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A Microstructure-Informed Sintering Stress Formulation

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LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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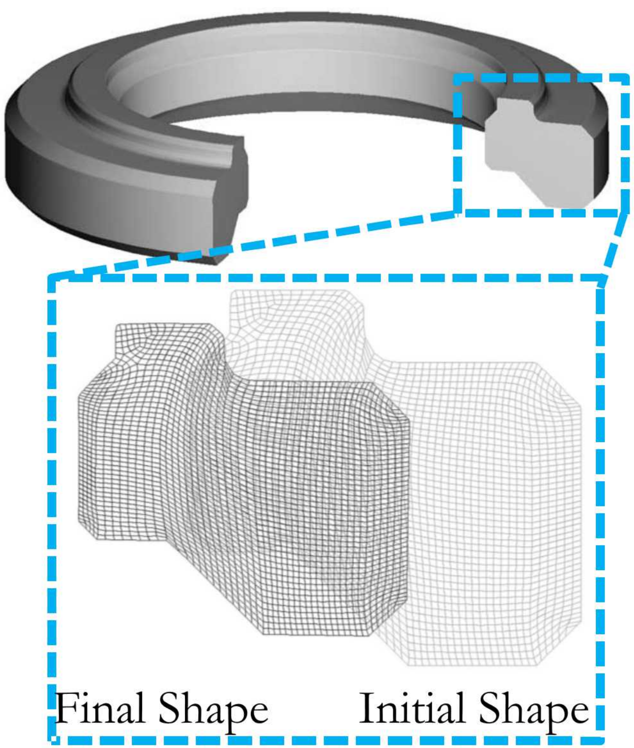
Continuum Sintering Modeling

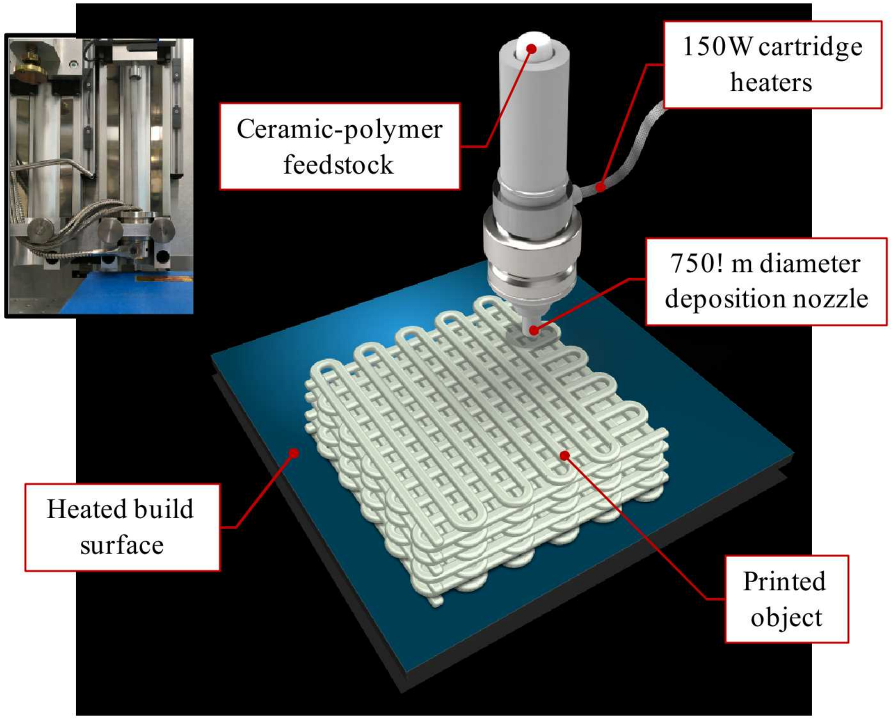
- Sintering is an important manufacturing step in both traditional and additive manufacturing
- Continuum modeling important for analysis and design

Traditional Processes



(Kraft and Riedel, 2004, *JECerS*, 24, p. 345-361)

"Direct Ink Write" Additive Manufacturing



(Abdeljawad *et al.*, 2019, *Acta Mat.*, In Press)

Sintering Stress

- Much of physics in sintering model through specification of *sintering stress*
- Forms exist for different stages; microstructure assumptions
- Limitations in terms of complex microstructure(s)

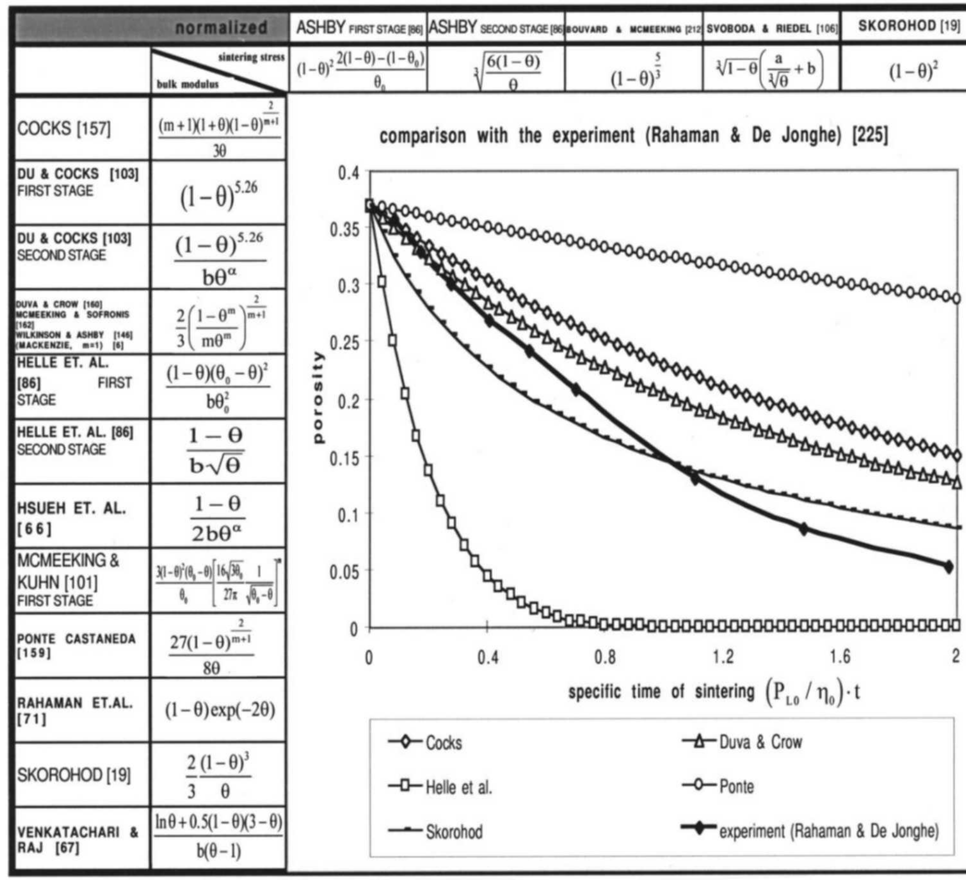
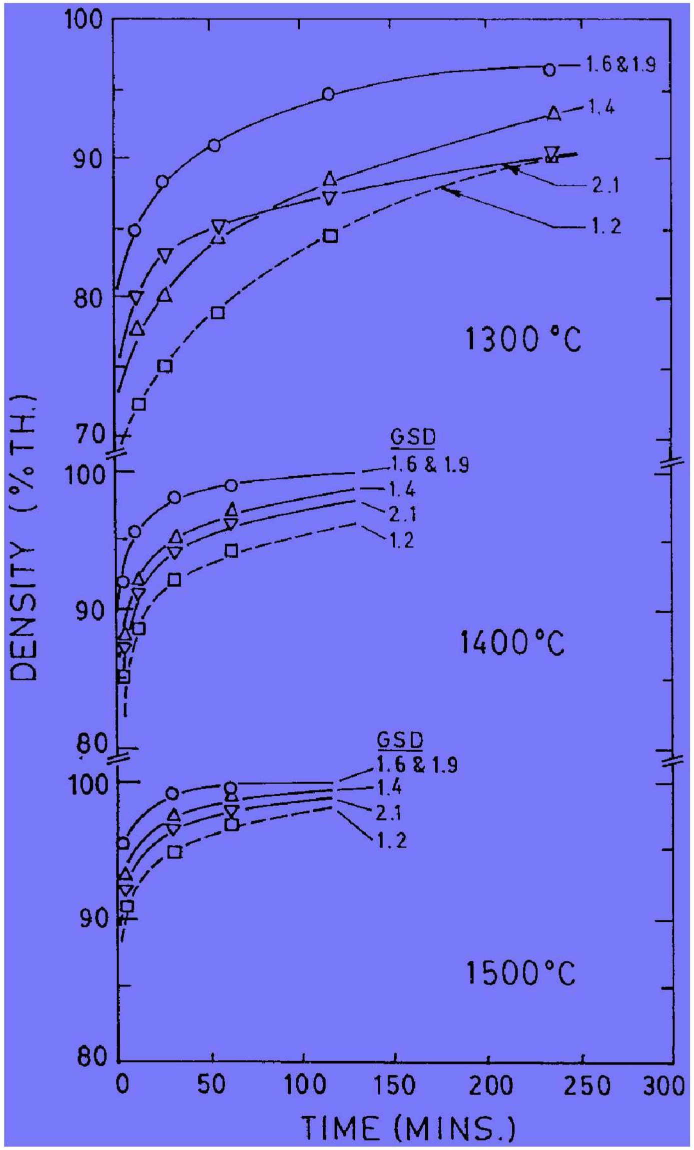


Fig. 2 of Olevsky giving various sintering stress forms

(Olevsky, 1998, “Theory of Sintering: From Discrete to Continuum”, *MSER*, R23, p. 41-100)

Objectives and Outline



- Common impact of microstructure seen through effects of *particle size distributions*
- Current constitutive models
  - Cannot capture this behavior
  - Require recalibration for each case
- Objective of current work:
  - Develop new sintering stress incorporating microstructure
    - Analytical form
    - Multiscale approach using phase field results
  - Investigate impact on continuum structure

(Ma and Lim, 2002, *Jrnl of the Euro. Cer. Soc.*, 22, p. 2197--2208)

Modeling

Skorohod-Olevsky Viscous Sintering (SOVS) Model

- Skorohod-Olevsky Viscous Sintering (SOVS) model is a common constitutive model for sintering analysis
  - Essentially derived assuming linear viscous, incompressible fluid
  - Thermodynamically based with specific volume as internal state variable (ISV)

ISVs

$$v = \frac{1}{\rho_t} = \frac{1}{\rho \rho_0} \qquad \rho = \frac{\rho_t}{\rho_0}$$

Evolution

$$\dot{\varepsilon}_{ij}^{\text{in}} = \frac{\sigma'_{ij}}{2\eta_0(T)\,\phi(\rho)} + \frac{\sigma_{kk} - 3\sigma_s(\rho)}{18\eta_0(T)\,\psi(\rho)}\delta_{ij} \qquad \dot{\rho} = -\rho\dot{\varepsilon}_{kk}^{\text{in}}$$

Functions

$$\phi(\rho) = a_1 \rho^{b_1}$$

$$\psi(\rho) = a_2 \frac{\rho^{b_2}}{(1-\rho)^{c_2}}$$

$$\eta_0(T) = a_4 \left(\frac{T}{T_0}\right)^2 + b_4 \left(\frac{T}{T_0}\right) + c_4$$

(Olevsky, 1998, *MSER*, 23, p. 41-100)

Sintering Stress

- Sintering stress is thermodynamically conjugate to specific volume

$$\sigma_s = \left(\frac{\partial F}{\partial v} \right)_T$$

- Assume a free energy, F , such that

$$F(T, v) = F_m(T) + F_s(v) \qquad F_s(v) = \alpha s(\rho(v)) v$$

- s is the specific surface that is interface area per unit volume

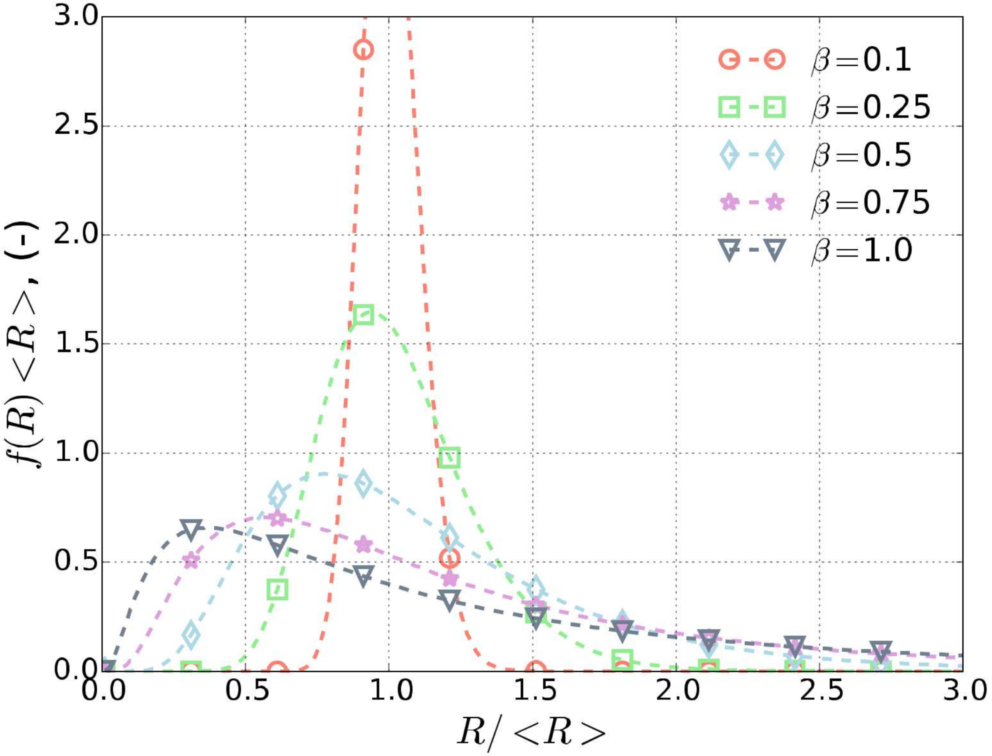
$$\sigma_s = \alpha s - \alpha \frac{ds}{d\rho} \rho$$

- Definition depends explicitly on specific surface and relative density
  - Flexible definition depending on forms of specific surface
  - Can directly incorporate microstructure information; details

Specific Surface Definitions

- Assume a log-normal distribution of particles
  - Distribution is controlled by specification of β
  - $\beta = 0$ is the monodisperse limit

$$f\left(R\right) = \frac{1}{R\sqrt{2\pi\beta^2}} \exp\left(-\frac{\left[\ln\left(\frac{R}{\langle R\rangle}\right)\right]^2}{2\beta^2}\right)$$



Specific Surface: Analytic Definition

- For analytic definitions, use two microstructure assumptions/simplifications from Torquato (2000)

Fully Penetrable Spheres

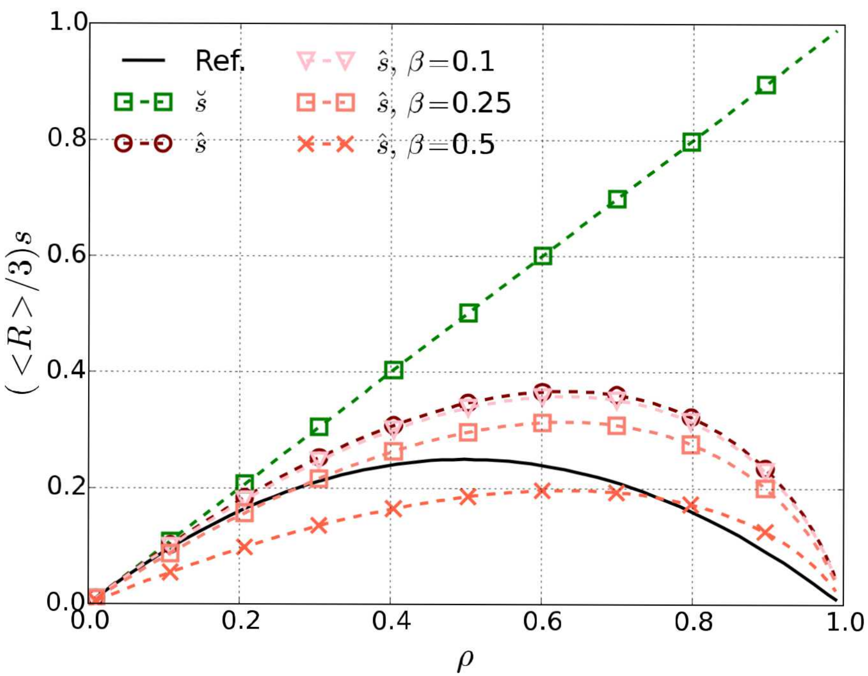
$$\hat{s} = \frac{3}{\langle R \rangle} \exp\left(-\frac{5}{2}\beta^2\right) \left((\rho - 1) \ln(1 - \rho)\right)$$

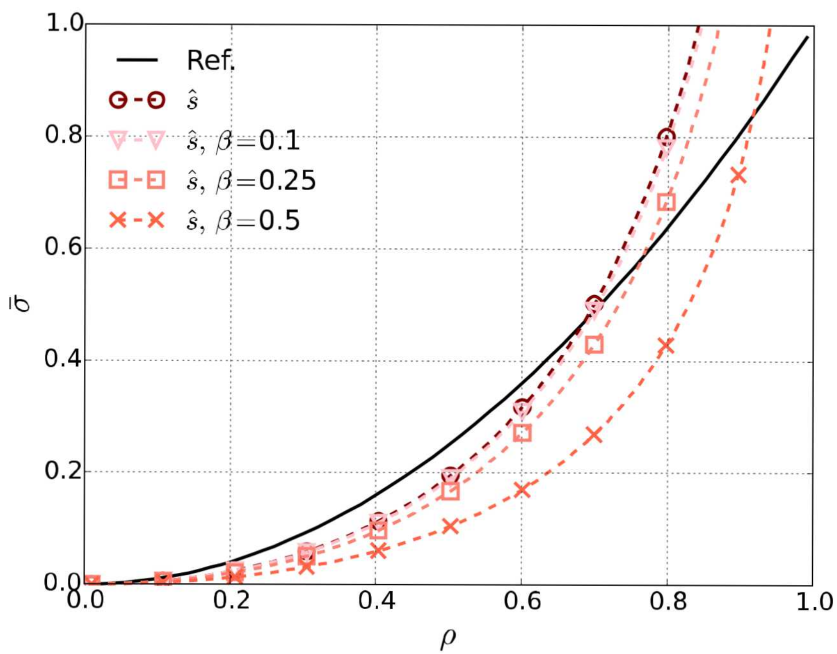
$$\hat{\sigma}_s = -\frac{3\alpha}{\langle R \rangle} \exp\left(-\frac{5}{2}\beta^2\right) \left(\rho + \ln(1 - \rho)\right)$$

Totally Impenetrable Spheres

$$\breve{s} = \frac{3}{\langle R \rangle} \exp\left(-\frac{5}{2}\beta^2\right) \rho$$

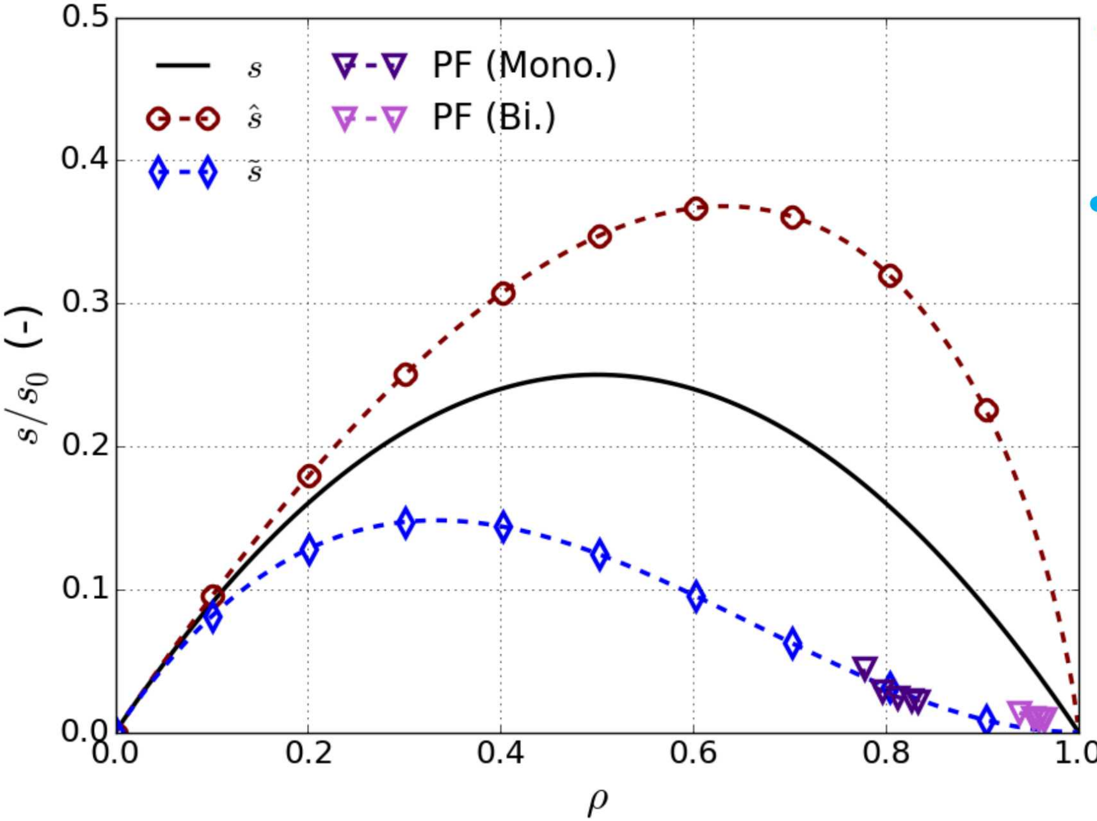
$$\breve{\sigma}_s = 0$$





Specific Surface: From Phase Field

- Lower micro-/mesoscale simulations can provide detailed analysis of microstructure evolution
- Look at recent phase field results of Abdeljawad *et al.* (2019, *Acta Mat*)



- Existing/analytic approaches do not match data
- Propose new form based on differences

$$\tilde{s} = s_0 \left(\rho - 2\rho^2 + \rho^3 \right)$$

$$\tilde{\sigma}_s = \frac{6\alpha}{\langle R \rangle} \exp\left(-\frac{5}{2}\beta^2 \right) \rho^2 (1 - \rho)$$

Results

Constitutive Response

- Look at free-sinter response
  - No-load w/ specified temperature history
  - Reduced to an ODE for relative density

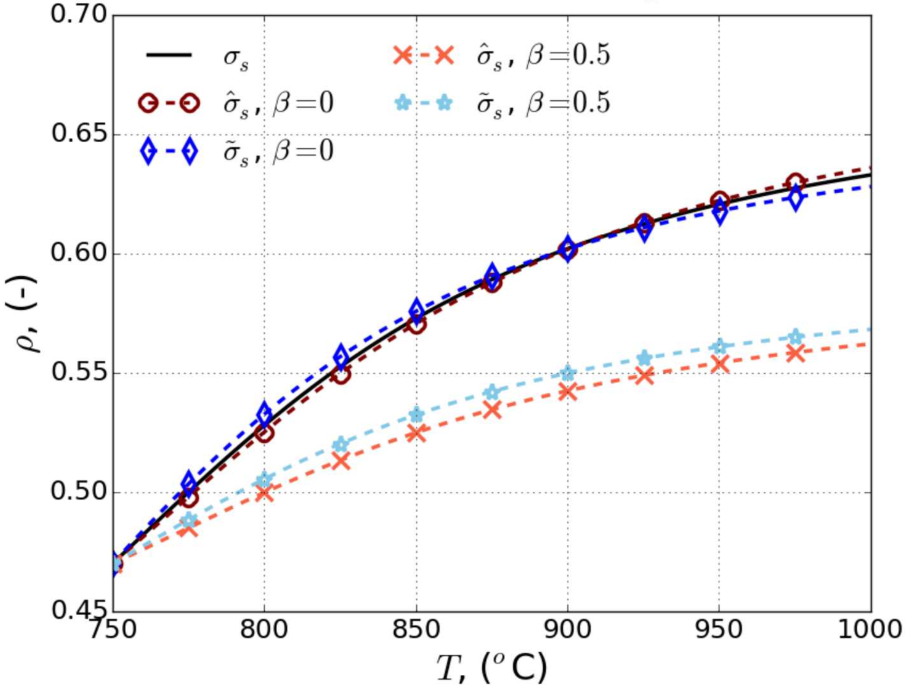
$$\dot{\rho} = \rho \frac{\sigma_{s0}\bar{\sigma}(\rho)}{2\eta_0(T)\,\psi(\rho)}$$

Material/Particle characteristics/parameters

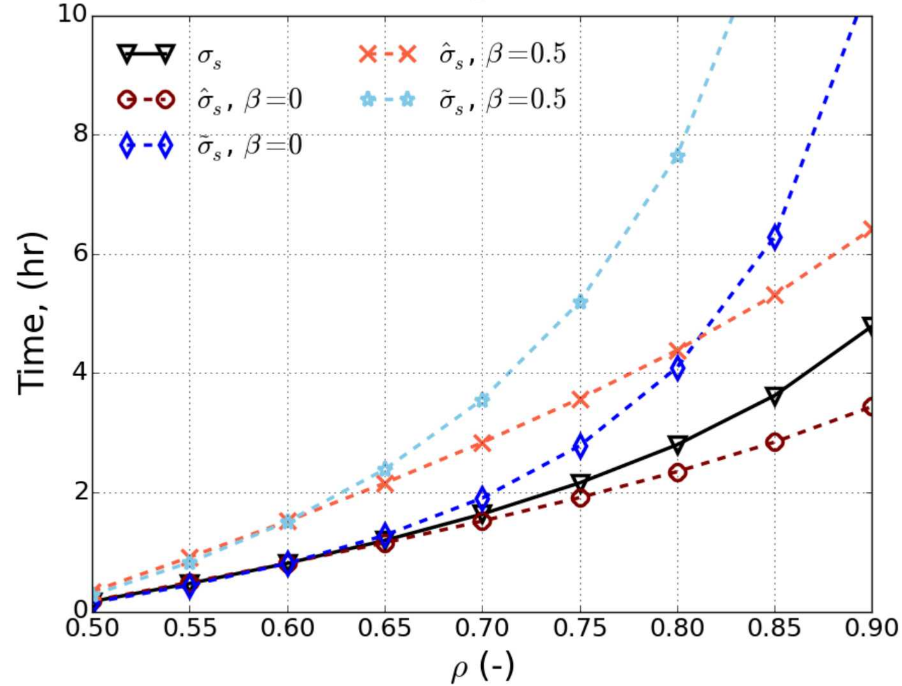
$$\sigma_s = \sigma_{s0}\bar{\sigma}(\rho)$$

Rel. Density Dependence

Sintering profile through constant, linear ramp



Sintering times to specified density at constant temperature (900°C)



Scaling Law

- The scaling laws of Herring provide useful relationships on impact of different features
- Consider two sets of particles exactly the same but of different radii, $r_2 = \lambda r_1$

$$\frac{\dot{\rho}_2}{\dot{\rho}_1} = \frac{\rho \frac{\sigma_{s0(2)}\bar{\sigma}}{2\eta_0 \psi}}{\rho \frac{\sigma_{s0(1)}\bar{\sigma}}{2\eta_0 \psi}} = \frac{r_1}{r_2} \qquad \dot{\rho} = \frac{\Delta\rho}{\Delta t} \Rightarrow \frac{\Delta t_2}{\Delta t_1} = \lambda$$

- Now consider the case two particle distributions, $r_2 = r_1$, $\beta_2 \neq \beta_1$

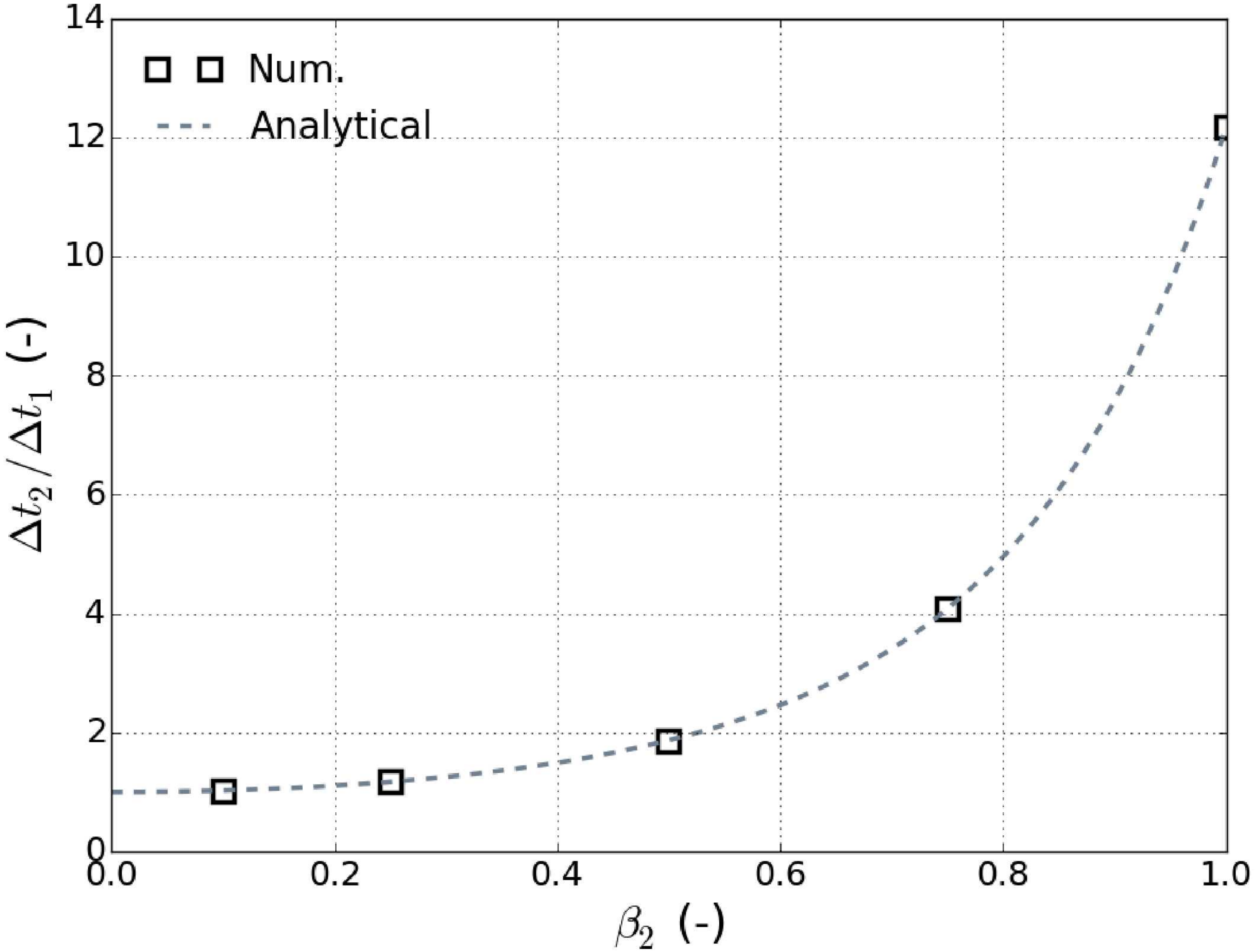
$$\frac{\dot{\rho}_2}{\dot{\rho}_1} = \frac{\rho \frac{\sigma_{s0} \exp\left[-(5/2)\beta_2^2\right]\bar{\sigma}_s}{2\eta_0 \psi}}{\rho \frac{\sigma_{s0} \exp\left[-(5/2)\beta_1^2\right]\bar{\sigma}_s}{2\eta_0 \psi}}$$

$$\frac{\Delta t_2}{\Delta t_1} = \exp\left[\frac{5}{2}\left(\beta_2^2 - \beta_1^2\right)\right] \rightarrow \exp\left(\frac{5}{2}\beta_2^2\right)$$

(Herring, 1950, *Jrnl. Appl. Phy.*, **21**, p. 301-303)

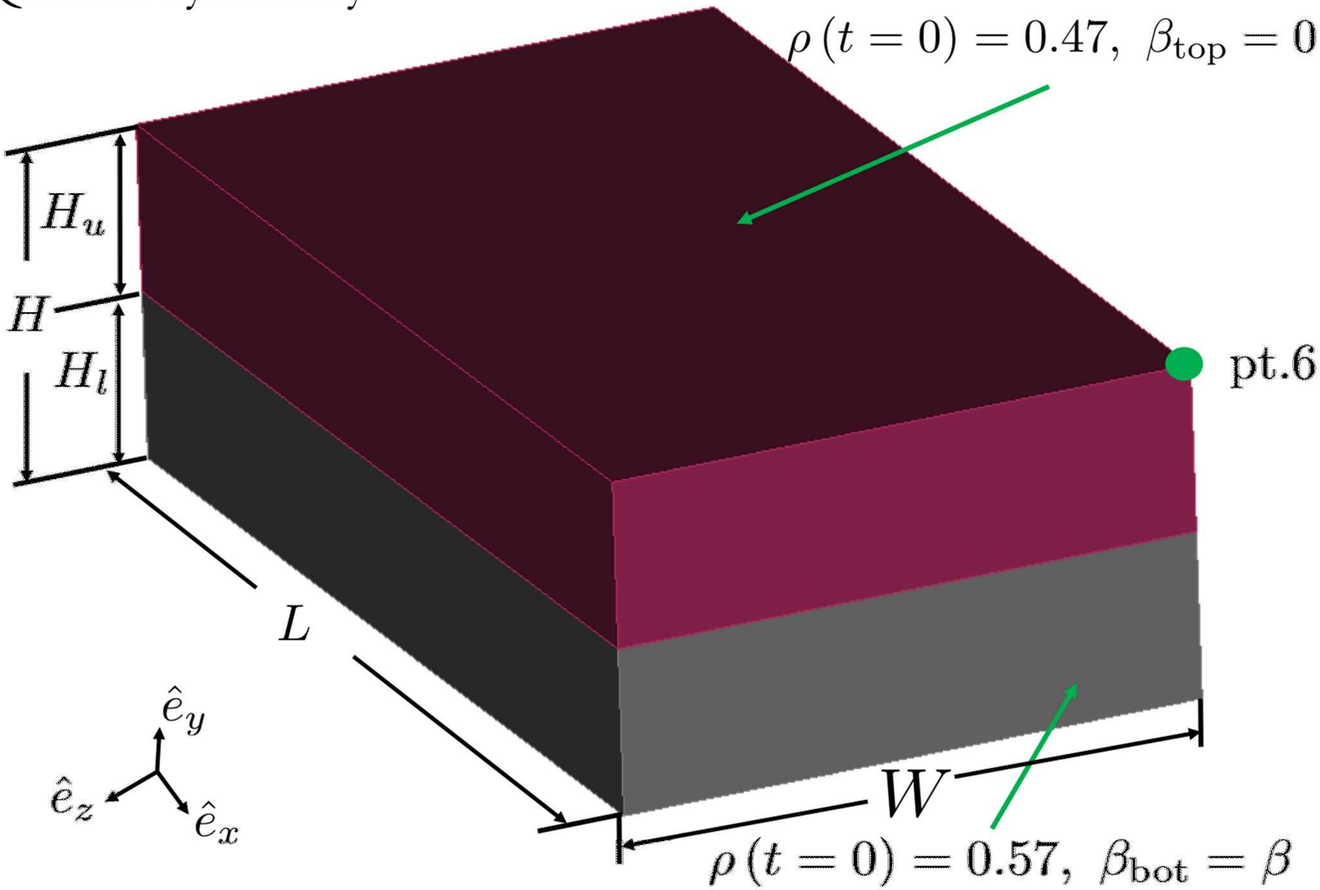
Scaling Law Results

- Increasing the breadth of the distribution can greatly increase sintering time for equivalent initial green densities



Structural Impact

- Consider the bilayer bar problem of Argüello *et al.*
  - Constant linear ramp temperature profile
  - No applied load
  - Quarter Symmetry

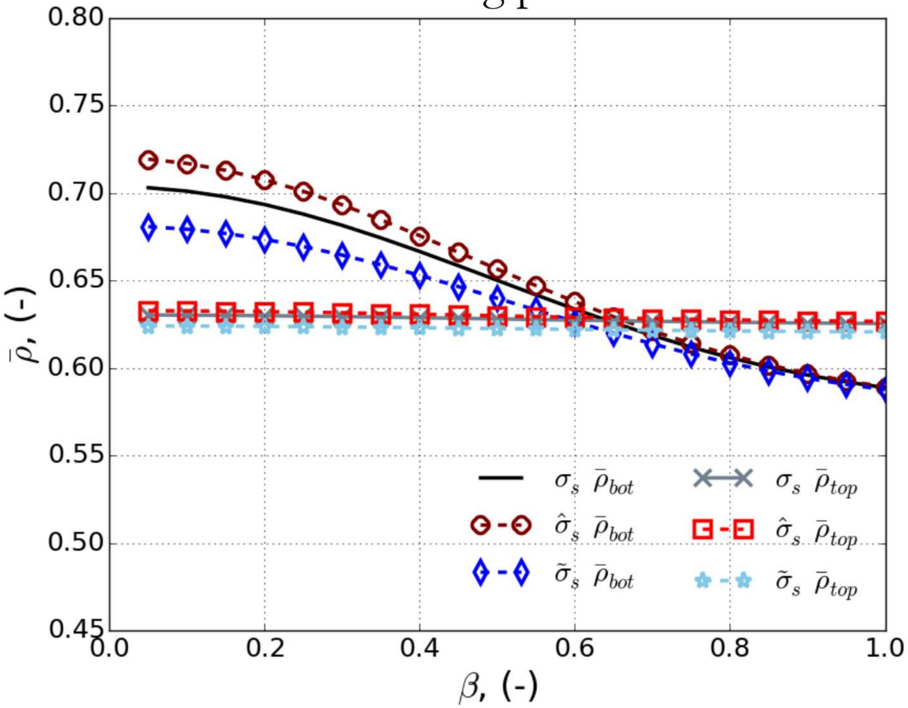


(Argüello *et al.*, 2009, *JACerS*, **92**(7), p. 1442-1339)

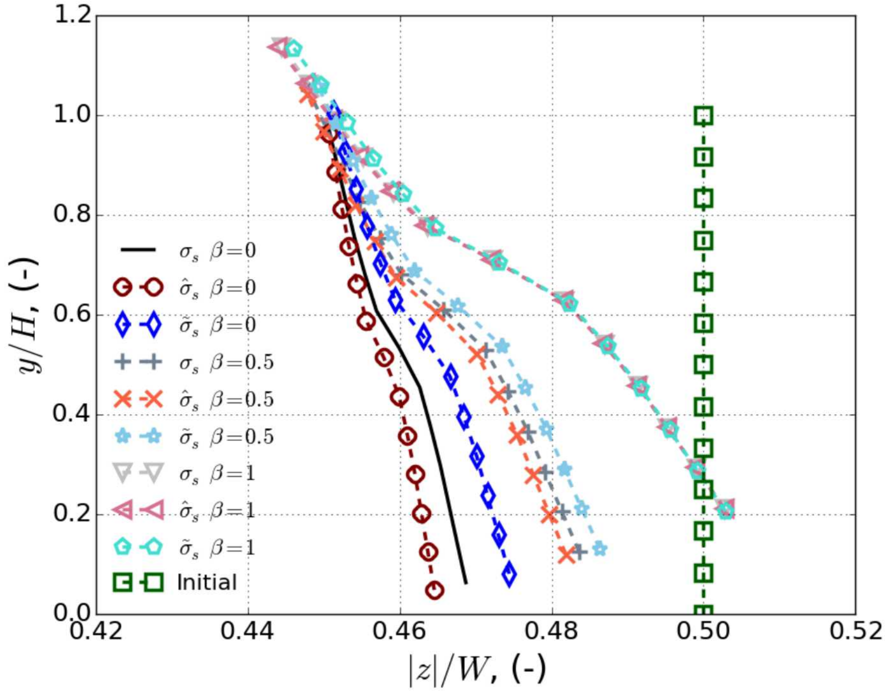
Bilayer Bar Results

- Changing the particle size distribution of the bottom layer can have a large impact on structural response
  - Avg. relative density of bottom can be greater or lower than top
  - Large differences in final shape

Avg. relative density at the end of the sintering profile

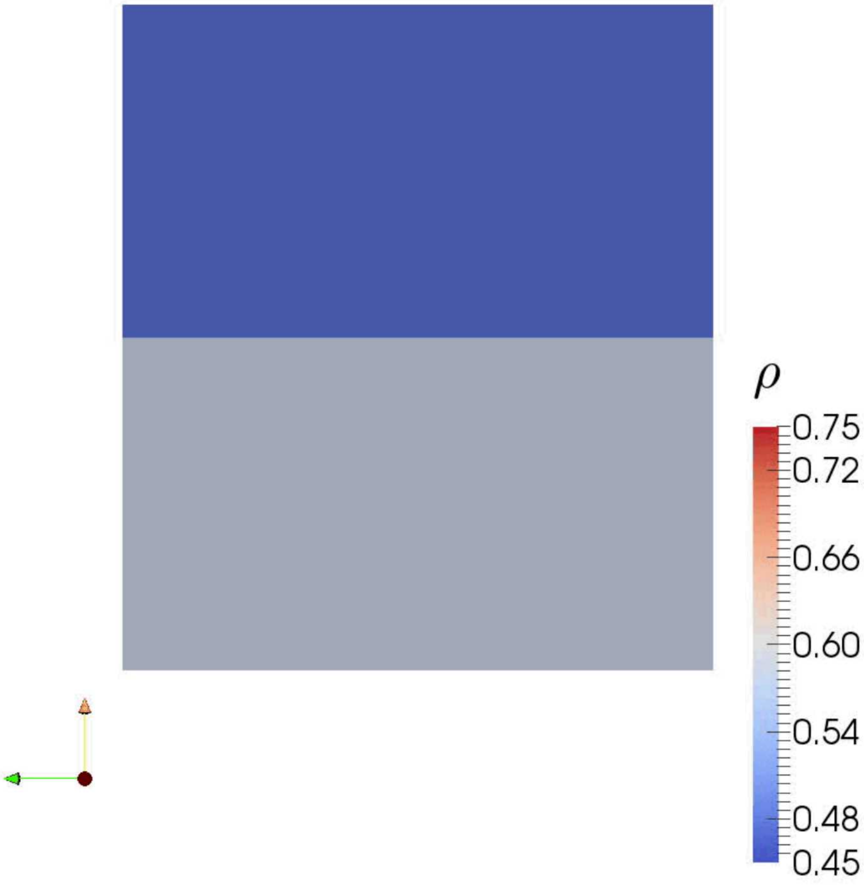


Final edge profile of bilayer bar with different sintering stresses

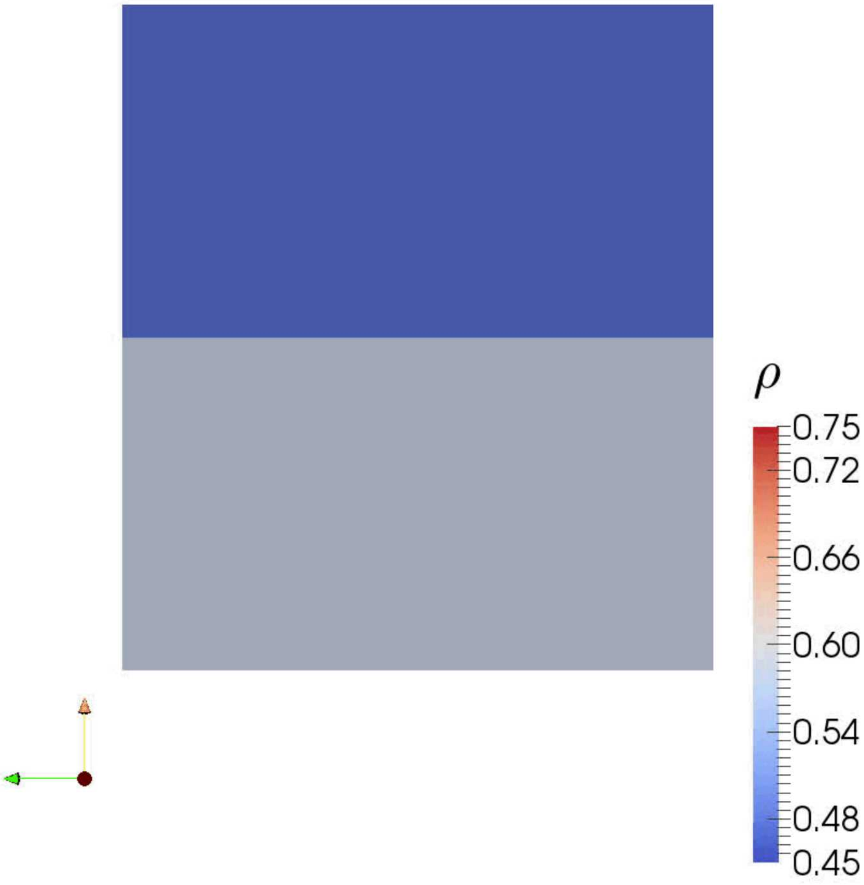


Relative Density Profile

$$\beta = 0$$



$$\beta = 1$$



Summary and Conclusions

- Developed a new expression for the sintering stress
  - Analytical expressions based on simplifying assumptions
  - A microstructure informed expression leveraging lower scale phase field results
- New expressions can directly incorporate quantified microstructure parameters including particle size distribution
- Polydispersity can have a strong impact on constitutive and structural behaviors
- Propose a new exponential scaling law

- Future work
  - Experimental validation
  - Extension to incorporate stages of sintering; micromechanical impact on relative viscosity terms

- B. T. Lester, F. Abdeljawad, and J. E. Bishop, “A Sintering Stress Formulation Incorporating Particle Size Distributions”, Submitted

Acknowledgements

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