SAND2022-14181C

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Experimentally Informed Model Development of Glass-Ceramic Materials

32nd Rio Grande Symposium on Advanced Materials, Albuquerque, NM, October 24, 2022

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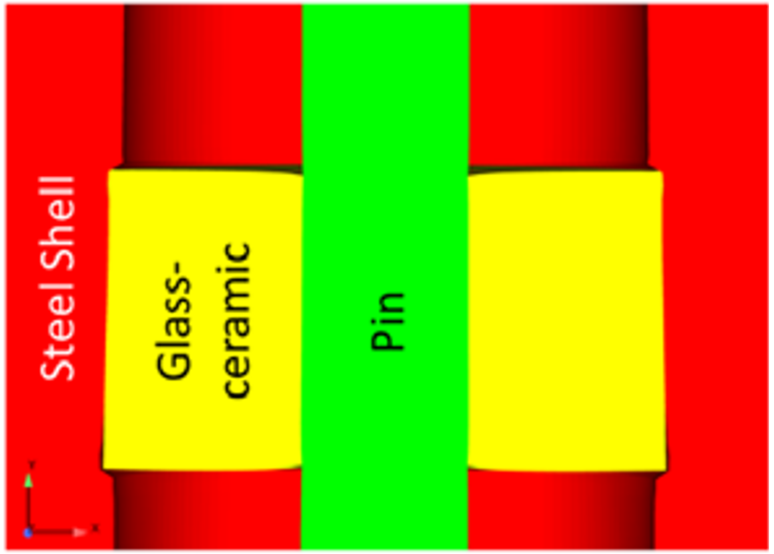
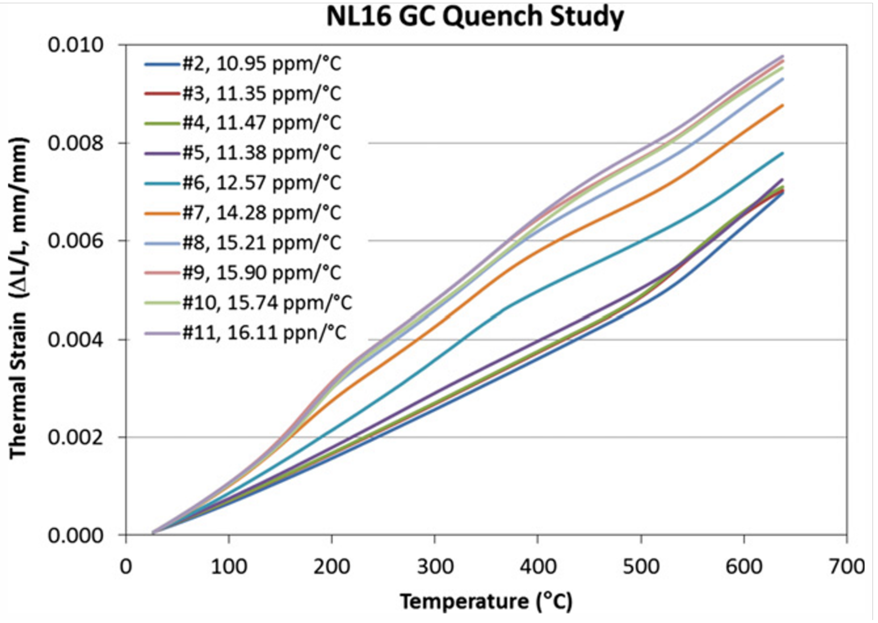
Glass-ceramic to Metal Seals (GcTMS)

- Variety of industrial applications for glass-ceramics
  - Hermetic glass-ceramic to metal seals (GcTMS)
  - Subject to complex thermomechanical histories



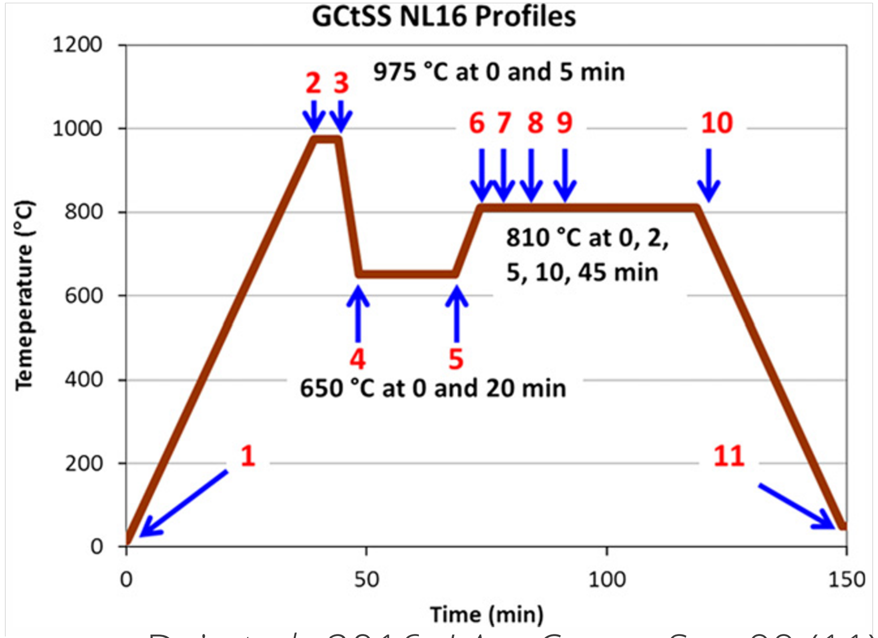
Dai *et al.*, 2017, *J Am Ceram Soc*, 100, pp.3652-3661



Dai *et al.*, 2016, *J Am Ceram Soc*, 99, pp.3719-3725

Glass-Ceramics - Microstructure

- Glass-ceramics are produced by inducing a ceramic phase(s) in an inorganic base glass
- Advantageous features arise from microstructure
  - Up to 5 constituents
  - Inelasticity from residual glass and silica polymorphs



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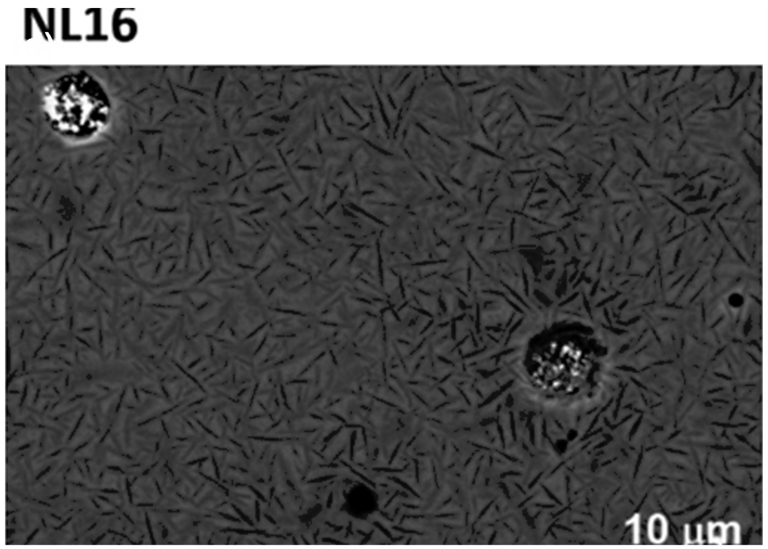


Rodriguez *et al.*, 2016, *J Am Ceram Soc*, 99 (11), pp.3726-3733

Objective

- Understanding actuation response essential for intended use

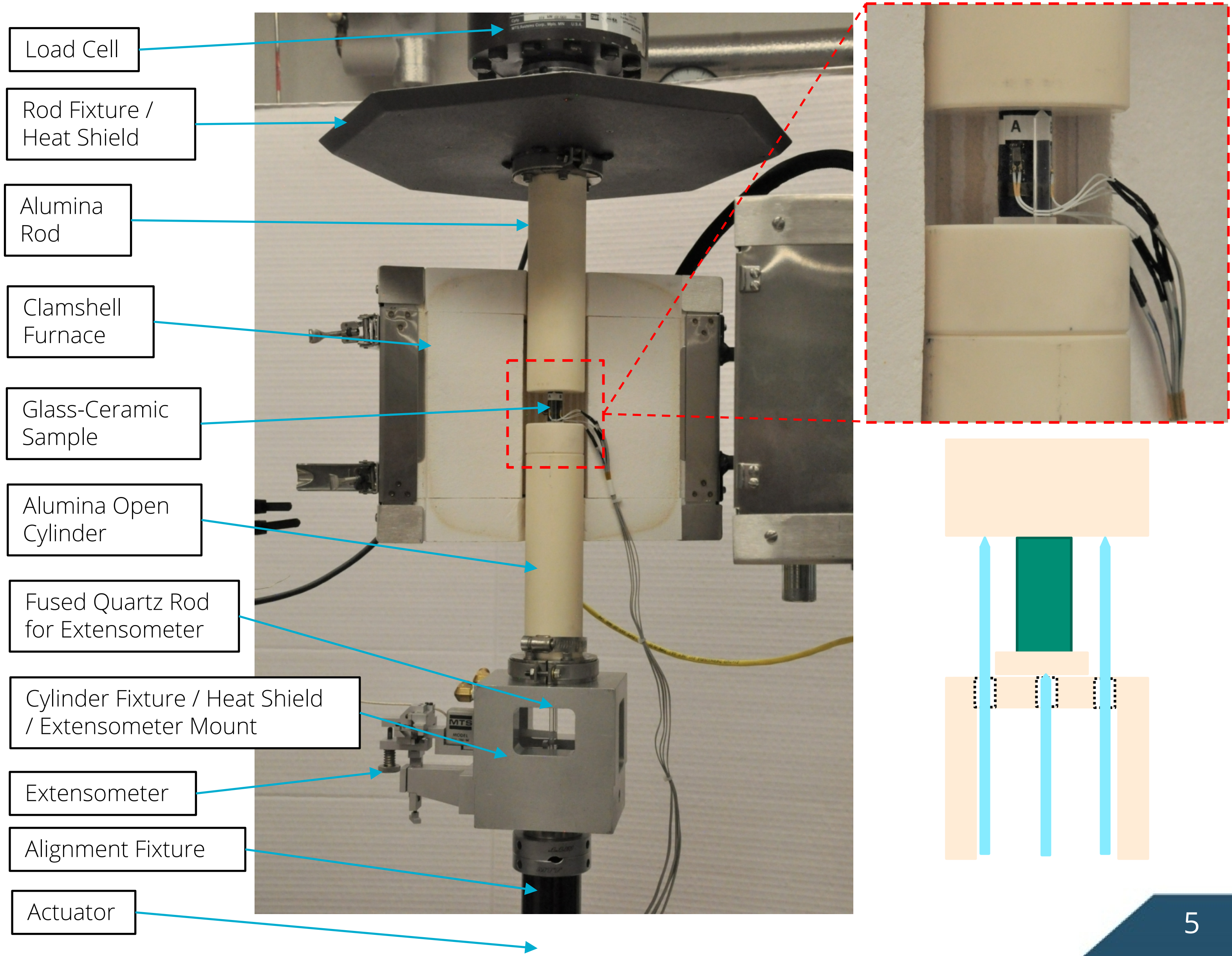
- Actuation not well understood experimentally or modeled
  - Experimental studies focused on other features (e.g. dilatometry, DMA)
  - Models leverage alternative phenomenologies

- Objective: Elucidate and enhance understanding of actuation response
  - Perform first of the kind experiments to characterize thermomechanical response
  - Develop new model capable of describing coupled phase-transformation and viscoelasticity

Experimental Set-up

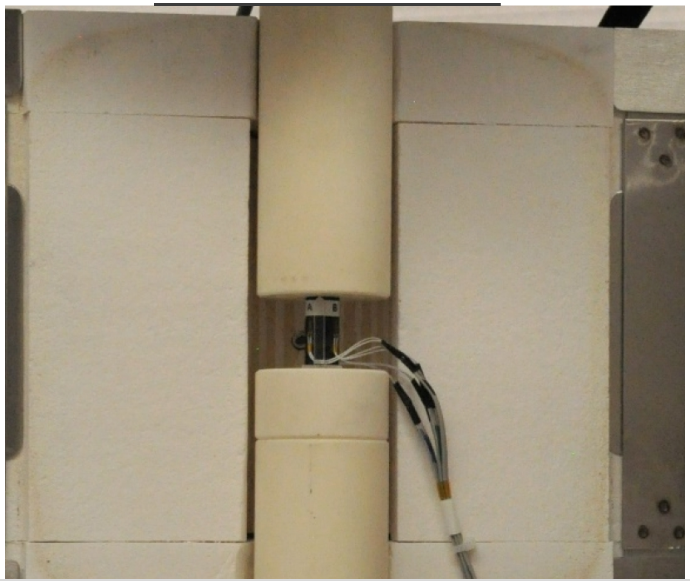
- Experimental challenges:
  - Thermal homogeneity
  - Precise strain measurement
  - Higher loads

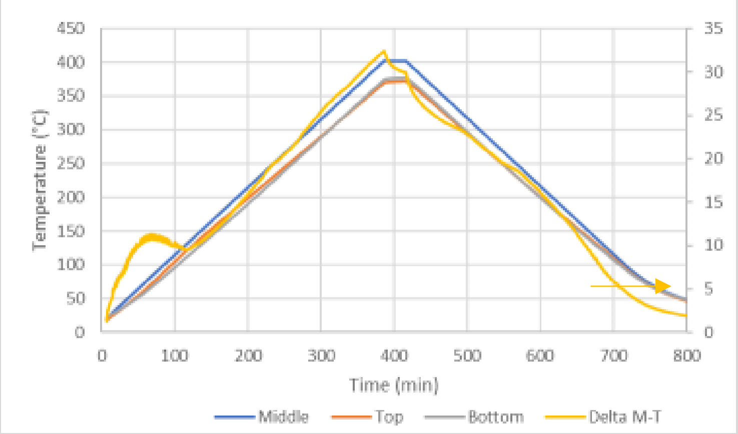
- Developed novel thermomechanical test chamber
  - Novel extensometer and stage design
  - Clamshell furnace



Experimental Thermal Control

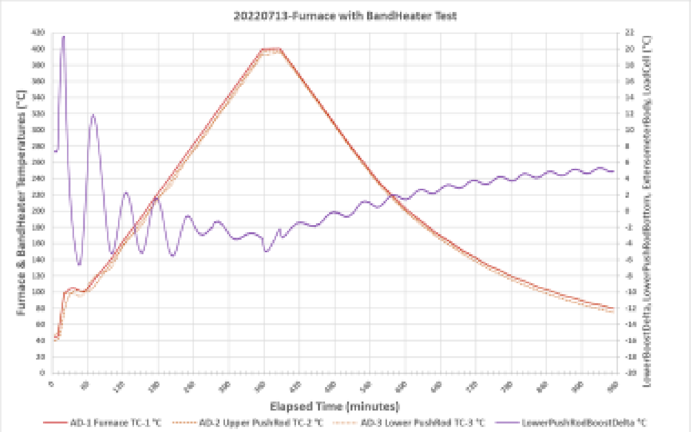
Alumina Top and Bottom
No Band Heater





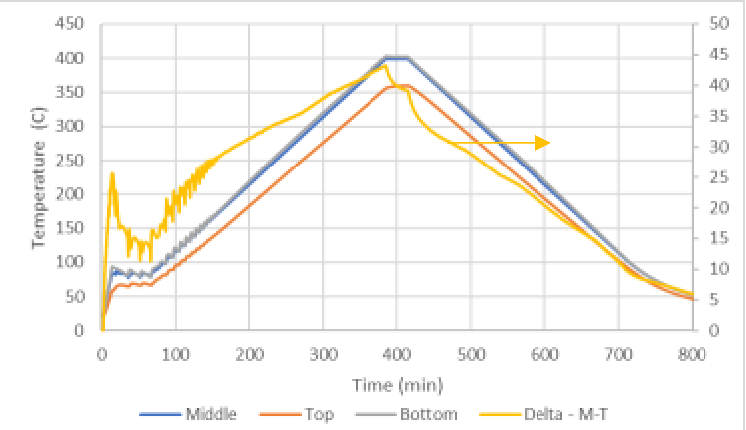
Thermal Gradient Across the Sample

Quartz Top Alumina Bottom
Band Heater



No Thermal Gradient

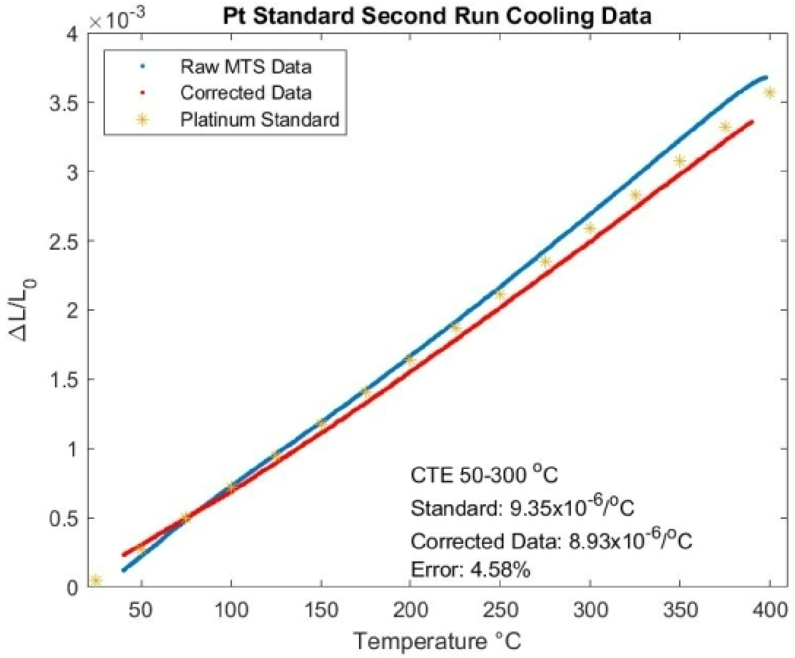
Alumina Top and Bottom
Band Heater



Minimal Thermal Gradient

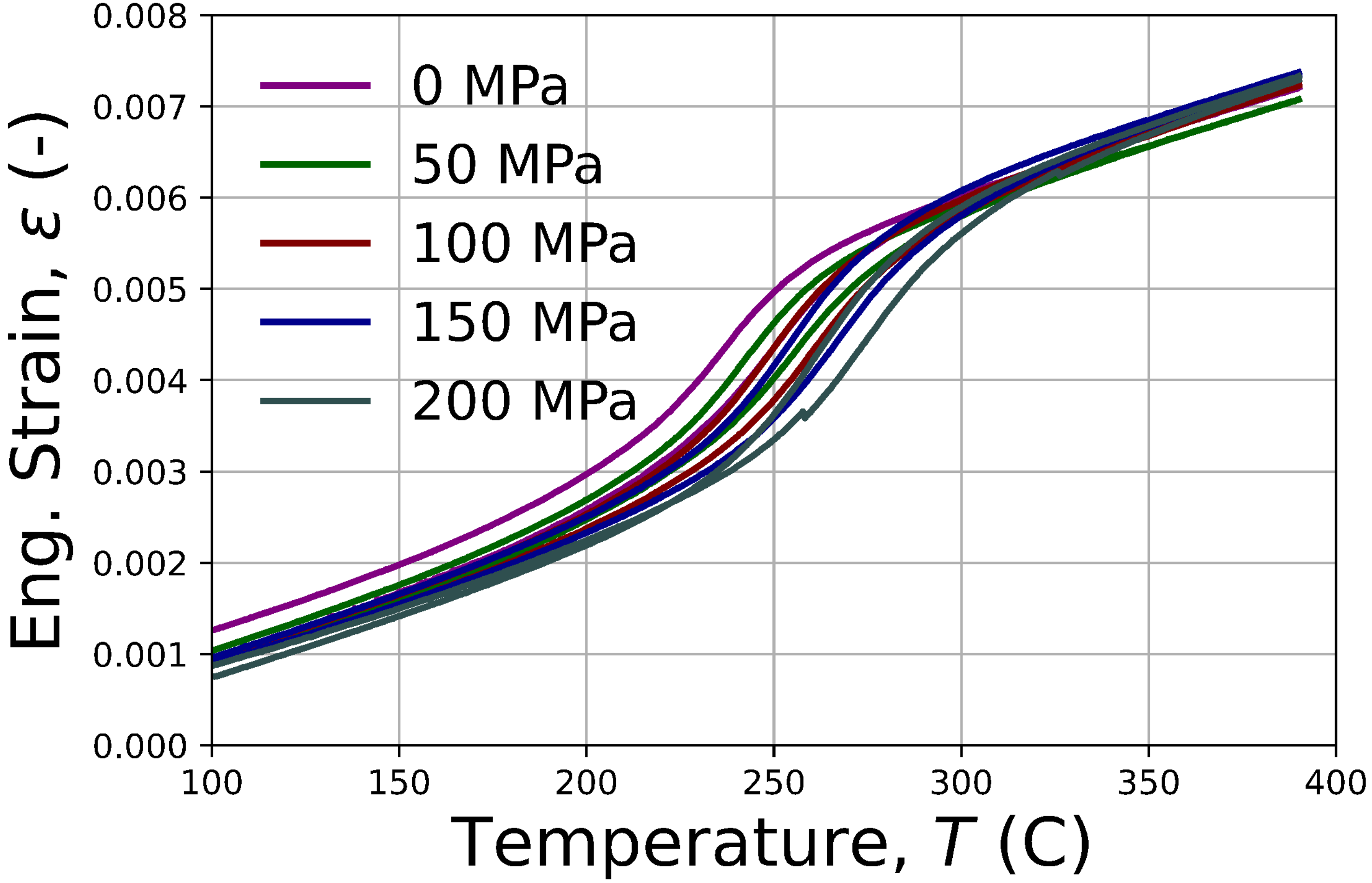
Experimental Results

- Obtained thermal strain data accounting for thermal issues



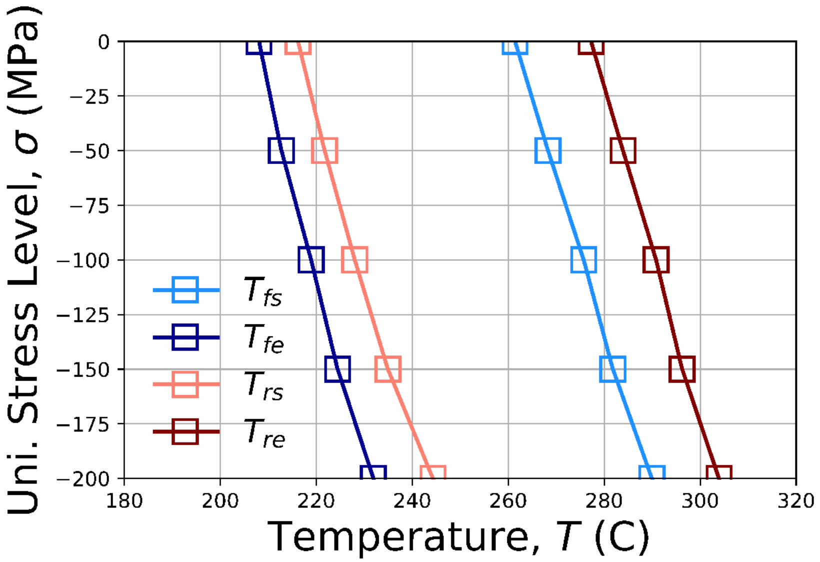
$$\frac{\Delta L}{L_0}(T)_{Correction} = \frac{\Delta L}{L_0}(T)_{\substack{Raw\\Data\ Std.}} - \frac{\Delta L}{L_0}(T)_{\substack{Known\\Standard}}$$

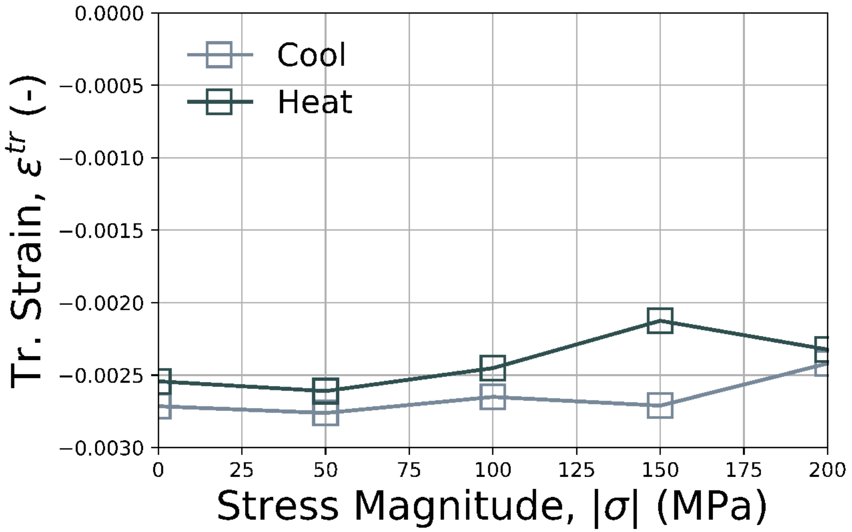
$$\frac{\Delta L}{L_0}(T)_{\substack{Corected\\Raw\ Data}} = \frac{\Delta L}{L_0}(T)_{\substack{Raw\\Data}} - \frac{\Delta L}{L_0}(T)_{Correction}$$

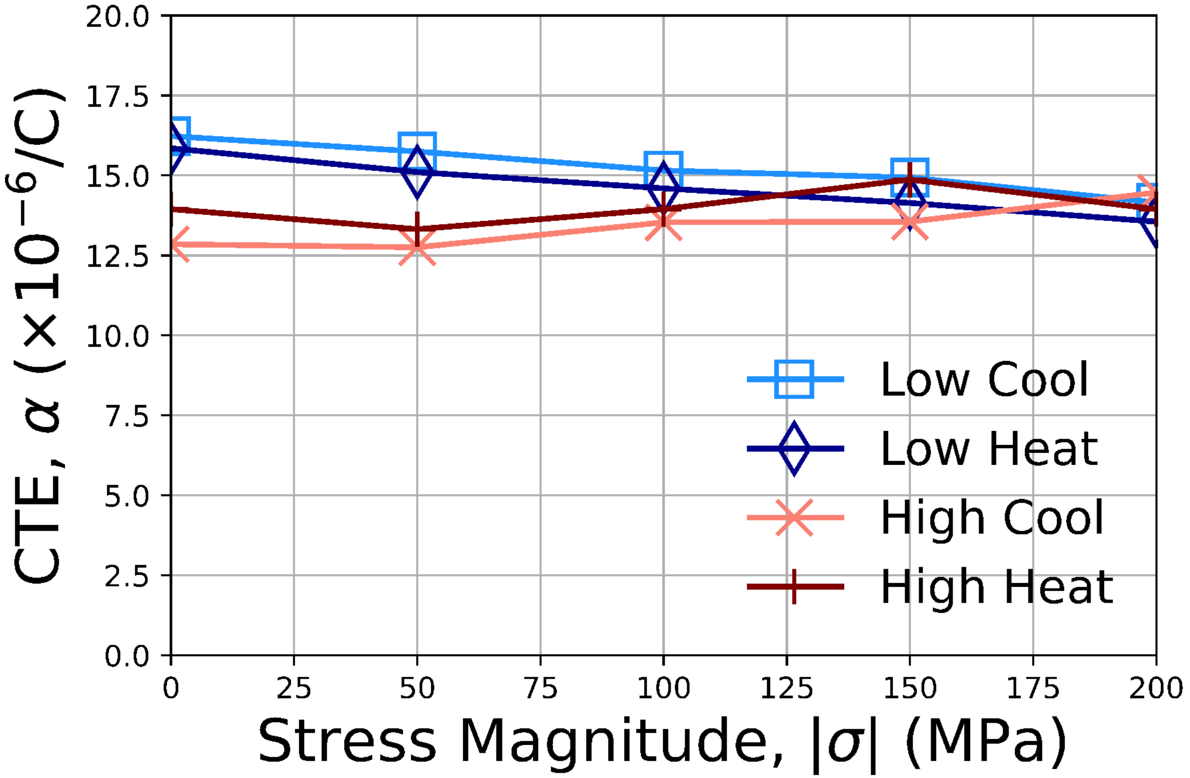


Experimental Observations

- Able to obtain stress and thermomechanical dependencies of GCs for first time







Glass-Ceramic Model

- Seek macroscale representation of glass-ceramics via use of internal state variable/continuum thermodynamics theory
  - Thermoviscoelastic theory for response of glass
  - Utilize shape memory alloy (SMA) theory as basis (Lagoudas model) for phase transformations
  - Details in Lester and Long, 2021, Mech Mat., 158, 103849

Free Energy

$$G\left(\sigma_{ij}, T, t, \xi, \varepsilon^{t}_{ij}; \delta^{i}\right) = G^{\mathrm{te}}\left(\sigma_{ij}, T, \xi; \delta^{i}\right) + G^{\mathrm{in}}\left(\sigma_{ij}, T, t, \xi, \varepsilon^{t}_{ij}; \delta^{i}\right)$$

Total Strain

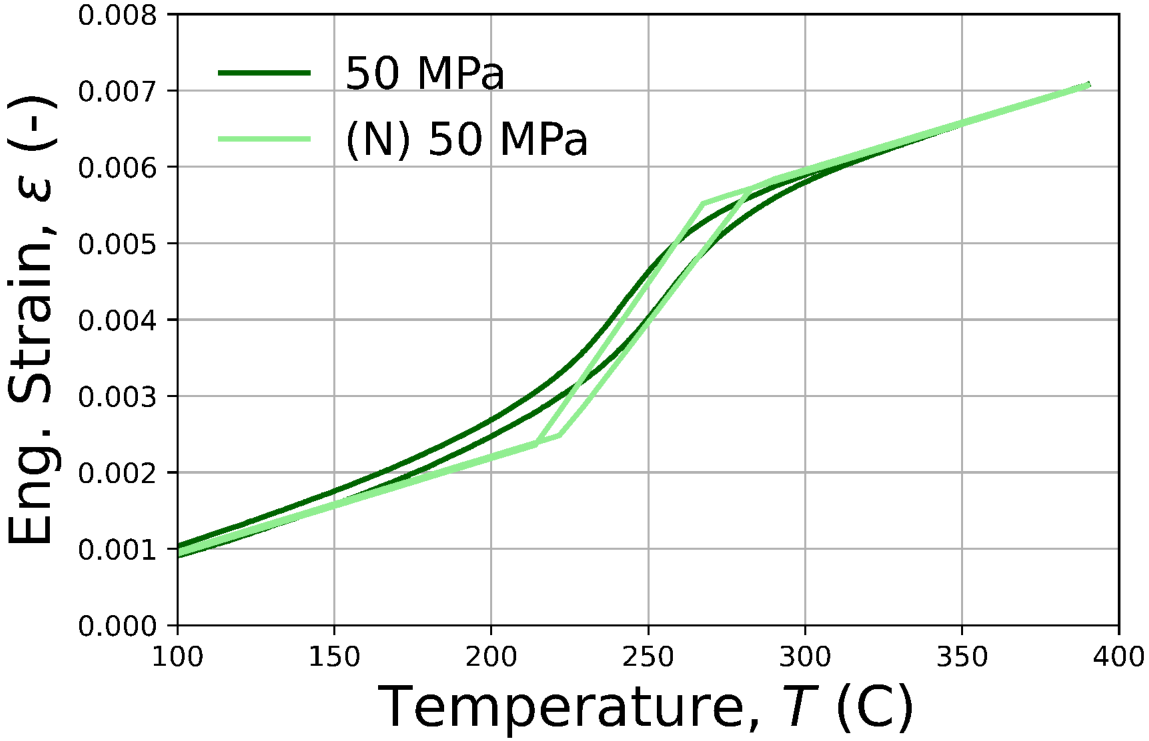
$$\varepsilon_{ij} = \frac{1}{2\bar{\mu}}\sigma'_{ij} + \frac{1}{9\bar{K}}\sigma_{kk}\delta_{ij} + g_{\varepsilon}\varepsilon^{\mathrm{t}}_{ij} + \bar{\alpha}\left(T - T_0\right)\delta_{ij} - g_v\frac{\Delta\mu}{2\mu^{\mathrm{eq}}\mu^{\mathrm{g}}}H^2_{ij} - g_v\frac{\Delta K}{9K^{\mathrm{eq}}K^{\mathrm{g}}}H^1\delta_{ij} + g_v\Delta\alpha H^3\delta_{ij}$$

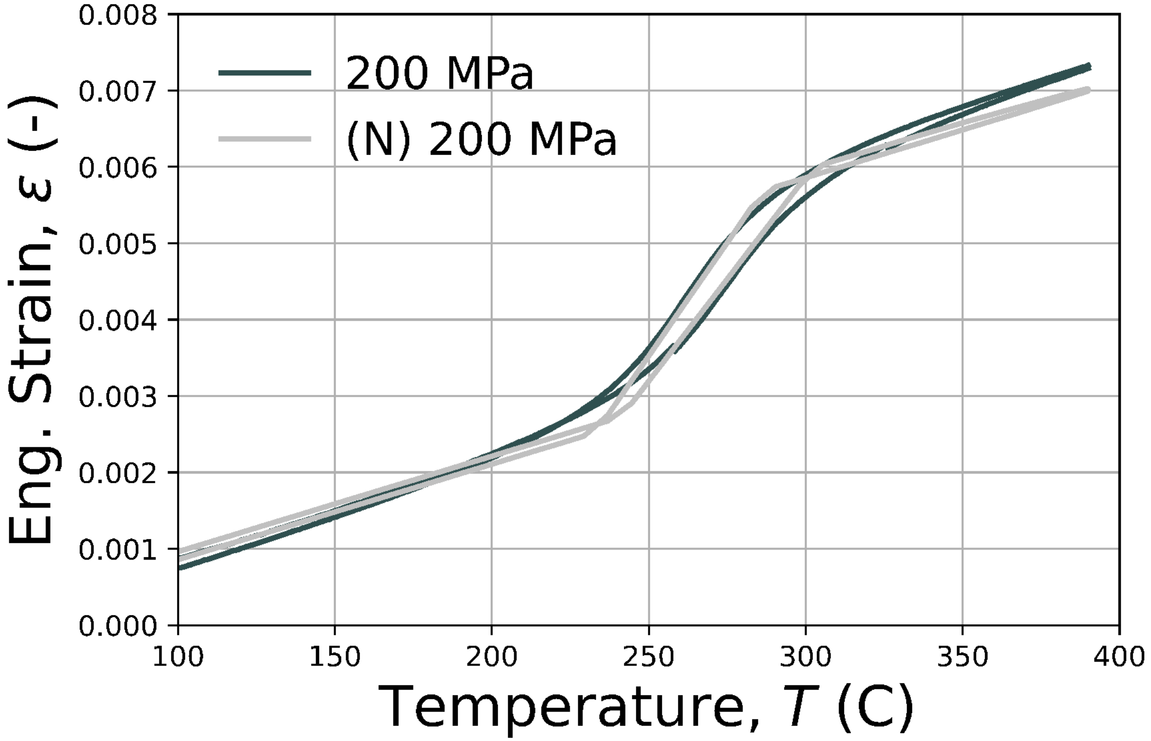
Shift Factor

$$\log_{10} a = \frac{-C_1\left(T - T_{\mathrm{ref}}\right)}{C_2 + \left(T - T_{\mathrm{ref}}\right)}, \qquad \log_{10} a^{\mathrm{WLF\_Lag}} = \frac{-C_1\left(T - T_{\mathrm{ref}} - \int_0^t \left(1 - j_v\left(t^* - s^*, 0\right)\right)\frac{\partial T}{\partial s}\mathrm{d}s\right)}{C_2 + \left(T - T_{\mathrm{ref}} - \int_0^t \left(1 - j_v\left(t^* - s^*, 0\right)\right)\frac{\partial T}{\partial s}\mathrm{d}s\right)}$$

Calibration and Exp. Simulation

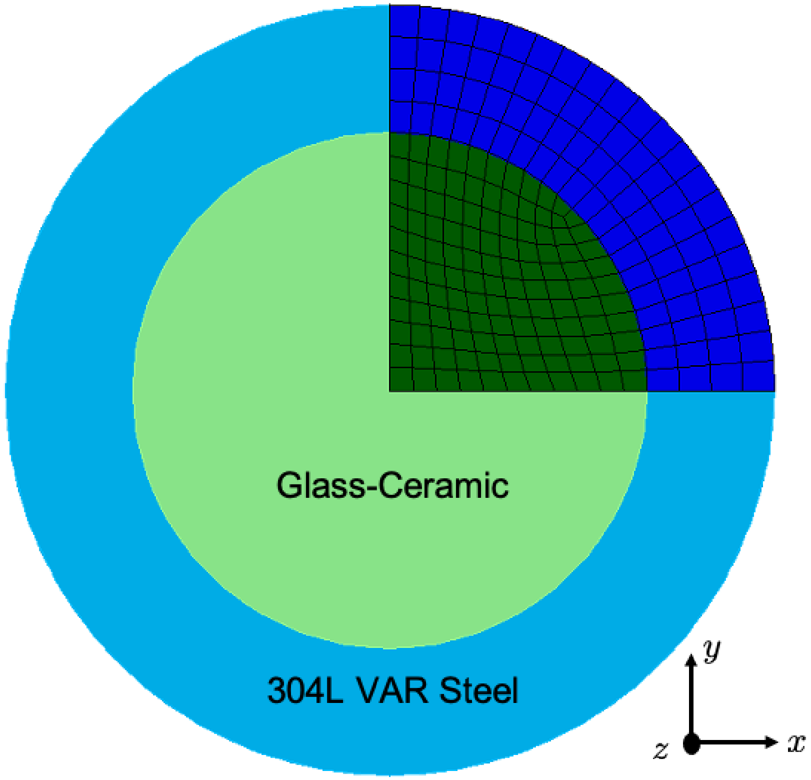
- Fit transformation terms to new actuation data
- Viscoelastic data from prior study
- Good agreement between experimental and simulation results observed



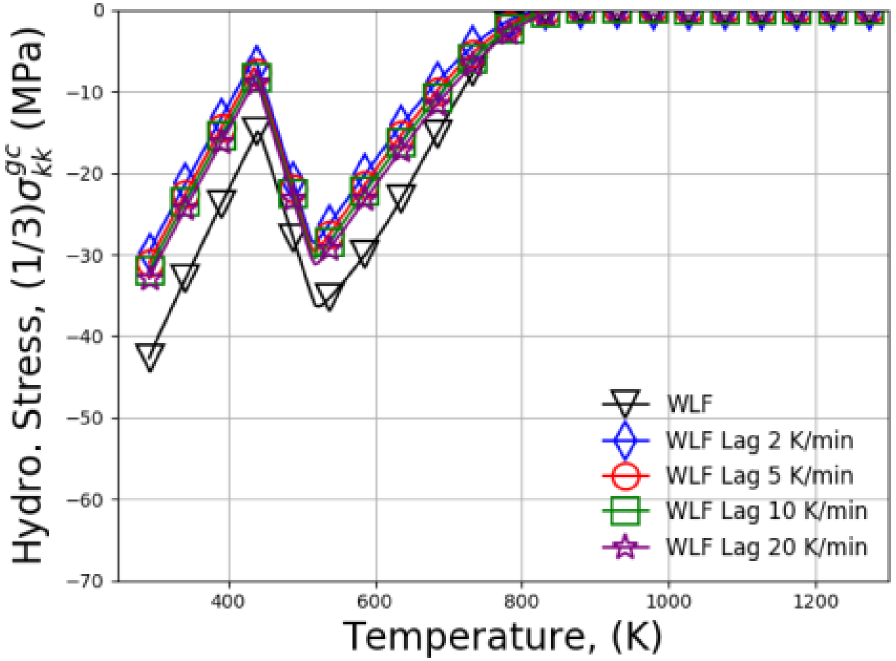


Example Problem – Simple Seal

- Simple seal used as representative example problem
  - Common test for prediction and measurement of residual stress
  - GC Seal enclosed in concentric metal (stainless steel) shell
  - Cooled from above T_g to RT



Volume averaged hydrostatic stress through cooling



Summary and Conclusions

- Actuation behavior of glass-ceramics explored for first time
  - Novel thermomechanical test chamber
  - New coupled constitutive model

- Have first measurements of stress dependence on different behaviors
  - Preparing second set of experiments to elucidate additional phenomenology
  - Used for updating model form

- Thermomechanical model demonstrated on representative problem
  - Examines coupling between different mechanisms
  - Essential tool for examining performance of engineered product

Acknowledgements

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APPENDIX

Numerical Implementation

- 3D numerical implementation formulated and implemented
  - Sierra/SolidMechanics FE code constitutive library (LAMÉ)
  - Fully implicit integration, line-search augmented Newton-Raphson

Non-Linear Solve

$$\sigma_{ij}^{n+1} = \sigma_{ij}^{n} + \Delta t \dot{\sigma}_{ij}^{n+1}$$

$$\varepsilon_{ij}^{\mathrm{t}(n+1)} = \varepsilon_{ij}^{\mathrm{t}(n)} + \Delta t \dot{\varepsilon}_{ij}^{\mathrm{t}(n+1)}$$

$$\xi^{n+1} \rightarrow f\left(\sigma_{ij}^{n+1}, T^{n+1}, \xi^{n+1}\right) = 0$$

Direct Solve

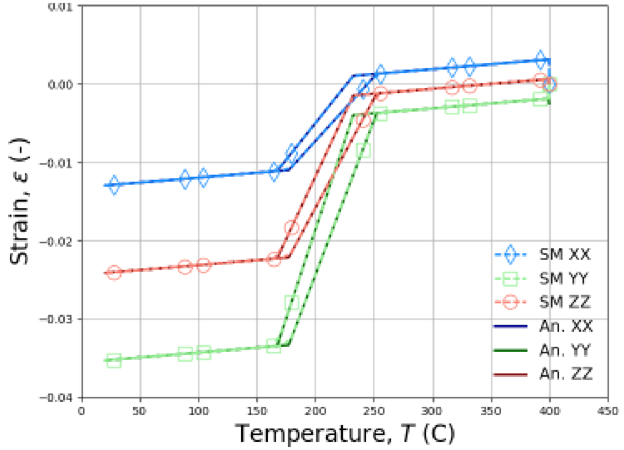
$$H_{n+1}^{1} = H_{n}^{1} + \Delta t \dot{H}_{n+1}^{1}$$

$$H_{ij}^{2(n+1)} = H_{ij}^{2(n)} + \Delta t \dot{H}_{ij}^{2(n+1)}$$

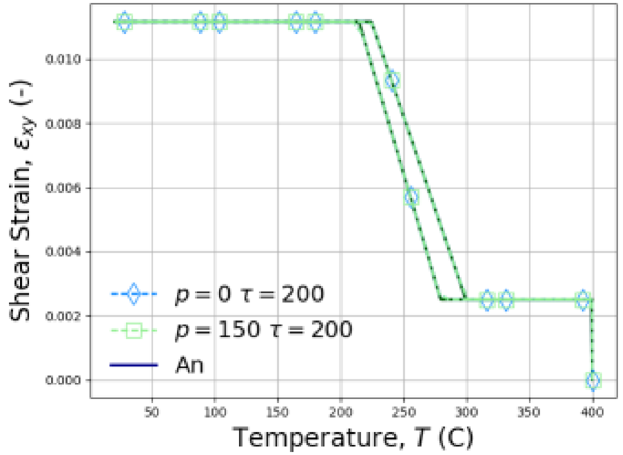
$$H_{n+1}^{3} = H_{n}^{3} + \Delta t \dot{H}_{n+1}^{3}$$

Example Verification Tests

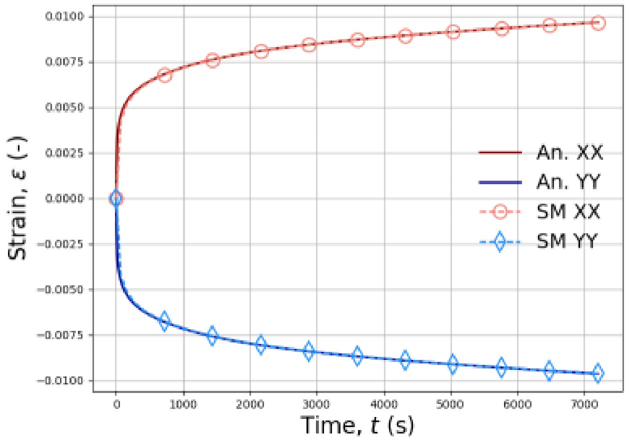
Balanced Biaxial Thermal Sweep



Pure Shear w/ Pressure



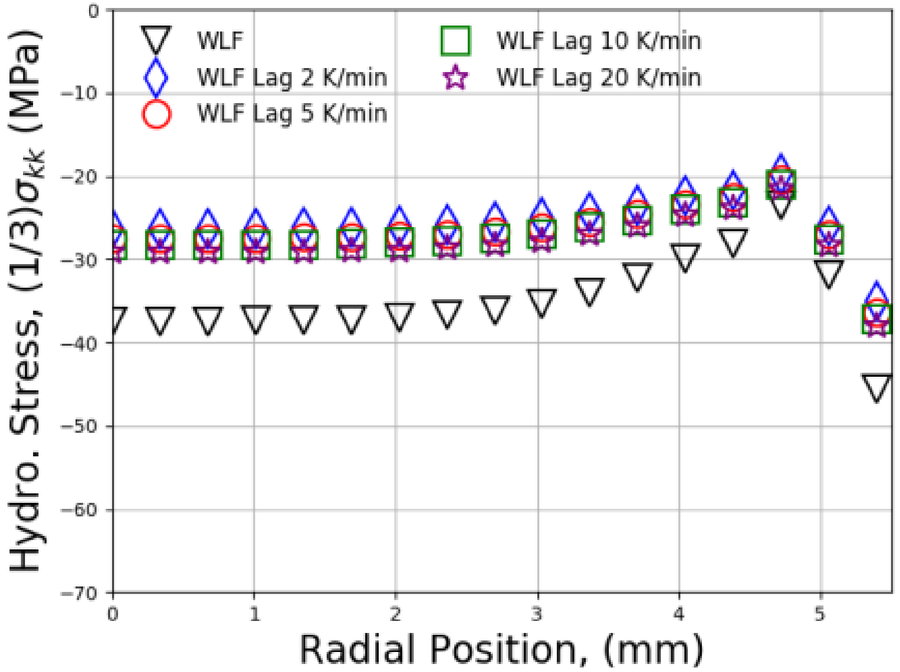
Balanced Biaxial Creep



Impact of Heating Rate

- Investigate simple seal with multiple shift factor
  - WLF-Lag at different cooling rates
  - WLF cooled at 2 K/min
  - Purely volumetric flow rule $\gamma_1^0 = 0, \ \gamma_2^0 = \bar{\gamma}$

Hydrostatic stress along top seal surface



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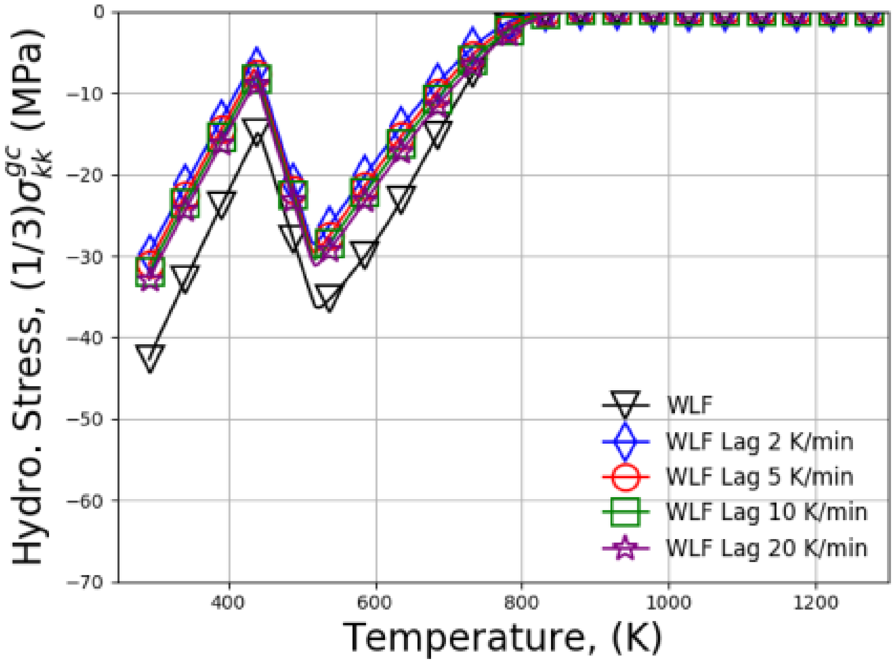

- Impact of both viscoelastic and transformation mechanisms may be observed

Lester and Long, 2021, *Mech Mat.*, 158, 103849