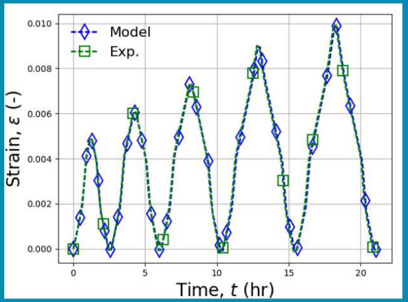
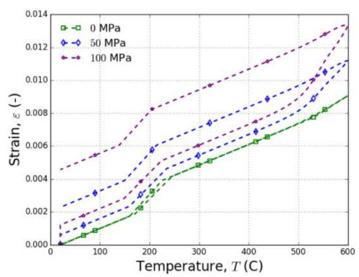
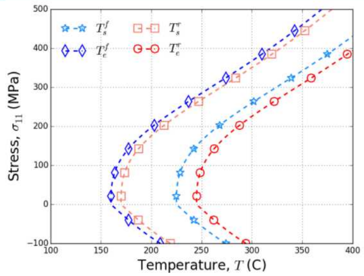
SAND2020-9435C

Modeling of Glass-Ceramic Materials and Applications







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2020 Virtual Technical Meeting of the Society of Engineering Science

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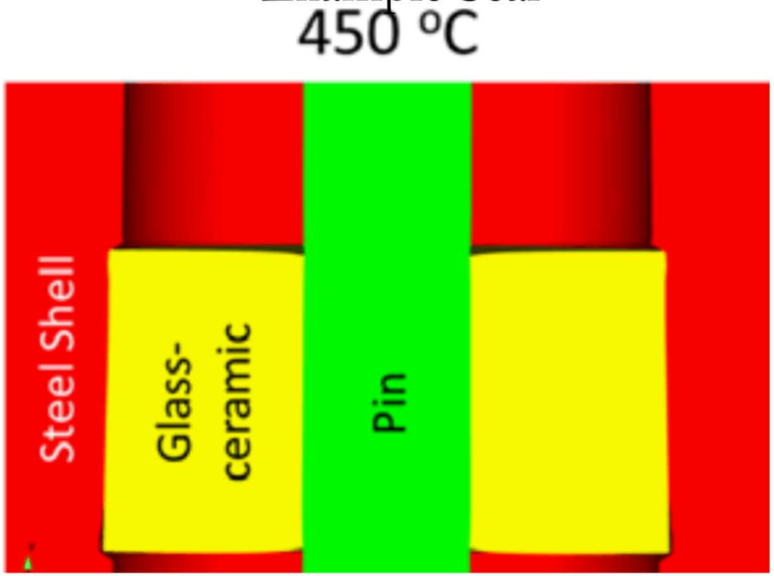
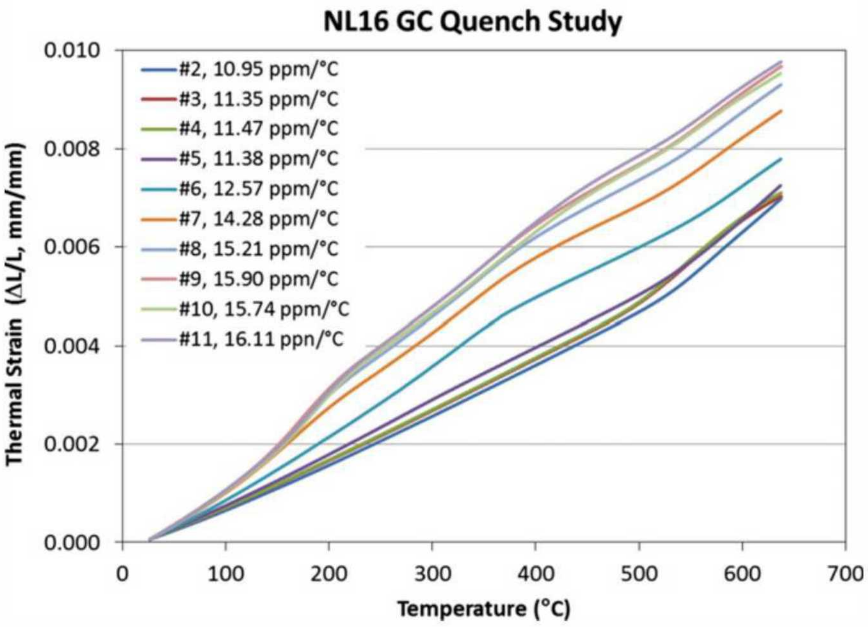
Glass-ceramic to Metal Seals (GcTMS)

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

Example Seal



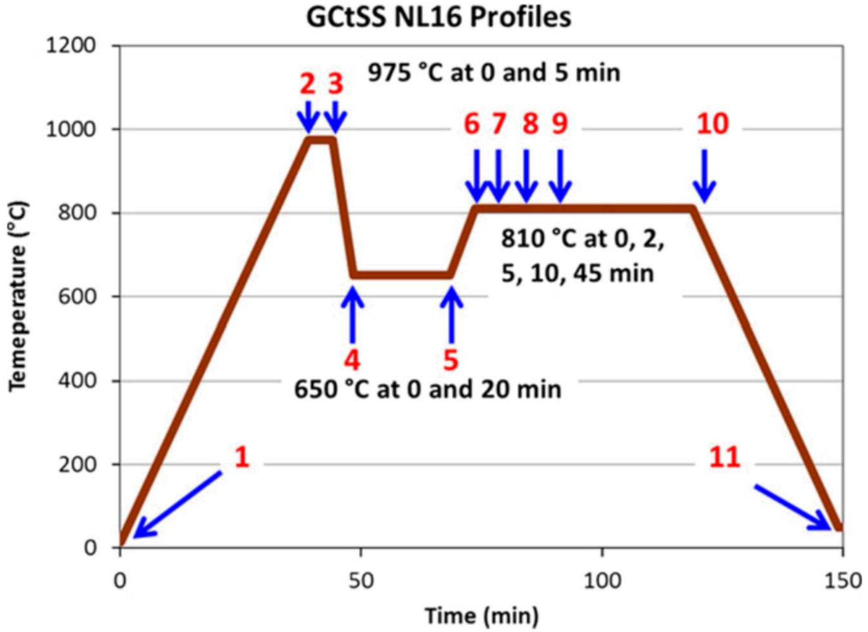
Dai *et al.*, 2017, *J Am Ceram Soc*, 100, pp.3652-3661



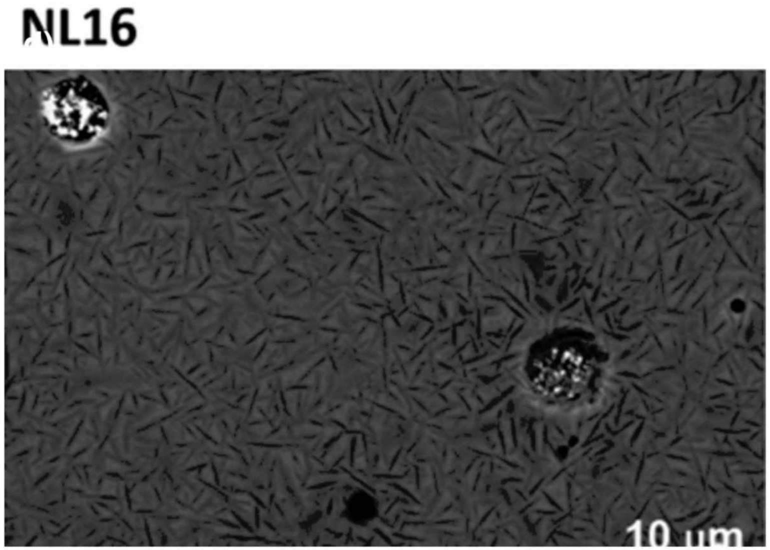
Dai *et al.*, 2016, *J Am Ceram Soc*, 99, pp.3719-3725

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

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

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

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

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

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

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)

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

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

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

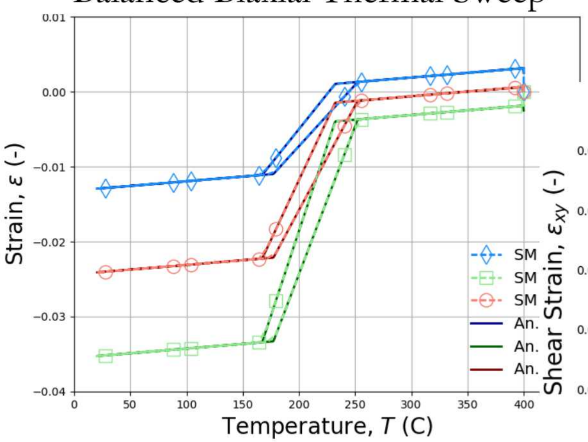
$$H_{n+1}^{1} = H_{n}^{1} + \Delta t \dot{H}_{n+1}^{1}$$

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

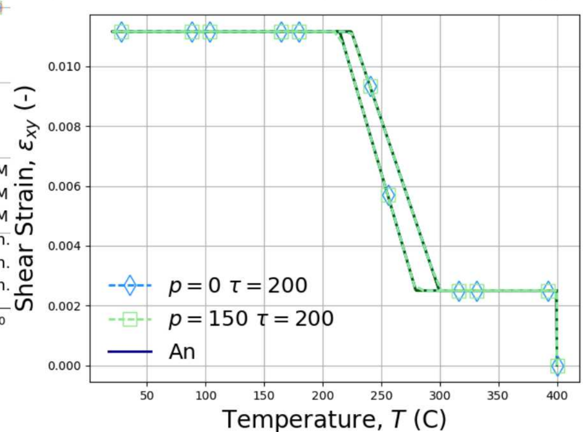
$$H_{n+1}^{3} = H_{n}^{3} + \Delta t \dot{H}_{n+1}^{3}$$

Example Verification Tests

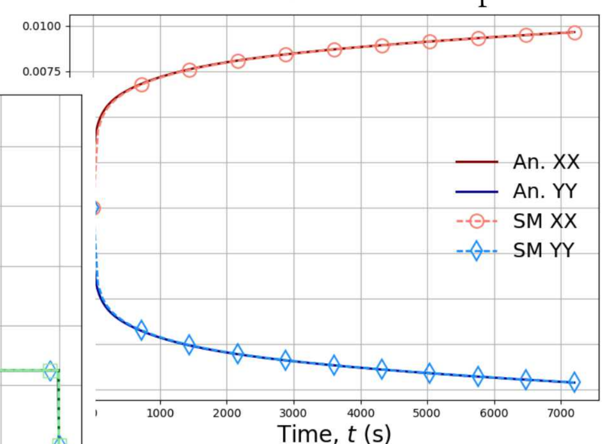
Balanced Biaxial Thermal Sweep



Pure Shear w/ Pressure

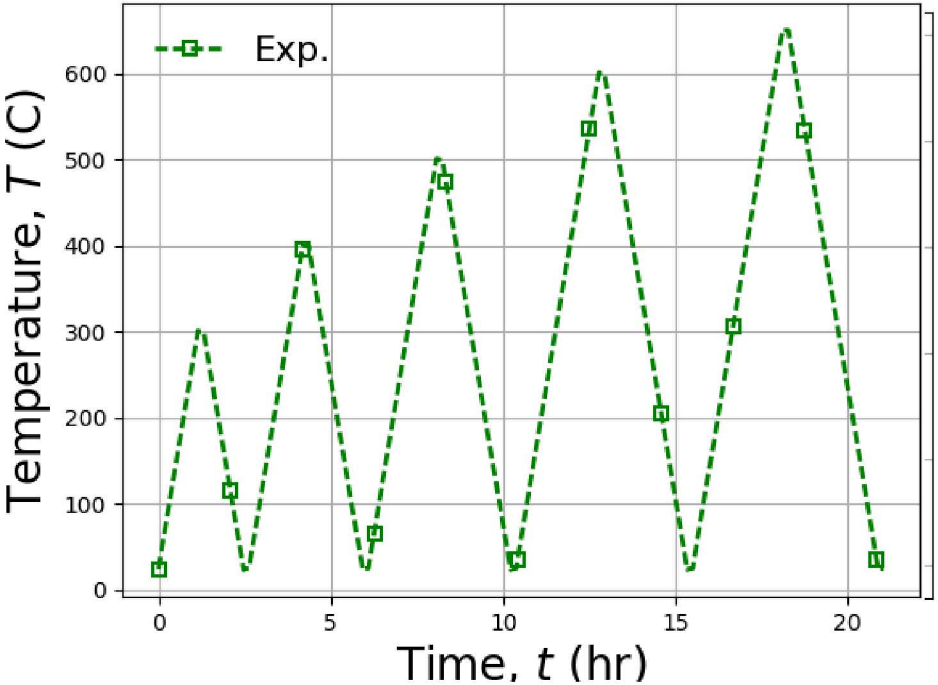


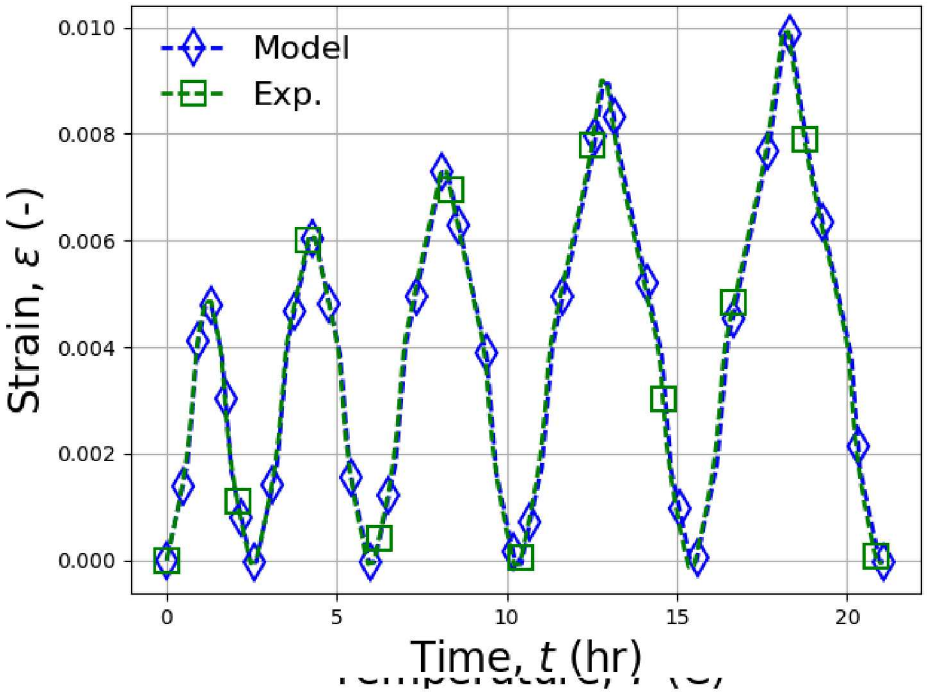
Balanced Biaxial Creep



Validation

- Consider response through no-load thermal sweeps
  - "Ladder"/ratcheting tests
  - Dilatometer (courtesy S. Dai, SNL)

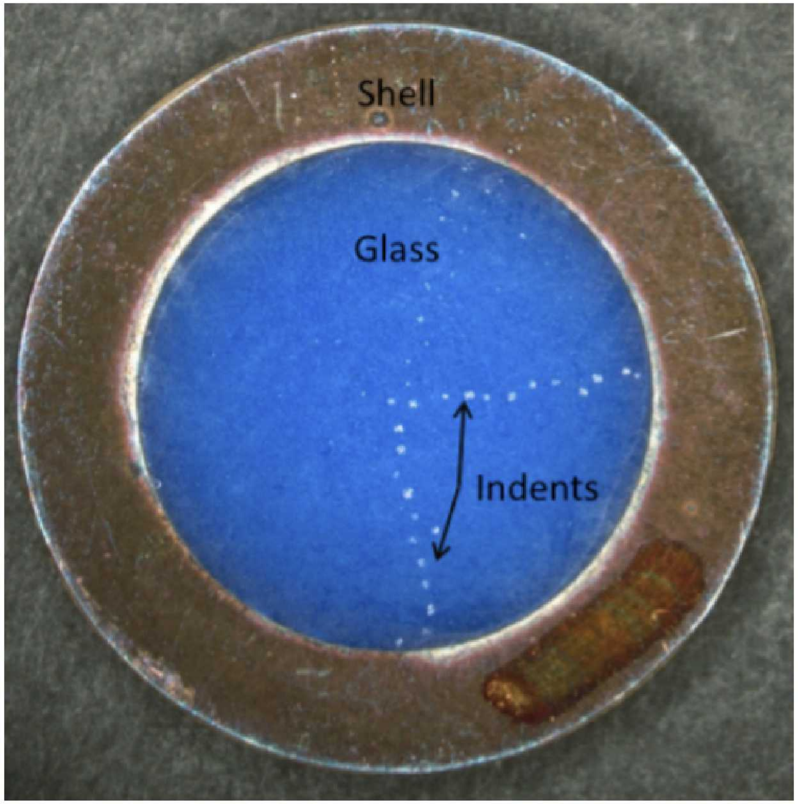




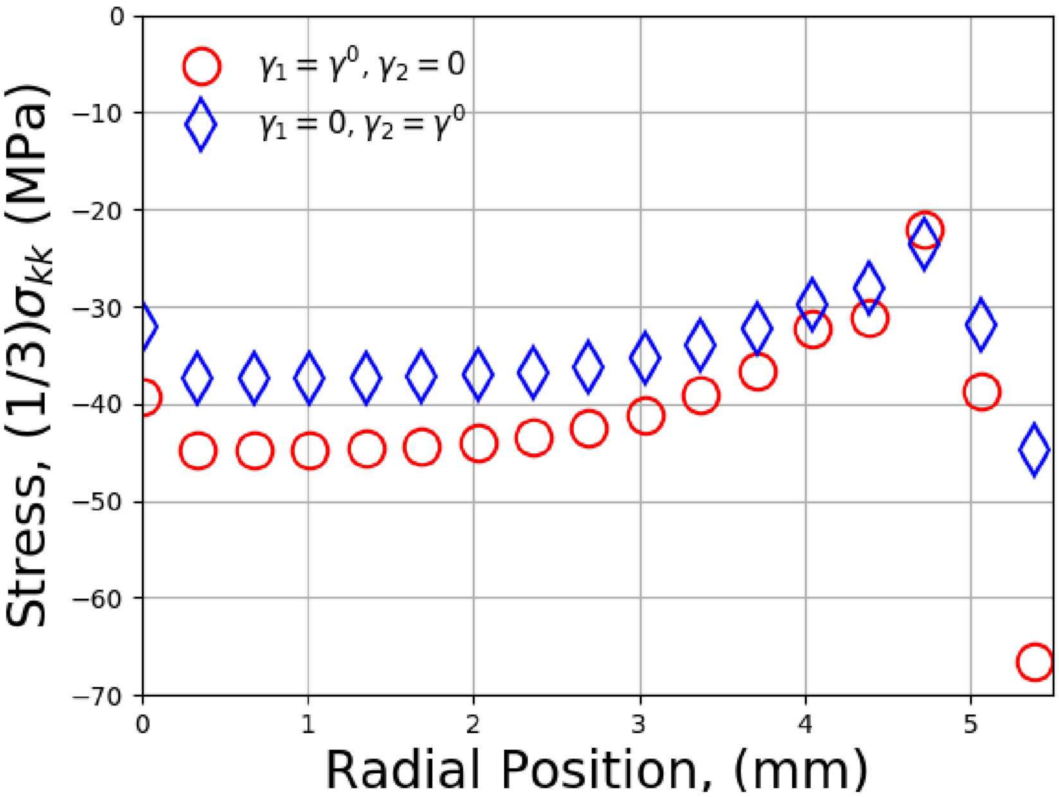
- Working on extending validation against other experiments

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
  - Consider both pure volumetric and pure deviatoric transformation strain



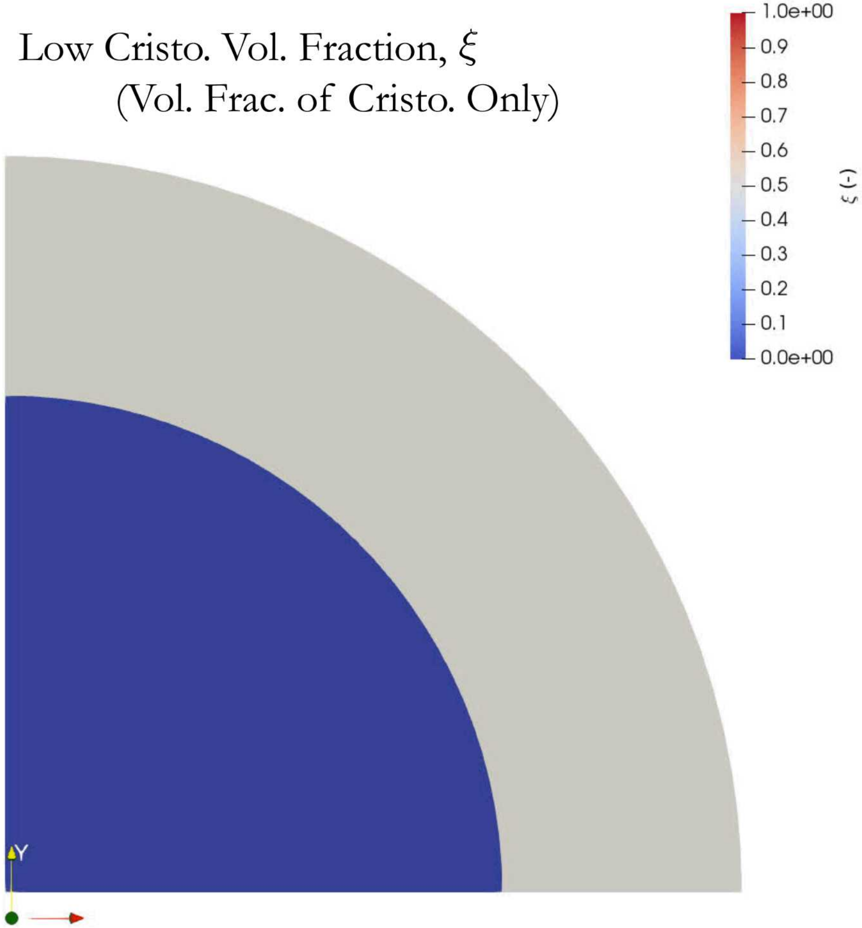
Jamison et al., SAND2017-10894



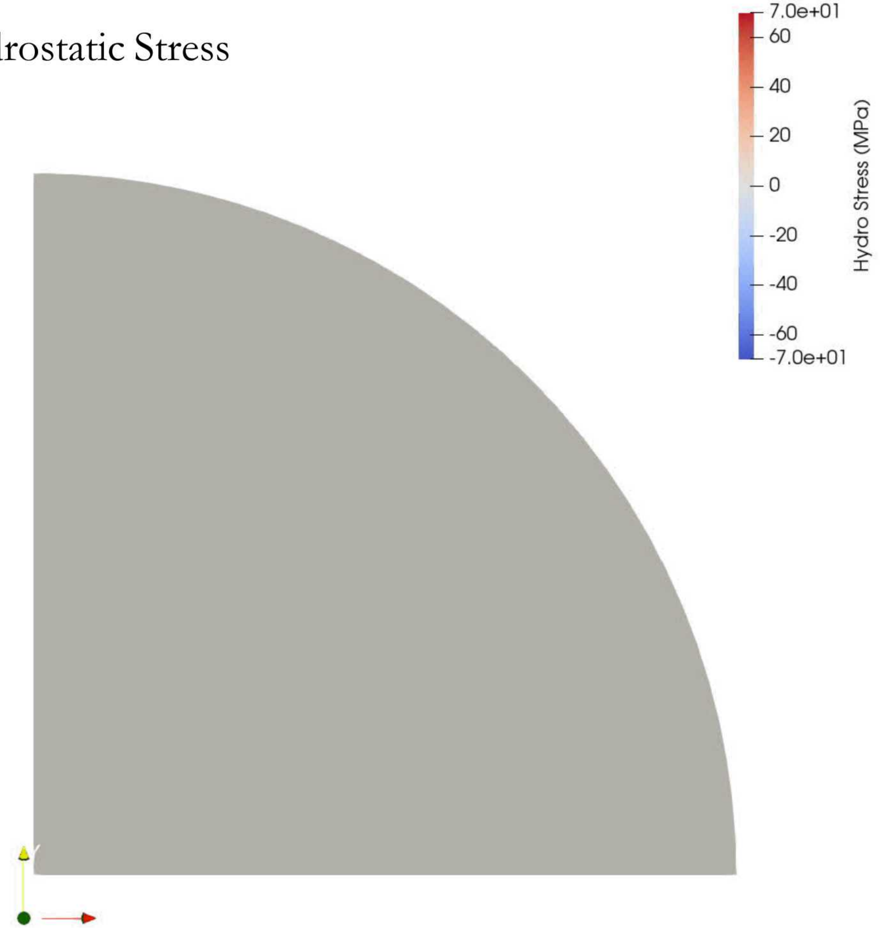
Simple Seal Results

- Look at time evolution of stress profiles
  - Consider interaction of viscoelasticity and transformation
  - Consider case of deviatoric flow rule
  - Constant cooling (2°C/min) from above T_g (700°C) to RT (20°C)

Low Cristo. Vol. Fraction, ξ
(Vol. Frac. of Cristo. Only)



Hydrostatic Stress



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

- Future work
  - Expanded validation exercises
  - Study impact of different flow-rules/shift factors

Acknowledgements

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Questions?