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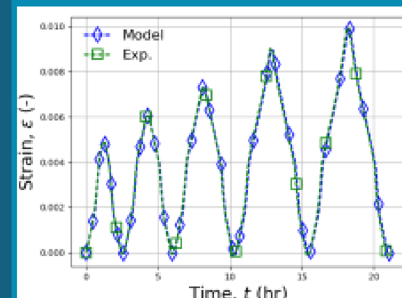
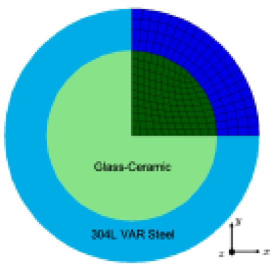
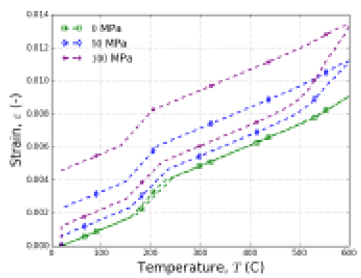
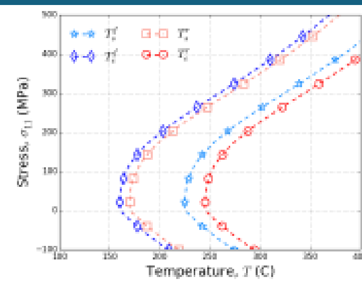
Constitutive and Application Modeling of Glass-Ceramic Materials









Brian T. Lester
Kevin Long

Sandia National Laboratories

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2021 US National Congress on Computational

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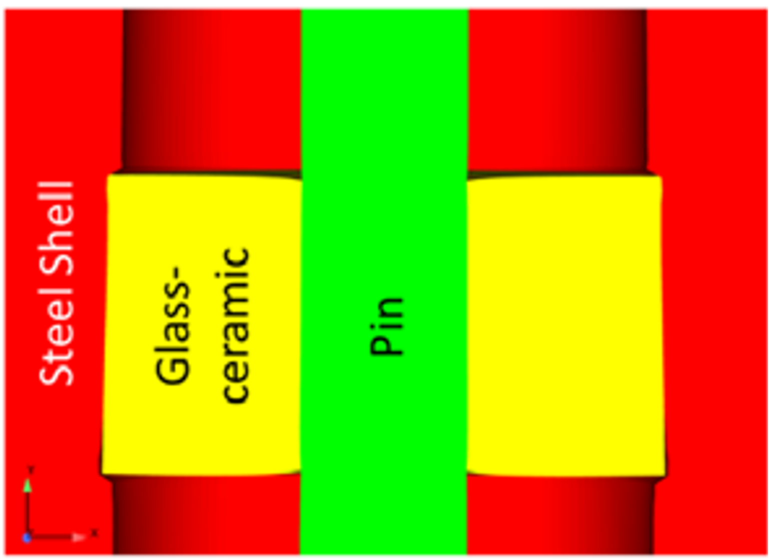
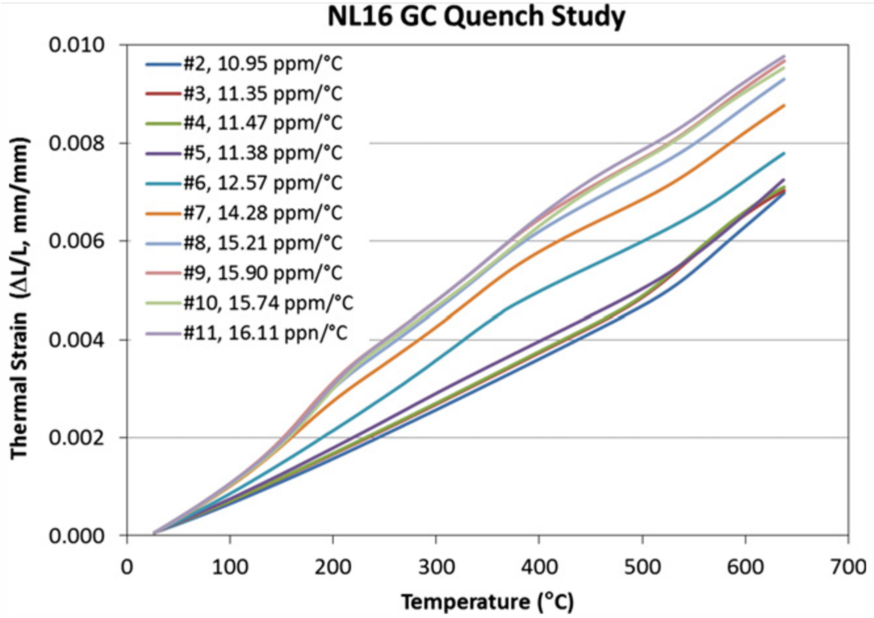
Glass-ceramic to Metal Seals (GcTMS)

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

Example Seal



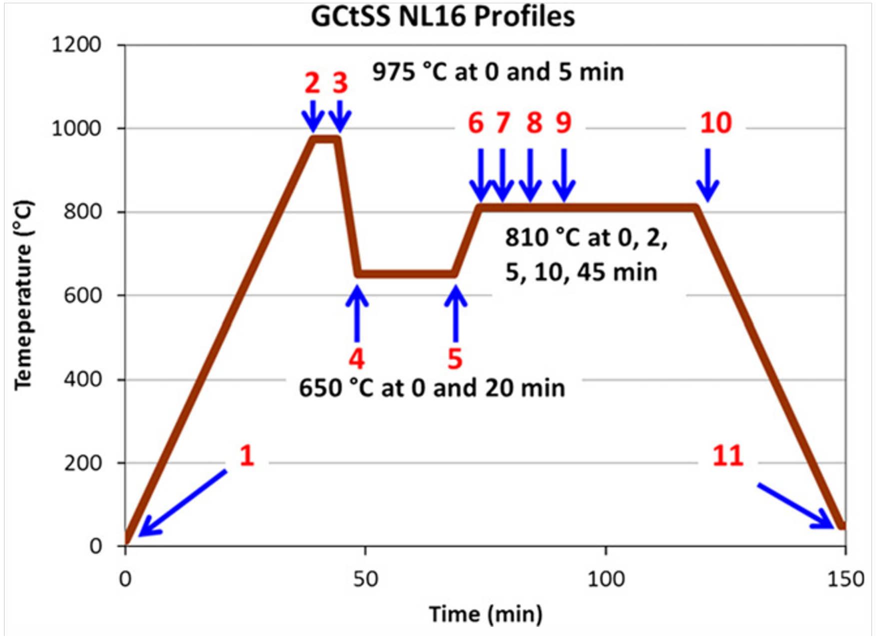
Dai *et al.*, 2017, *J Am Ceram Soc*, 100, pp.3652-3661



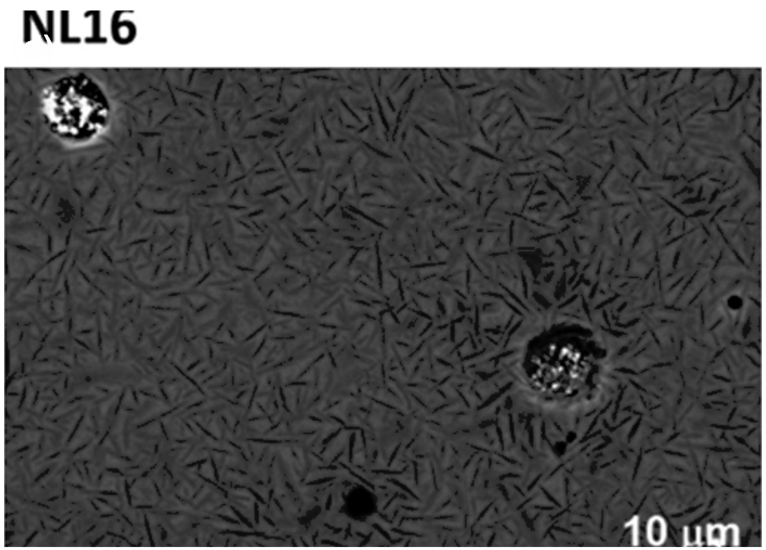
Dai *et al.*, 2016, *J Am Ceram Soc*, 99, pp.3719-3725

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



Dai *et al.*, 2016, *J Am Ceram Soc*, 99 (11), pp.3719-3725



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

Objective

- Need to be able to simulate sealing process
  - Predict residual stress states
  - Optimize thermal profile during sealing

- Need appropriate constitutive model for glass-ceramic
  - No existing specialized glass-ceramic constitutive models
  - Existing efforts adapt other model forms (e.g. non-linear viscoelastic)
  - Neglect complexity and details of current combination of mechanisms

- The objective of the current work is to develop a glass-ceramic constitutive model
  - Theory coupling viscoelastic and phase-transformation response
  - Robust 3D numerical implementation
  - Use model to simulate sealing process

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

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

σ_{ij}, T, t	External State Variables
$\xi, \varepsilon_{ij}^{\mathrm{t}}$	Internal State Variables
δ^{i}	Constituent Volume Fractions

$$G^{\mathrm{te}}\left(\sigma_{ij}, T, \xi; \delta^{i}\right) = \sum_{\mathrm{r=Q,LO,LM,A}} \delta^{r} G^{r}\left(\sigma_{ij}, T\right) + \delta^{C} G^{C}\left(\sigma_{ij}, T, \xi\right)$$

$$G^{\mathrm{in}}\left(\sigma_{ij}, T, t, \xi, \varepsilon_{ij}^{\mathrm{t}}\right) = G^{\mathrm{in\text{-}t}}\left(\sigma_{ij}, \xi, \varepsilon_{ij}^{\mathrm{t}}\right) + G^{\mathrm{neq}}\left(\sigma_{ij}, T, t\right)$$

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

Constitutive Behavior

- Coleman-Noll and 2nd Law arguments produce:
  - All constituents/phases assumed isotropic

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

$$- \; g_v \frac{\Delta\mu}{2\mu^{\mathrm{eq}}\mu^{\mathrm{g}}} H^2_{ij} - g_v \frac{\Delta K}{9K^{\mathrm{eq}}K^{\mathrm{g}}} H^1\delta_{ij} + g_v \Delta\alpha H^3 \delta_{ij}$$

- Transformation functions
  - Utilize $J_2 - I_1$ model
  - Combines parts of Qidwai & Lagoudas (IJP, 2000) and Lagoudas *et al.* (IJP, 2012)

$$f\left(X_{ij}, p\right) = \left[\phi\left(X_{ij}\right) - p\right]^2 - p_0^2$$

$$\phi\left(X_{ij}\right) = \gamma_1\left(J_2\right)\sqrt{3J_2} - \gamma_2 I_1$$

Viscoelasticity

- Hereditary integral based formulation
  - Creep – not relaxation – spectra needed for use of Gibbs free energy
  - Shift-factor relates "material" and "laboratory" time

$$t^* = \int_0^t \frac{\mathrm{d}s}{a\left(s\right)}$$

- Investigate impact of two shift factors
  - WLF – equilibrated shift factor

$$\log_{10} a = \frac{-C_1\left(T - T_{\mathrm{ref}}\right)}{C_2 + \left(T - T_{\mathrm{ref}}\right)},$$

  - WLF-Lag
    - Incorporate some history dependence
    - Sealing problem exhibits large temperature ranges of interest (RT << T_g)

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

Numerical Implementation

- 3D numerical implementation formulated and implemented
  - Sierra/SolidMechanics FE code constitutive library (LAMÉ)
  - Fully implicit integration
  - Line-search augmented Newton-Raphson
  - Verified through a variety of loadings

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

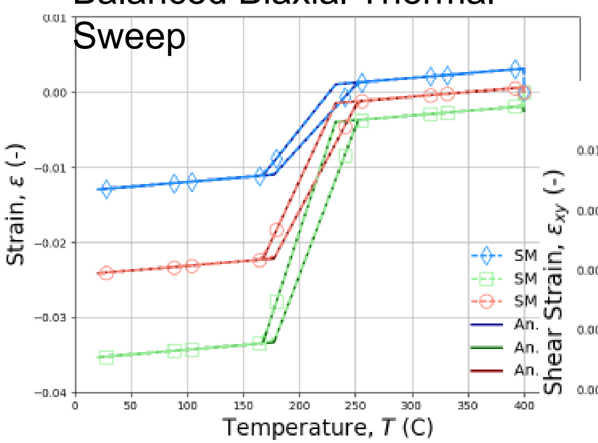
$$H_{n+1}^{1} = H_{n}^{1} + \Delta t \dot{H}_{n+1}^{1}$$

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

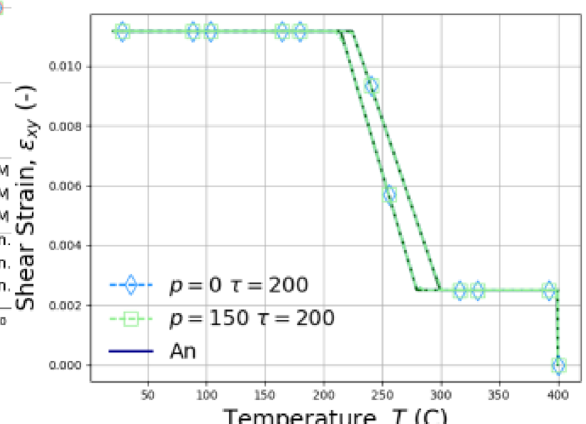
$$H_{n+1}^{3} = H_{n}^{3} + \Delta t \dot{H}_{n+1}^{3}$$

Example Verification Tests

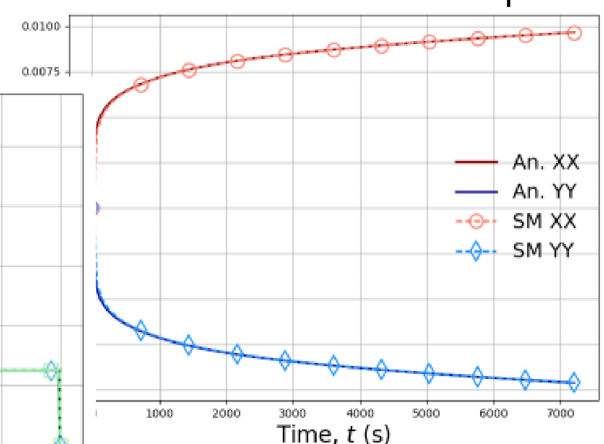
Balanced Biaxial Thermal Sweep



Pure Shear w/ Pressure

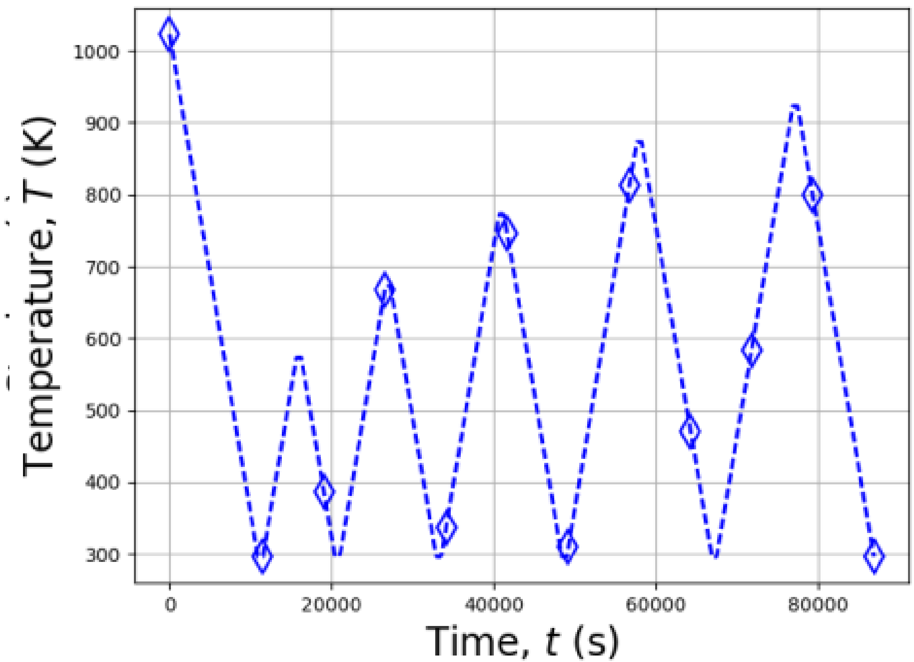


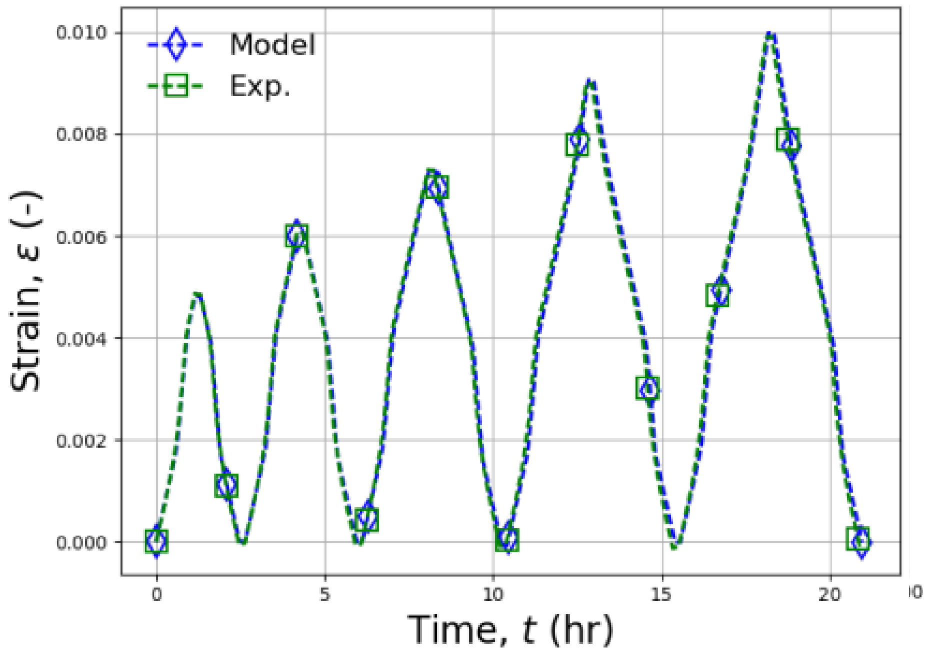
Balanced Biaxial Creep



Validation

- Consider response through “no”-load thermal sweeps
  - “Ladder”/ratcheting tests
  - Dilatometer (courtesy S. Dai, SNL)
    - Stress free thermal sweeps
    - Measures axial strain

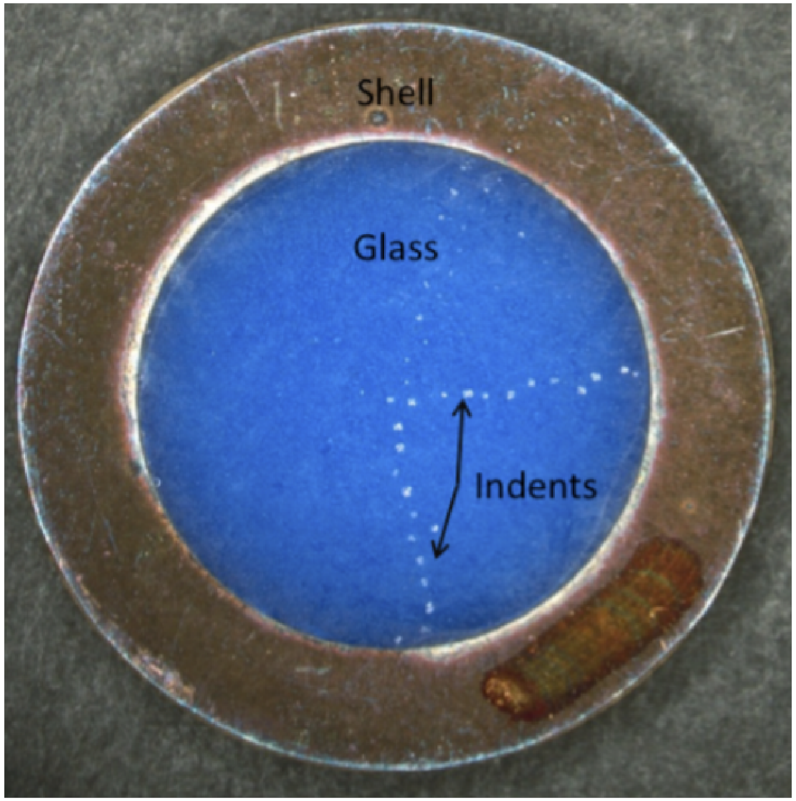


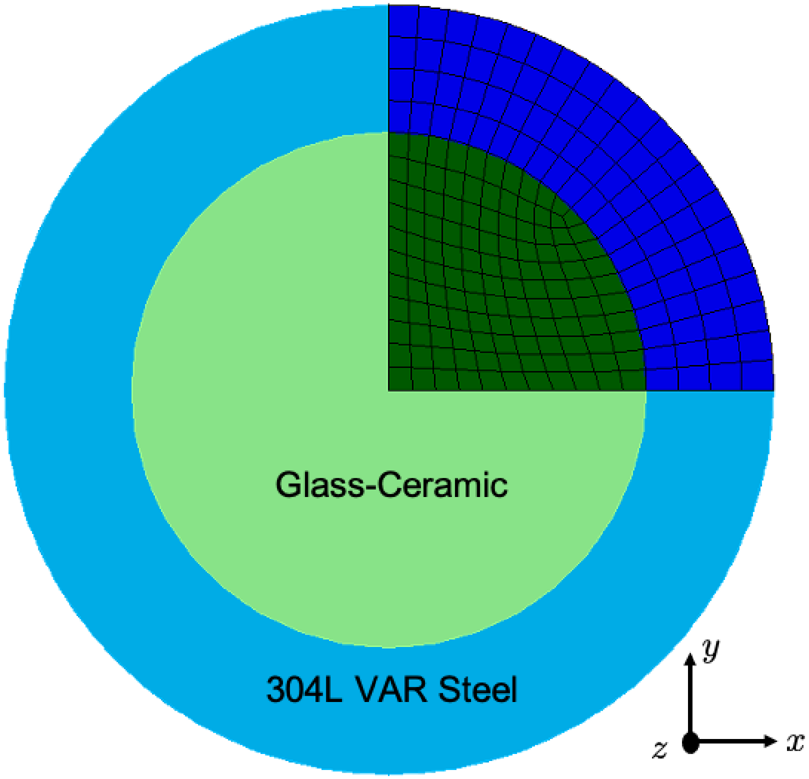


- Working on extending validation against other experiments

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



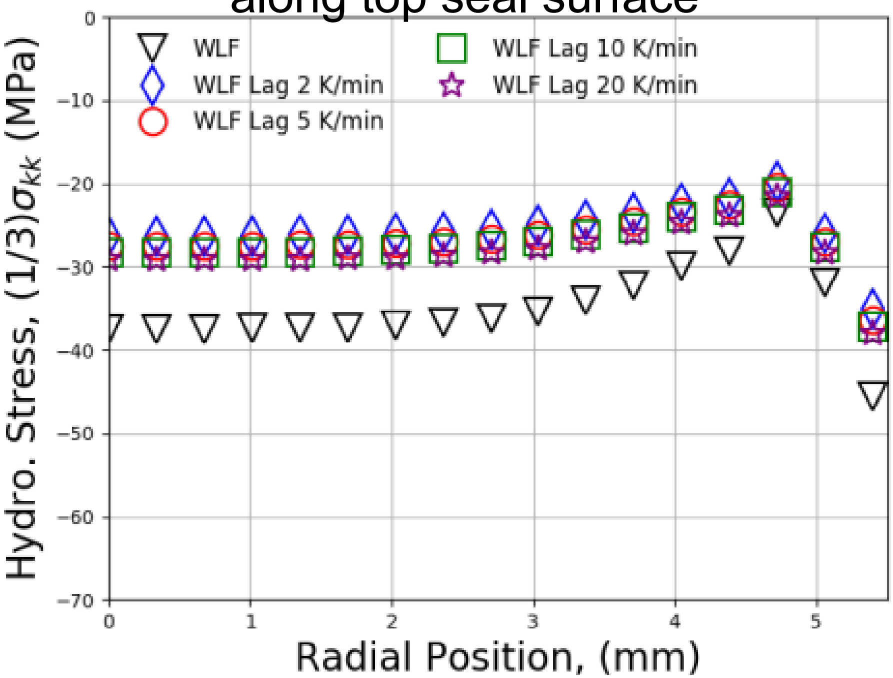


Jamison et al., SAND2017-10894

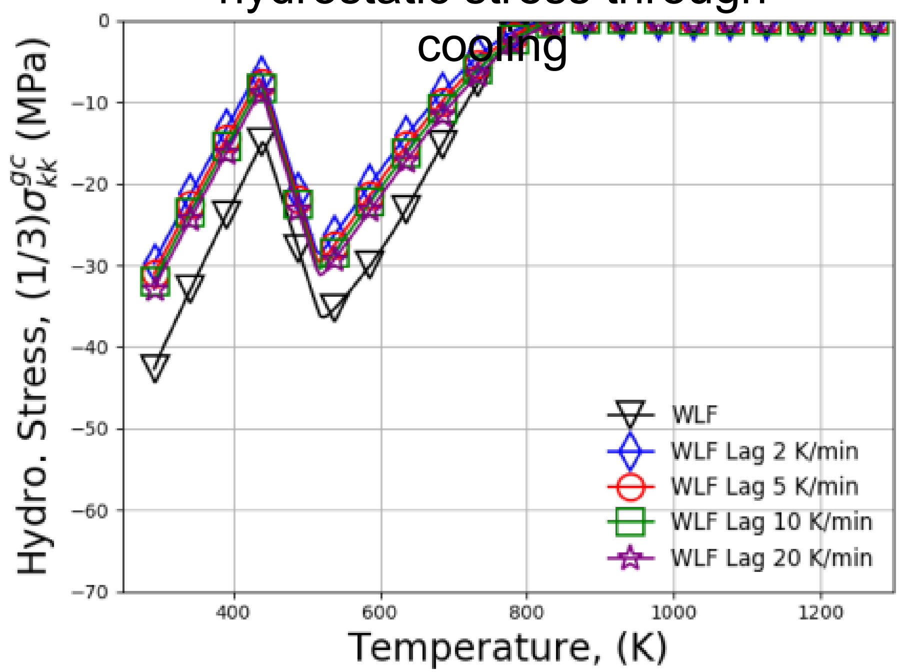
Impact of Shift Factor

- 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



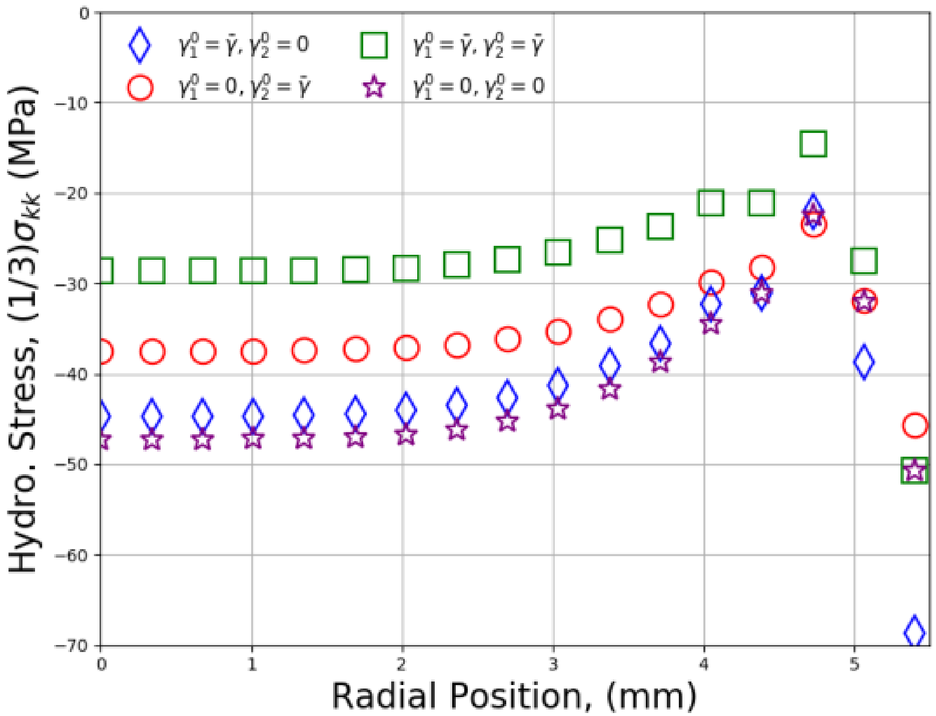
Volume averaged hydrostatic stress through cooling



- Stress state remains compressive through loading
- Impact of both viscoelastic and transformation mechanisms may be observed

Impact of Effective Stress

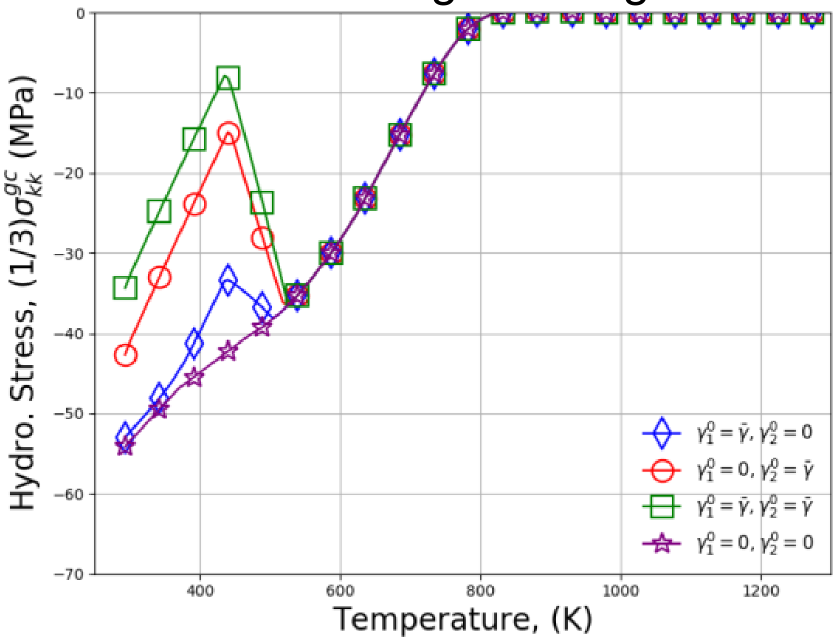
- Consider four different effective stress forms
  - Pure deviatoric, $\gamma_1^0 = \bar{\gamma},\ \gamma_2^0 = 0$
  - Pure volumetric, $\gamma_1^0 = 0,\ \gamma_2^0 = \bar{\gamma}$
  - Both volumetric and deviatoric, $\gamma_1^0 = \bar{\gamma},\ \gamma_2^0 = \bar{\gamma}$
  - No transformation, $\gamma_1^0 = 0,\ \gamma_2^0 = 0$



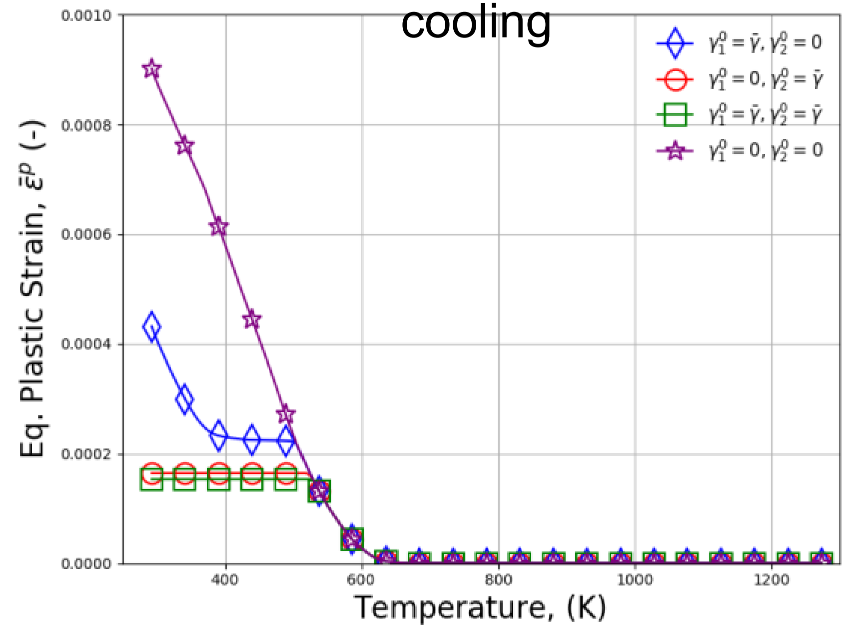
- Presence of hydrostatic strain yields lower hydrostatic stress magnitudes

Impact of Flow Rule

Vol. Avg. Hydrostatic stress through cooling



Vol. Avg. shell equiv. plastic strain through cooling



- Onset of transformation leads to differences in stress evolution
- Cases with hydrostatic stress decrease stress magnitudes and plastic strain evolution in shell
- Differences in shell versus seal dominated response

Conclusion and Summary

- Developed new phenomenological constitutive model for glass-ceramic materials
  - Coupled viscoelasticity and phase transformation
  - 3D numerical implementation

- Results show promise for use in modeling seal applications
  - Validation against simple, existing experiments
  - 3D form considered for simple seal case
  - Explored impact of shift factor and flow rule
  - Interesting interaction between different mechanisms

- Future work
  - Expanded validation exercises
  - Consideration of quartz response

Acknowledgements

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- Thanks to S. Dai (SNL) for dilatometer results

Questions?