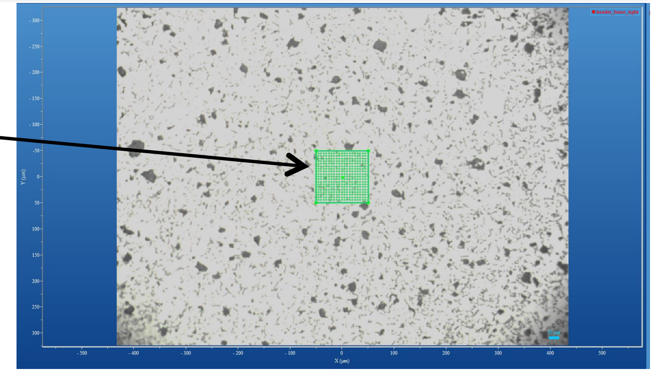
Modeling assumptions

- idealized geometry
- Ideal/bulk material behavior
- processing (e.g. uniform temperature)

Raman Spectroscopy Is Being Developed To Determine Residual Stress Across Length Scales

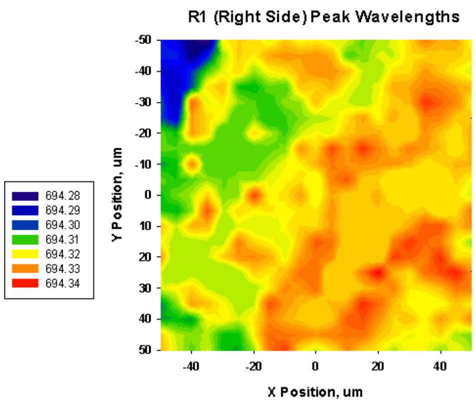


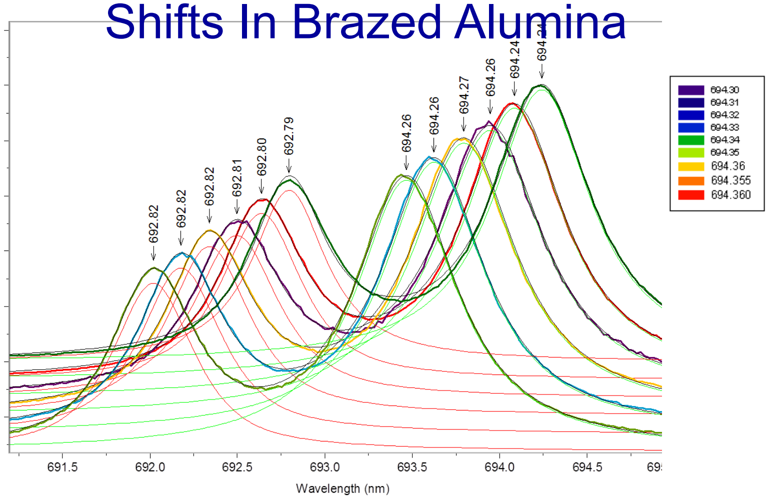
Analysis Area
(1 μm spots)

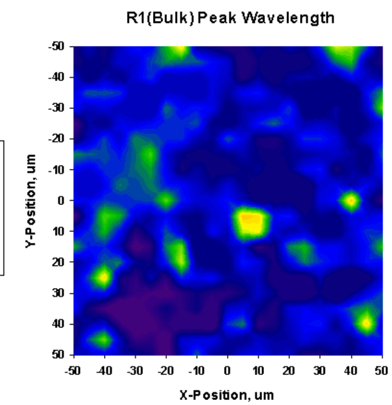


Raman Cr^{+3} Fluorescence Spectra Shifts In Brazed Alumina

Stress increase

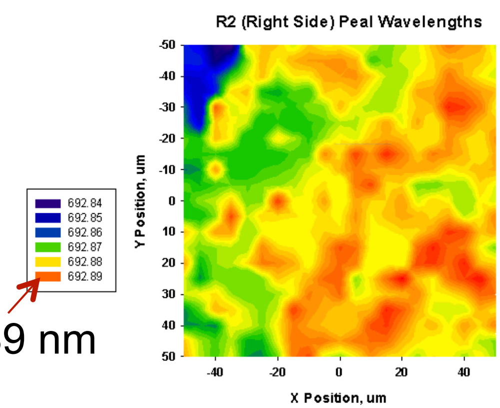




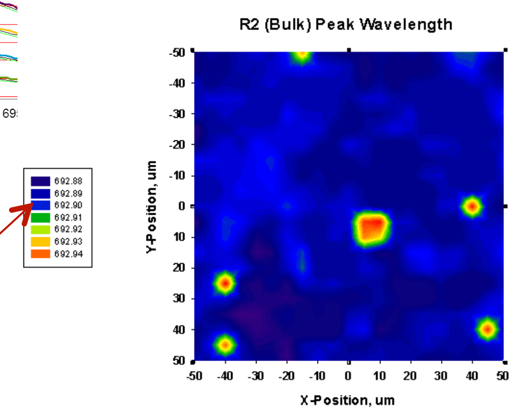


trace of stress tensor ~400 MPa
1 micron resolution

692.90 nm



692.89 nm



Technical Work

Focus Area: Stress/Loading

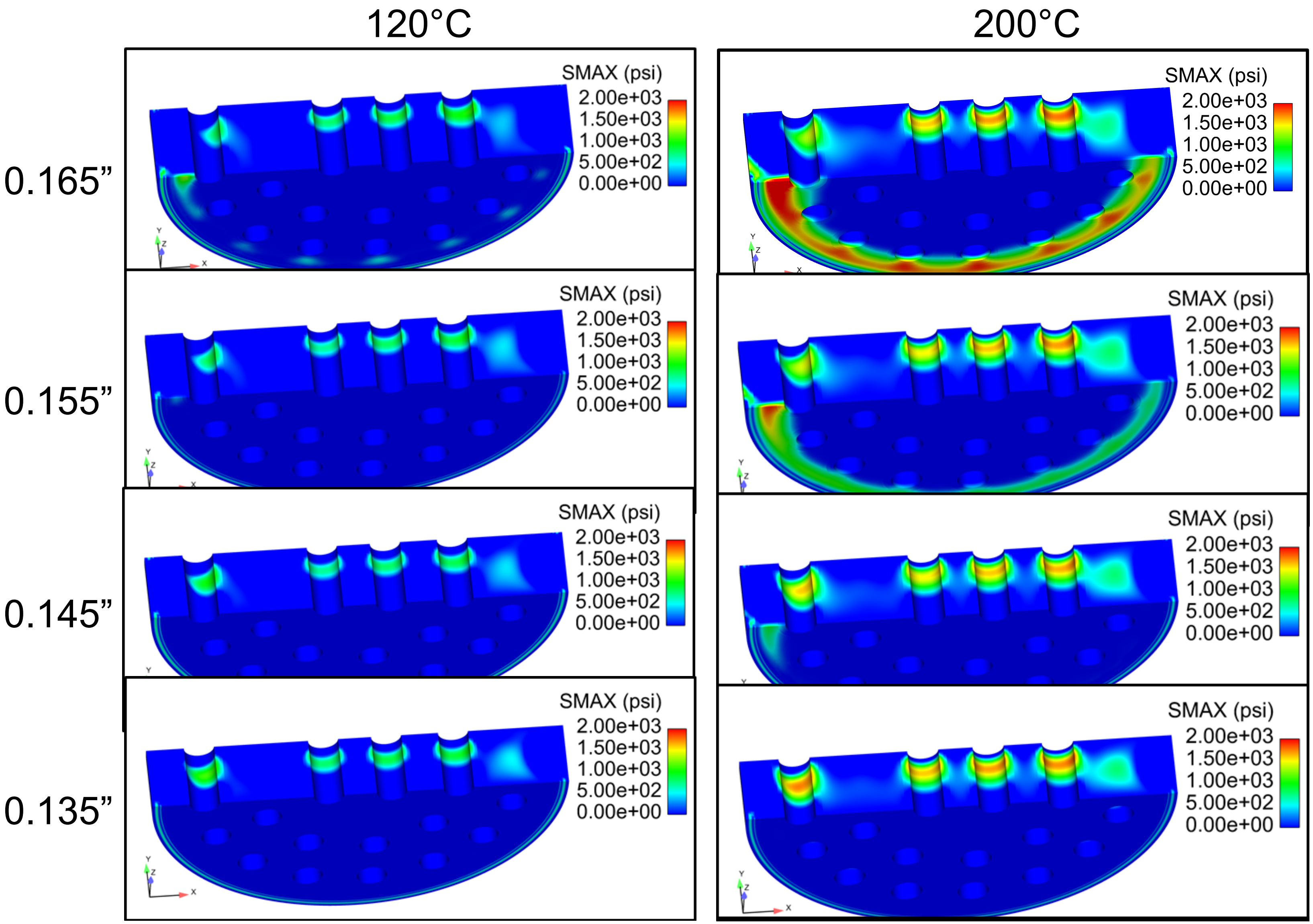
Enabling S&T:

Stress Modeling & Measurement, Property Determination, Fracture Testing/Analysis, and Fracture Mechanics

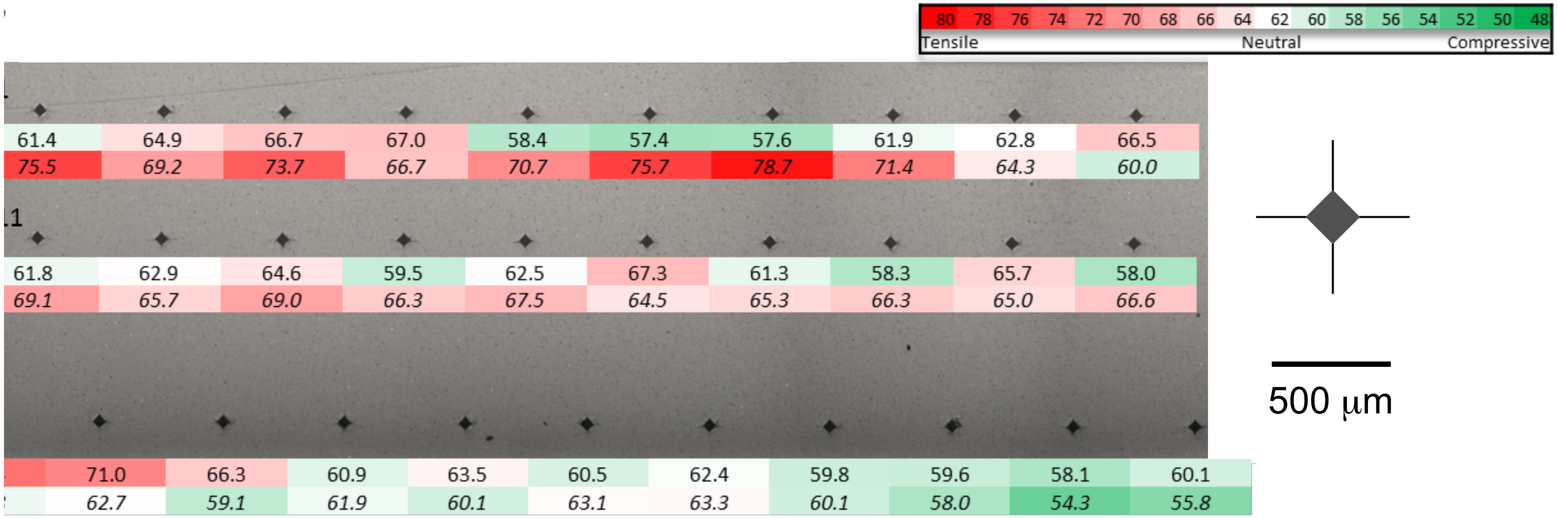
Engineering Application:

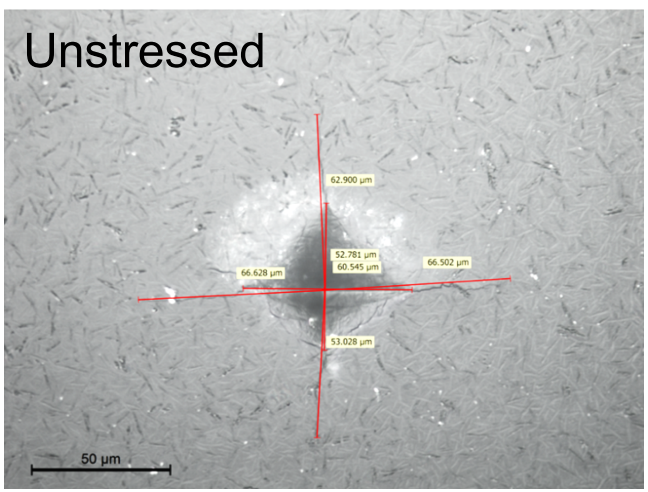
GtM Seal Design, Process Sensitivity, & Performance Assessment

GtM Seal Design Variability & Sensitivity Was Assessed Using FE Stress Modeling



Stress In GCtM Seals Was Mapped Using Indentation Crack Length Measurements





Technical Work

Focus Area: Fracture Mechanics

Enabling S&T:

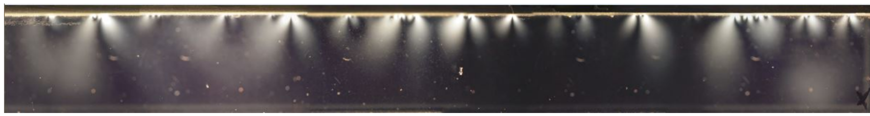
Crack Propagation, Failure & Reliability Testing & Modeling, Property Characterization

Engineering Applications:

GtM Seals and Brazed Alumina Connectors

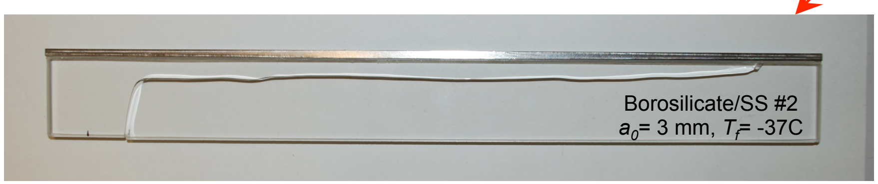
Model Bi-Material Beam Experiments Are Being Designed/Conducted To Understand Crack Propagation

Photoelasticity analysis shows residual stress

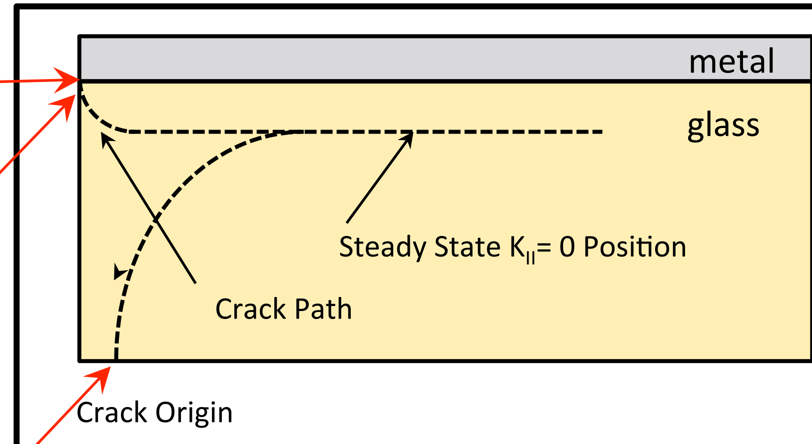


Edge crack initiated

Bottom crack initiated

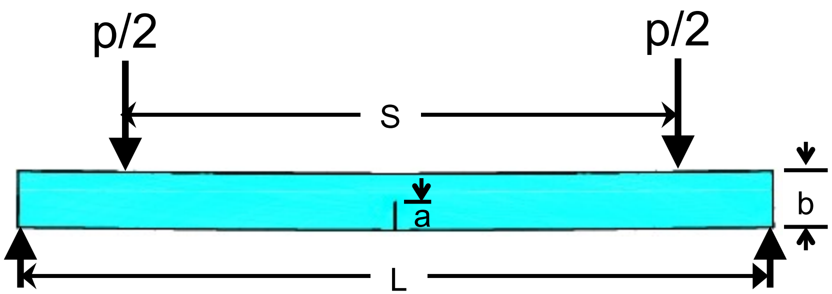


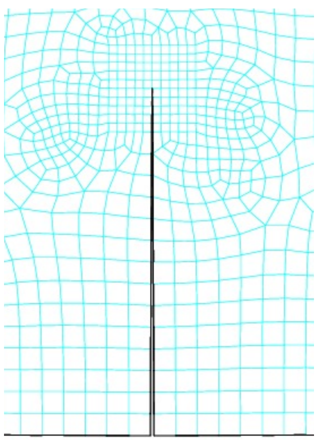
Specimen with different CTE materials to generate interface stress/crack growth.



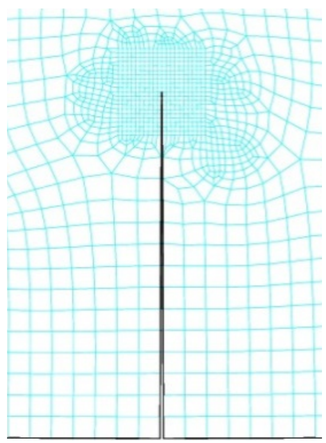
- The crack grows rapidly once initiated
- Initial tests show expected behavior.
  - But crack only roughly planar with out-of-plane tilt

Modeling Capabilities Were Tested/Refined By Calculating The Force Required To Propagate A Crack





standard mesh with Δ/b = 0.0125



refined mesh with Δ/b = 0.00625

FEA mesh used in calculations has:

a=1.5 mm, *b*=3 mm, *L*=40 mm, *S*=20 mm

Method	Δ/b	F(a/b)	% difference from reference solution
J-integral	0.01250	1.490	-0.3
J-integral	0.00625	1.493	-0.1
CZ analysis	0.01250	1.453	-2.8
CZ analysis	0.00625	1.486	-0.5

- Semi-analytical solution for plane stress $G=K^2/E$

$$F(a/b) = \frac{2b^2}{3P(L-S)}\sqrt{EG/3.14\,\mathrm{a}}$$

- Excellent agreement with reference solution (Cohesive Zone, CZ, model requires finer mesh).
  - J-integral is a one step, linear-elastic (LE) solution.
  - CZ length with Δ/b= .001250 only 2 elements long.
  - CZ analysis is nonlinear, multi-step crack growth.

Technical Work

Focus Area: Structure/Properties

Enabling S&T:

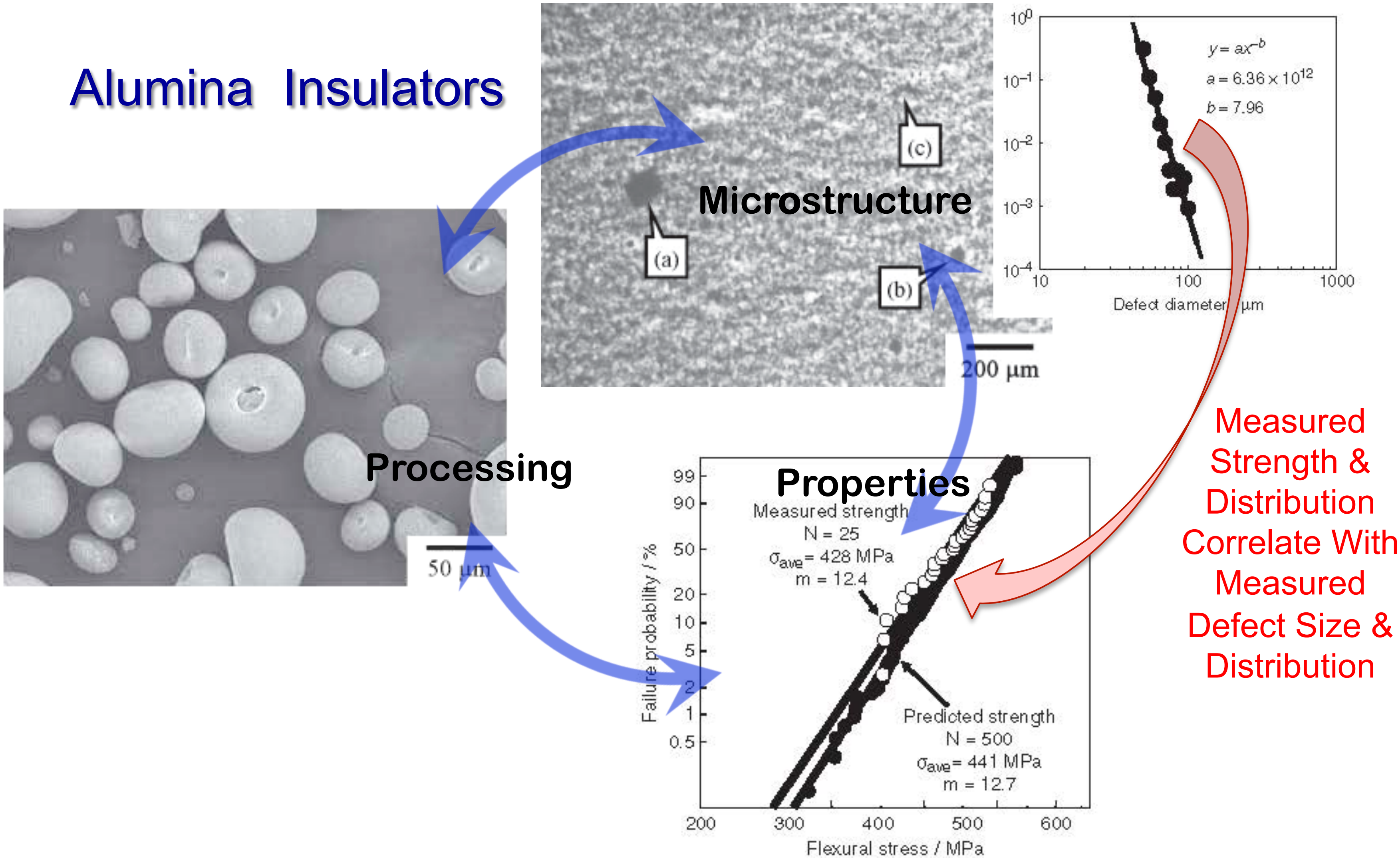
Property & Microstructure Characterization

Engineering Applications:

Crystalline Ceramics

(e.g., in GCtM Seals, Alumina Insulators, etc.)

Understanding/Controlling Process-Structure-Property Relations Will Be Critical To Failure Prediction



S. Nakamura, S. Tanaka, Z. Kato, & K. Uematsu, "Strength-Processing Defects Relationship Based on Micrographic Analysis & Fracture Mechanics in Al_2O_3 Ceramics," J. Am. Ceram. Soc., 92 [3] 688–693 (2009).

Experimentally-Validated Modeling Is Moving Us Toward Quantitative Brittle Failure/Reliability Prediction

$$K \sim \sigma a^{1/2} \sim K_{IC}$$