



Sandia
National
Laboratories

Statistical Modeling of Mechanical Lifetime in Glass and Ceramic

Scott Grutzik, Thomas Diebold, Kevin Strong

sjgrutz@sandia.gov

International Conference on Ceramics and Advanced Composites

January 22-27, 2023



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Statistical lifetime prediction for brittle materials



Brittle materials fail stochastically and interact with water for delayed failure or reduction in strength. How to combine these?

Probabilistic failure at short times

$$P_W = 1 - \exp \left[- \left(\frac{\sigma}{\sigma_0} \right)^\rho \right]$$

Single crack propagation at long times

$$v(K_I) = A \left(\frac{K_I}{K_{Ic}} \right)^n$$

$$K_I = Y(a) \sigma \sqrt{a}$$



$$t_f = \frac{2K_{Ic}^2}{A(n-2)Y^2\sigma_f^2} \left[\left(\frac{\sigma_i}{\sigma_f} \right)^{n-2} - 1 \right]$$

How do we predict probabilistic failure at long times? Solve the t_f equation for σ_f and assume that Weibull stress σ_0 evolves in the same way while shape ρ stays constant? Sometimes this is done, but can we do better?

Proposed method for probabilistic lifetime prediction



Solve the t_f equation for σ_i . This is the initial strength of a specimen that failed at time t_f and stress σ_f .

$$t_f = \frac{2K_{Ic}^2}{A(n-2)Y^2\sigma_f^2} \left[\left(\frac{\sigma_i}{\sigma_f} \right)^{n-2} - 1 \right] \quad \longrightarrow \quad \sigma_i = \left[\frac{A(n-2)Y^2\sigma_f^2 t_f}{2K_{Ic}^2} + 1 \right]^{\frac{1}{n-2}} \sigma_f$$

Since a Weibull distribution fit to strength data collected at beginning of life characterizes the un-aged flaw population we can substitute σ_i into the Weibull distribution as σ_0 .

$$P_f(\sigma_i) = P_f[\sigma_i(\sigma_f, t_f; A, n, K_{Ic}, Y)] = 1 - \exp \left(- \left\{ \frac{\left[\frac{A(n-2)Y^2\sigma_f^2 t_f}{2K_{Ic}^2} + 1 \right]^{\frac{1}{n-2}} \sigma_f}{\sigma_0} \right\}^\rho \right)$$

If we neglect the "1" in the numerator we can get effective aged Weibull properties, note that ρ is not constant during aging

$$\tilde{\sigma}_0 = \left[\frac{2K_{Ic}^2}{A(n-2)Y^2 t_f} \right]^{\frac{1}{n}} \sigma_0^{1-\frac{2}{n}}$$

$$\tilde{\rho} = \left(\frac{n}{n-2} \right) \rho$$

Validation experiment: static strength time to failure

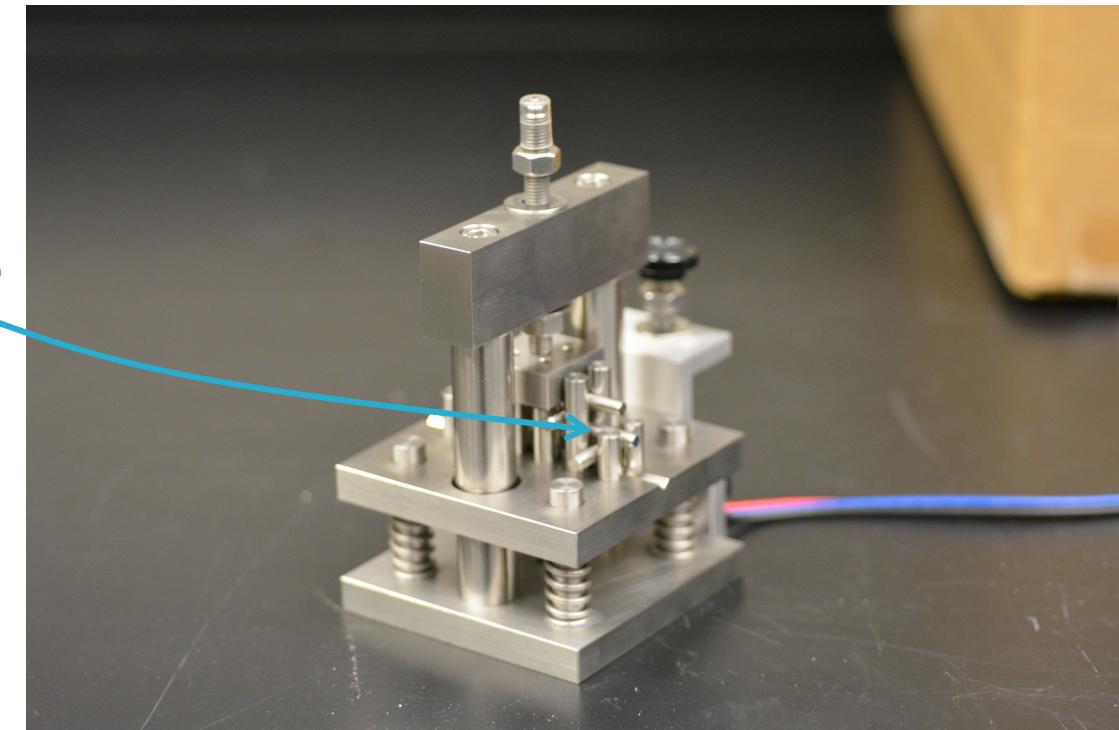
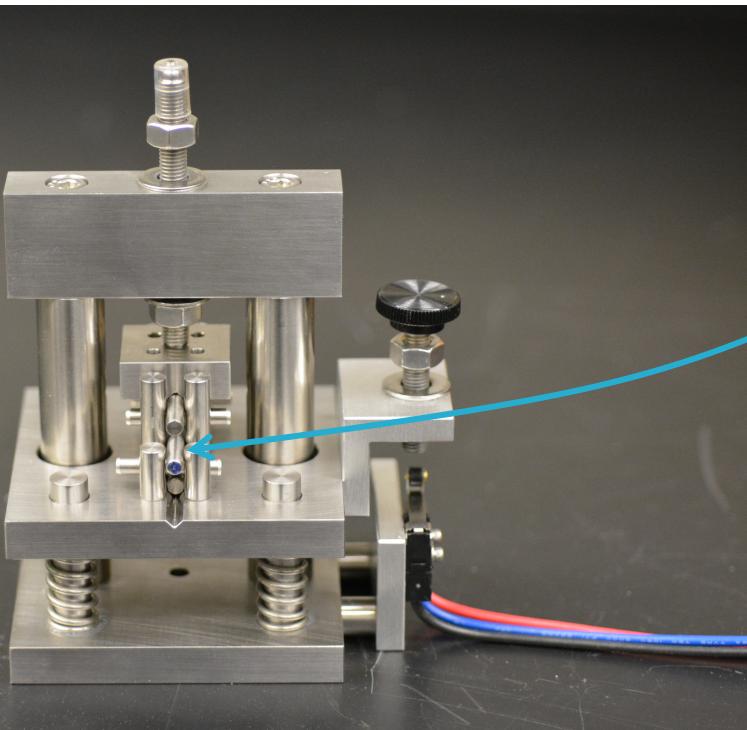


The proposed method seems reasonable, but we don't know if flaws actually age in this way.

As a validation, small screw loaded four point bending load frames were designed and fabricated. The specimen is fully articulated with roller contacts.

Load is applied with dead load weights to compress the springs. A calibrated force cell is used to verify the load. Then the top nut is tightened and dead weight is removed.

An electronic switch connected to a timing circuit detects bend bar failure.



Validation experiment: static strength time to failure

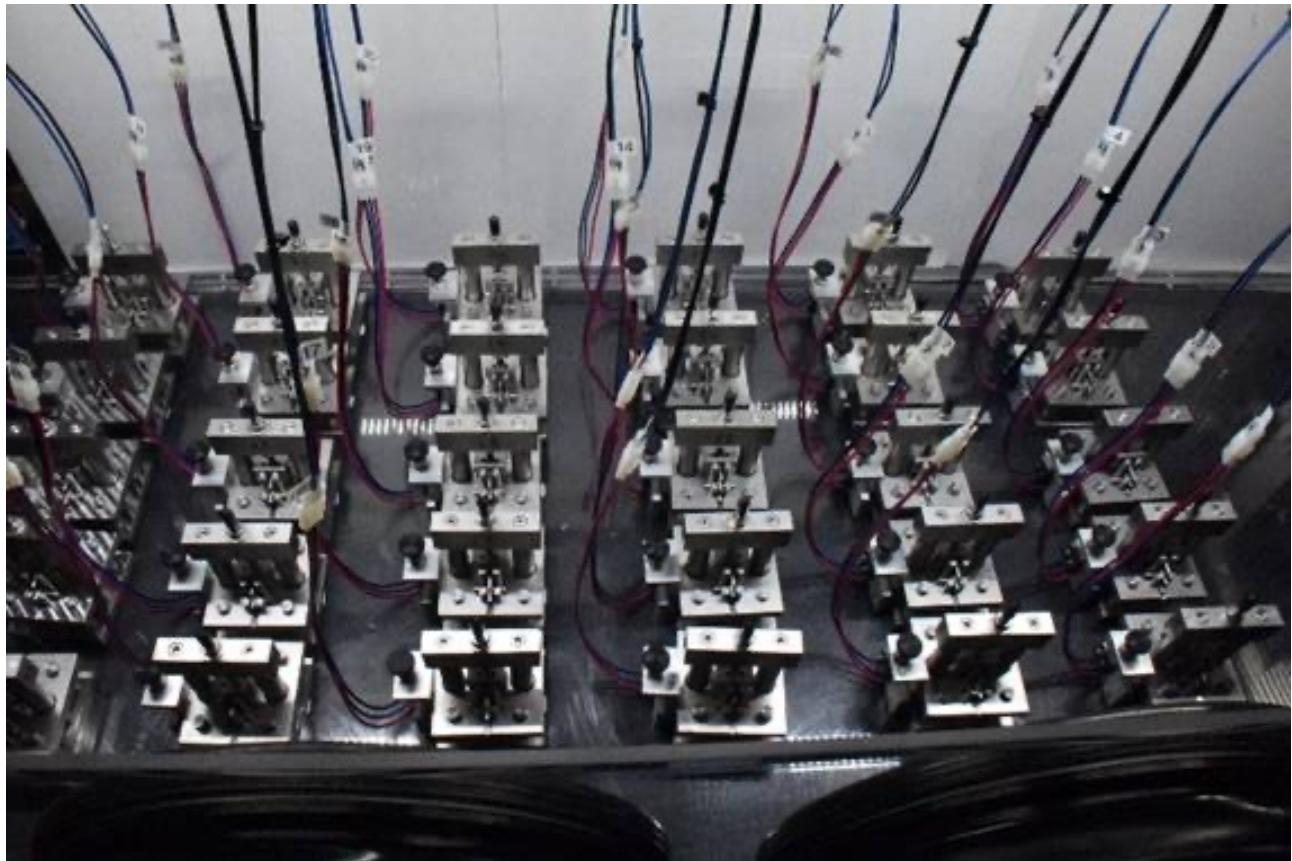


30 static load frames were aged in controlled atmosphere at constant 95% relative humidity and room temperature

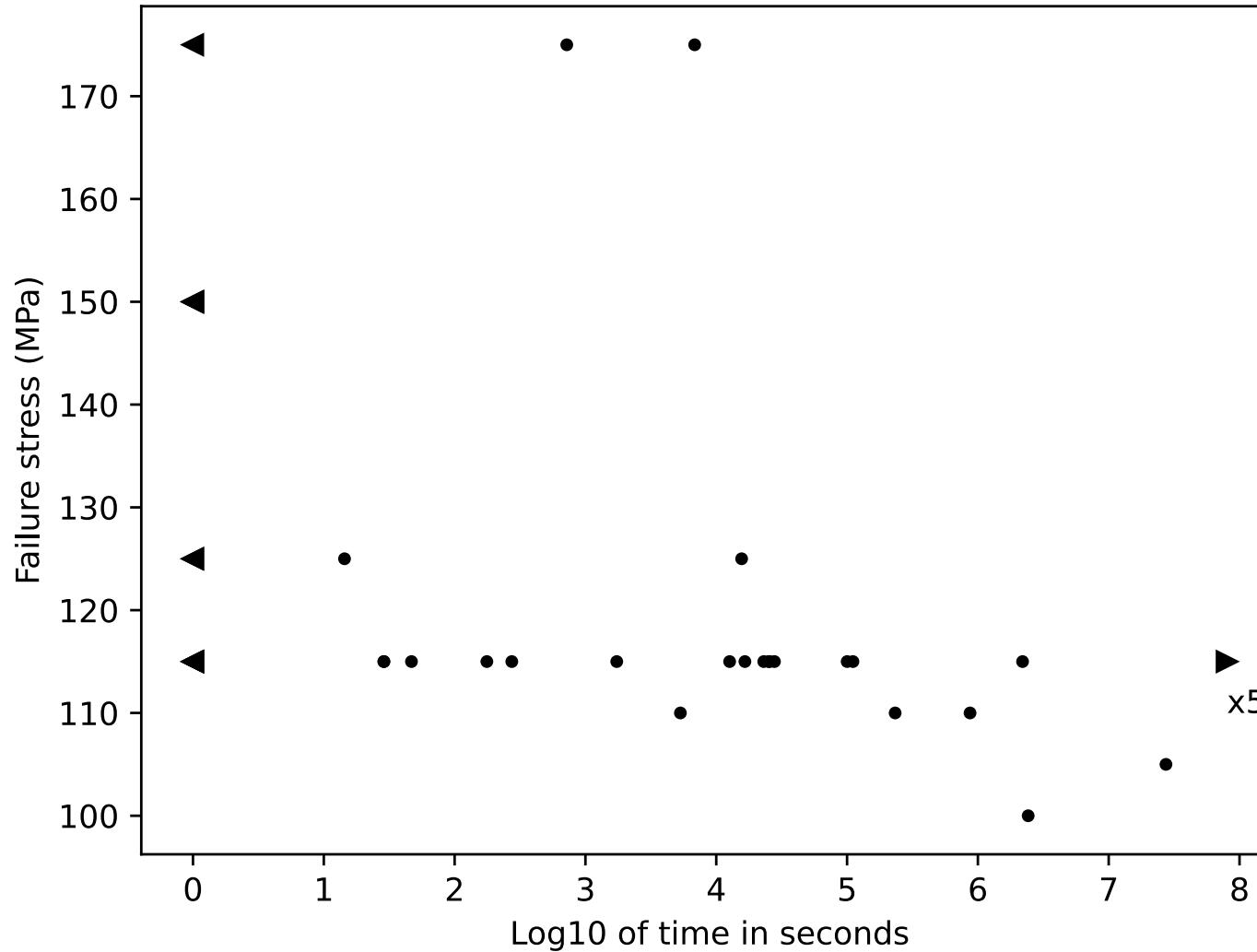
Failure times were measured at various load levels

ASTM size B bend bars were used in all cases

- 3 x 4 mm cross section
- 20 mm inner span
- 40 mm outer span
- 45 mm total length



Static strength time to failure results for barium titanate



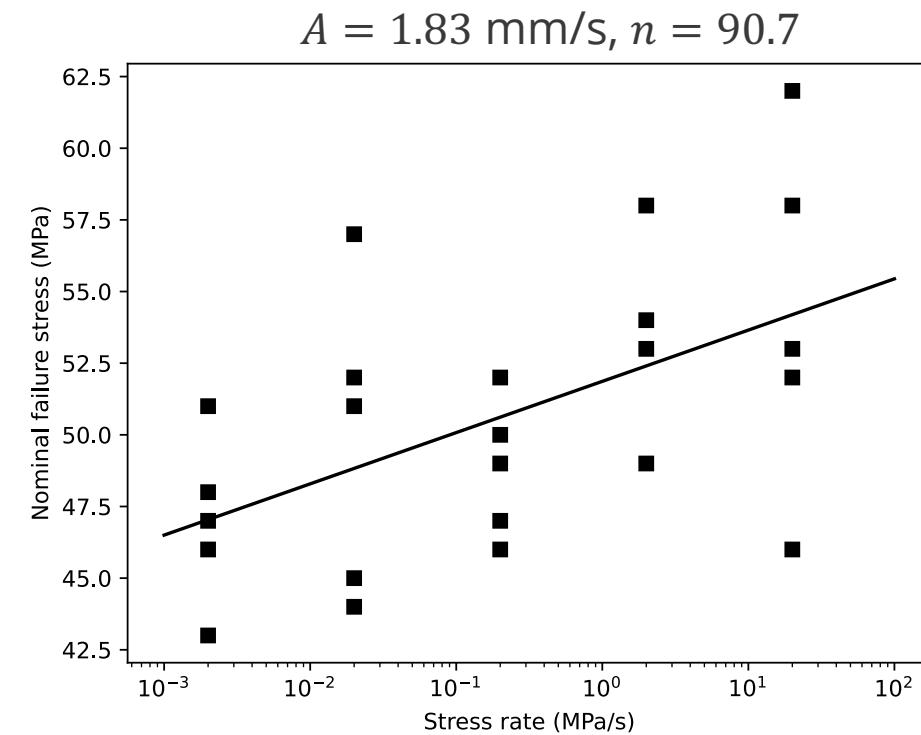
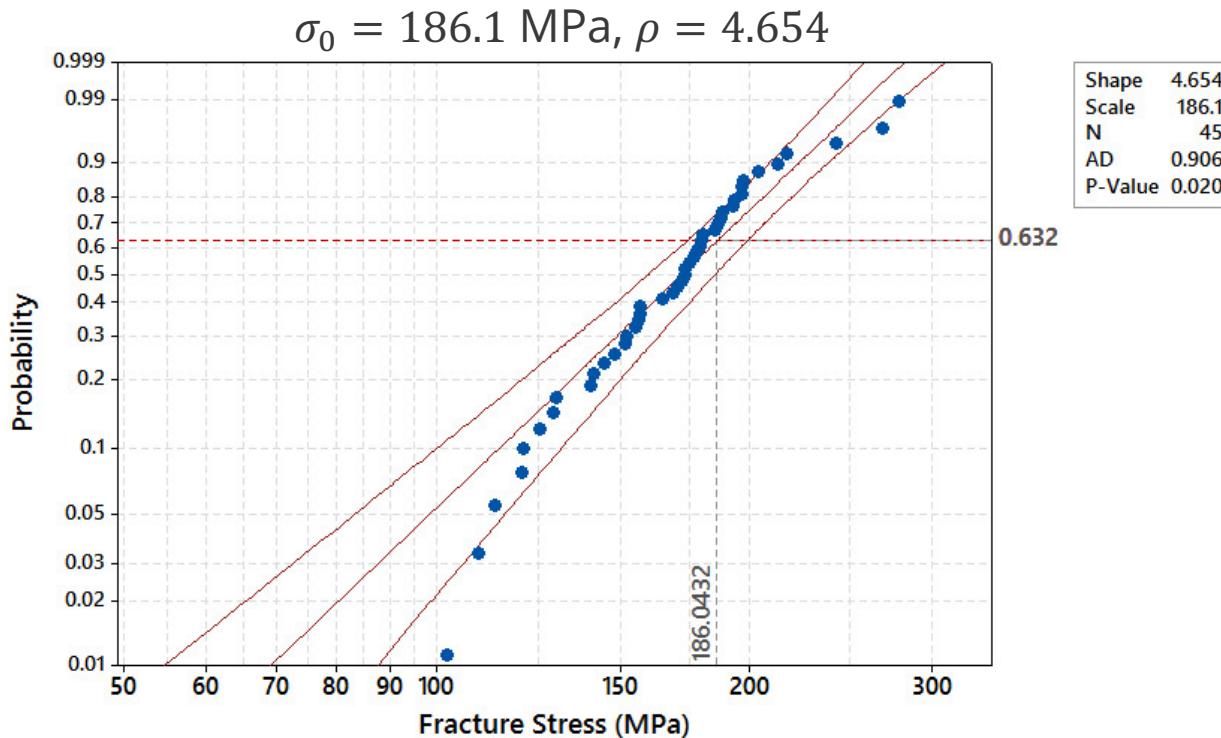
Barium titanate preliminary characterization

Inert Weibull data collected with 4-point-bend tests at 2% RH at various stress rates, no visible trend in failure stress versus stress rate.

SCG parameters fit to indented stress rate strength tests at 95% RH

$$P_f = 1 - \exp \left[- \left(\frac{\sigma}{\sigma_0} \right)^\rho \right]$$

$$\nu = \dot{a} = A \left(\frac{K_I}{K_{Ic}} \right)^n$$



Probabilistic prediction of measured data



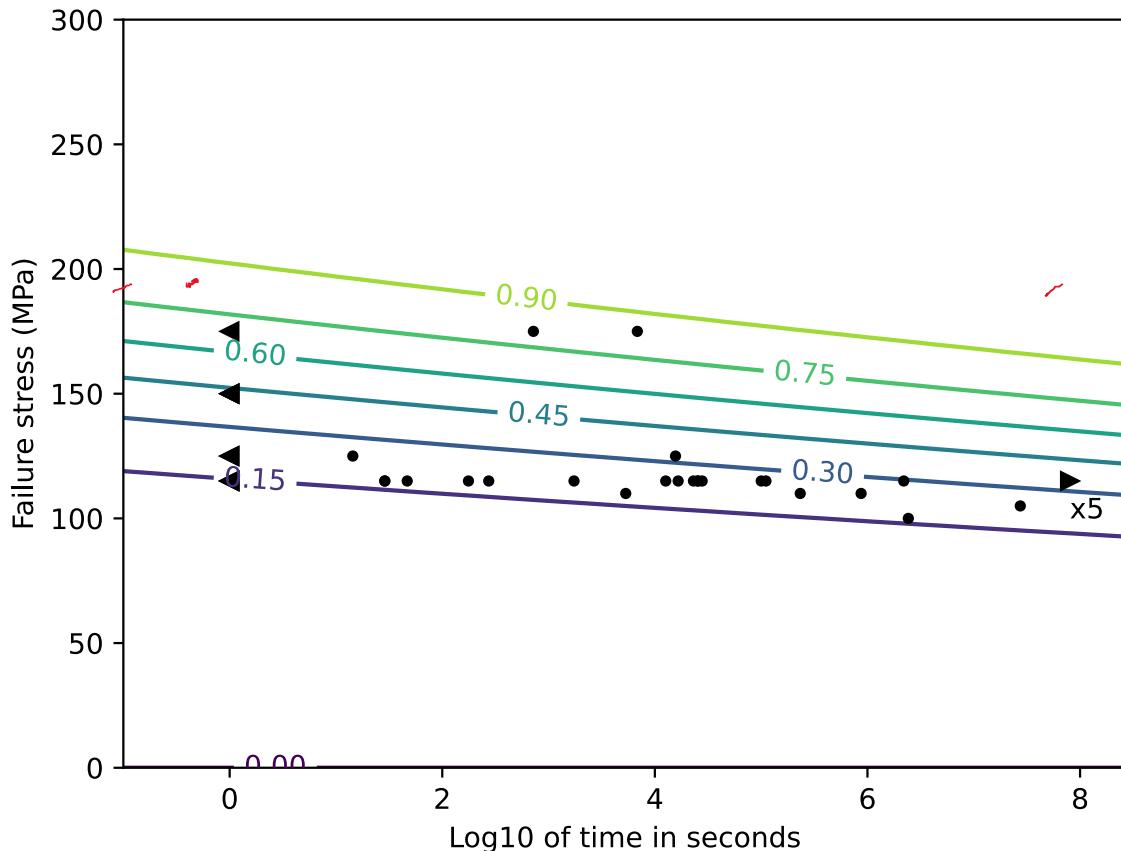
Measured BaTiO₃ parameters

- $\sigma_0 = 186$ MPa
- $\rho = 4.654$
- $A = 1.83$ mm/s
- $n = 90.7$

The resulting predicted probability distribution over time is shown at right

$$P_W = 1 - \exp \left[- \left(\frac{\sigma}{\sigma_0} \right)^\rho \right] \quad v(K_I) = A \left(\frac{K_I}{K_{Ic}} \right)^n$$

$$P_f = 1 - \exp \left(- \left\{ \frac{\left[\frac{A(n-2)Y^2\sigma_f^2 t_f}{2K_{Ic}^2} + 1 \right]^{\frac{1}{n-2}} \sigma_f}{\sigma_0} \right\}^\rho \right)$$



Fitting parameters to measured time-to-failure



Can we use our proposed P_f to calibrate parameters from static failure data?

Note $\lim_{t \rightarrow \infty} P_f = \lim_{\sigma_f \rightarrow \infty} P_f = 1$, so P_f is a cumulative failure function in both t and σ_f

Calculate marginal probability over $\log t$ as $\frac{\partial P_f}{\partial(\log t)}$

Time-to-failure should be conditional on surviving initial load application

Run-out specimens and those failing on load-up should also be included

$$P_f = 1 - \exp \left(- \left\{ \frac{\left[\frac{A(n-2)Y^2\sigma_f^2 t_f}{2K_{Ic}^2} + 1 \right]^{\frac{1}{n-2}} \sigma_f}{\sigma_0} \right\}^\rho \right)$$

$$P_W = 1 - \exp \left[- \left(\frac{\sigma}{\sigma_0} \right)^\rho \right]$$

$$p_{MLE} = \max_{\{\sigma_0, \rho, A, n\}} \text{loglike}(\sigma_0, \rho, A, n | t_f, \sigma_f)$$

$$= \max_{\{\sigma_0, \rho, A, n\}} \sum_{j \in \text{loadup}} \log P_W(\sigma_j | \sigma_0, \rho) + \sum_{j \in \text{delayed}} \log \left\{ \left[\frac{\partial P_f(\sigma_j, t_j | \sigma_0, \rho, A, n)}{\partial(\log t)} \right] [1 - P_W(\sigma_j | \sigma_0, \rho)] \right\} + \sum_{j \in \text{run-out}} \log [1 - P_f(\sigma_j, t_{cut} | \sigma_0, \rho, A, n)]$$

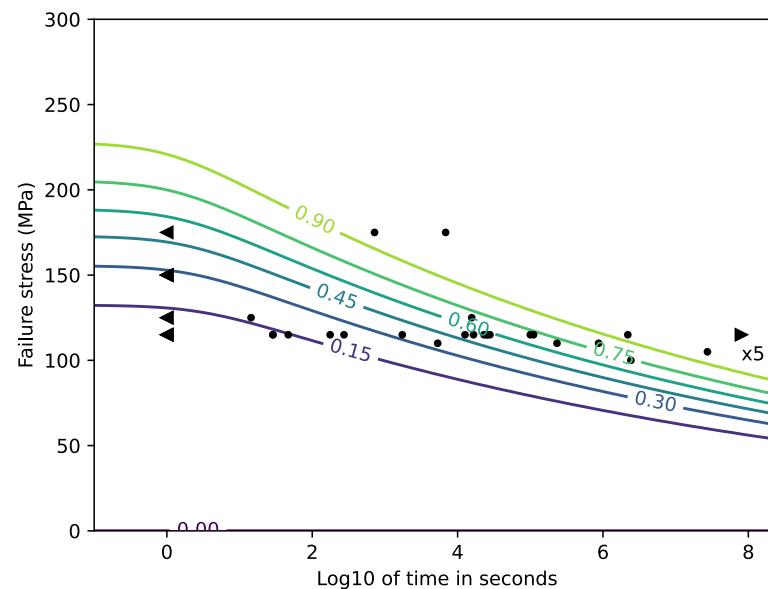
Fitting parameters to measured time-to-failure



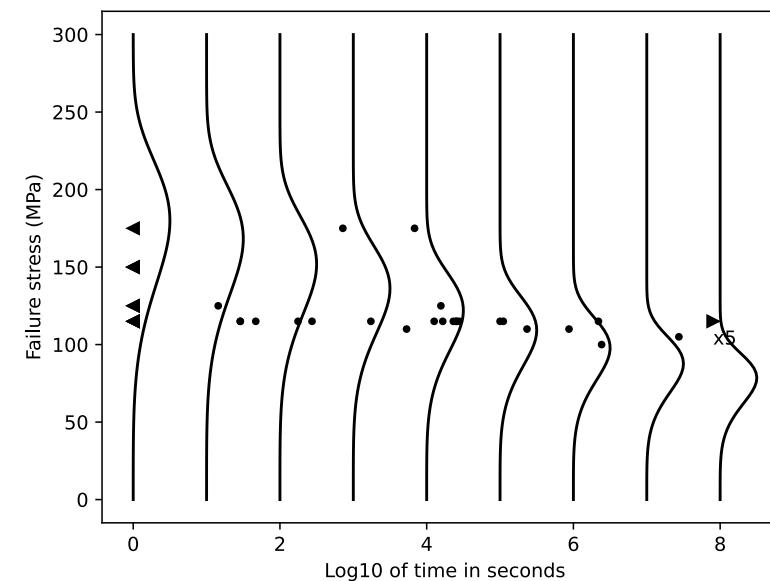
Prior parameters were $\sigma_0 = 186$ MPa, $\rho = 4.654$, $A = 0.00183$ m/s, $n = 90.7$

MLE fit parameters are $\sigma_0 = 192$ MPa, $\rho = 4.89$, $A = 10^{-5.92}$ m/s, $n = 20.9$

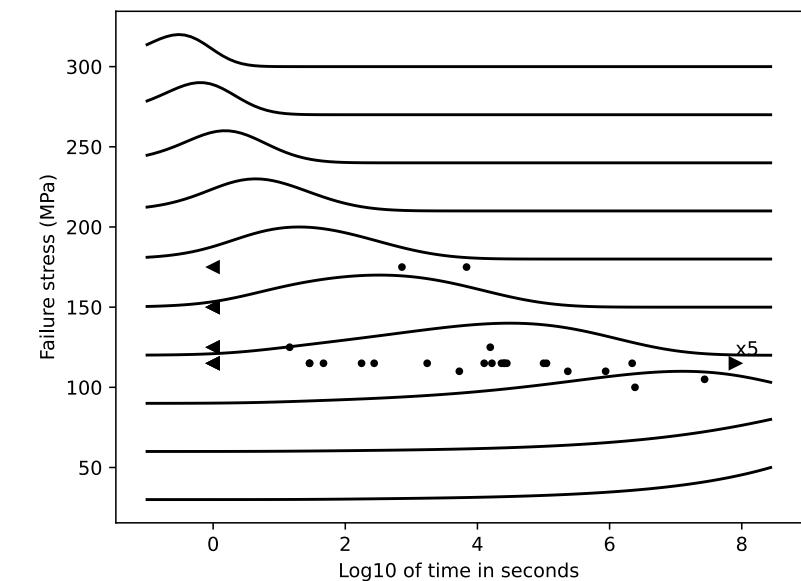
Cumulative failure probability, P_f



Marginal probability, $= p_{\sigma_f} = \frac{\partial P_f}{\partial \sigma_f}$



Marginal probability, $= p_{t_f} = \frac{\partial P_f}{\partial (\log t)}$



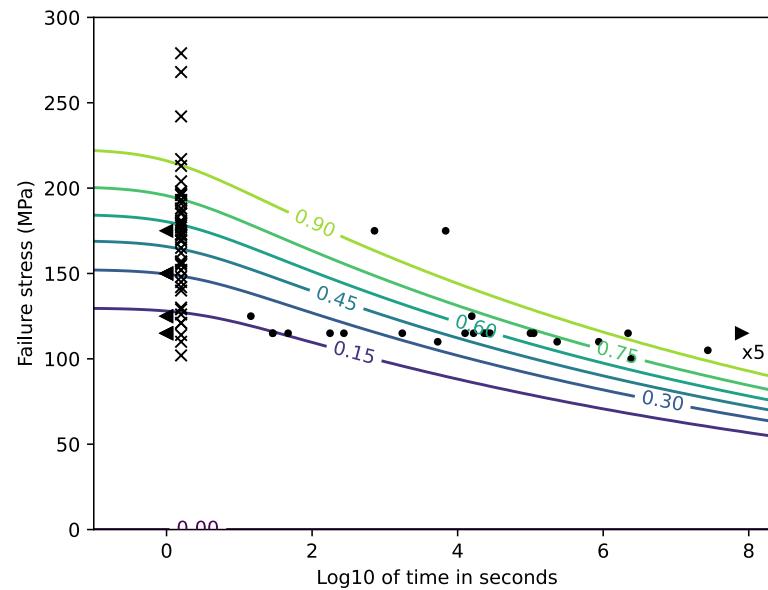
Fitting parameters including inert strength data



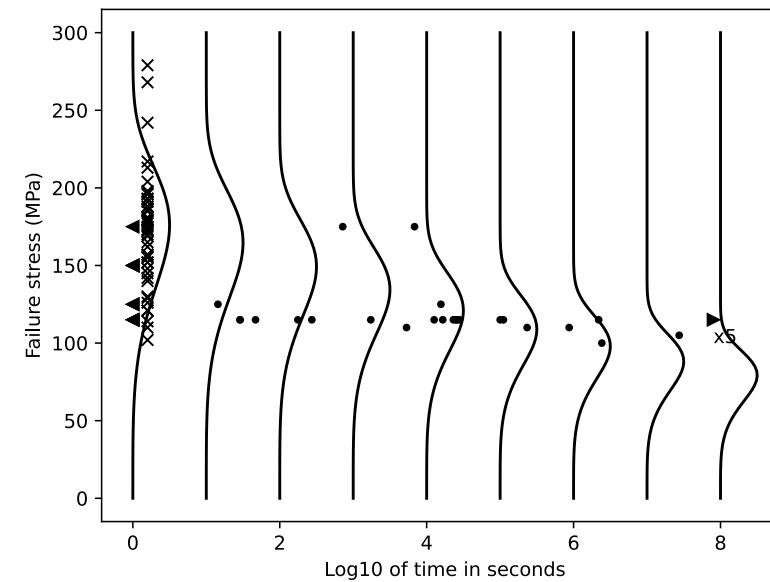
Prior parameters were $\sigma_0 = 186 \text{ MPa}$, $\rho = 4.654$, $A = 0.00183 \text{ m/s}$, $n = 90.7$

MLE fit parameters are $\sigma_0 = 188 \text{ MPa}$, $\rho = 4.90$, $A = 10^{-5.88} \text{ m/s}$, $n = 21.8$

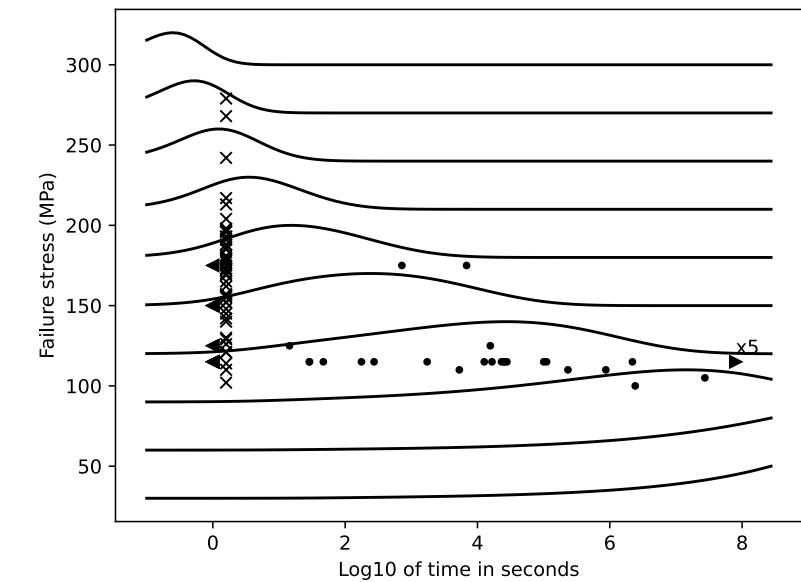
Cumulative failure probability, P_f

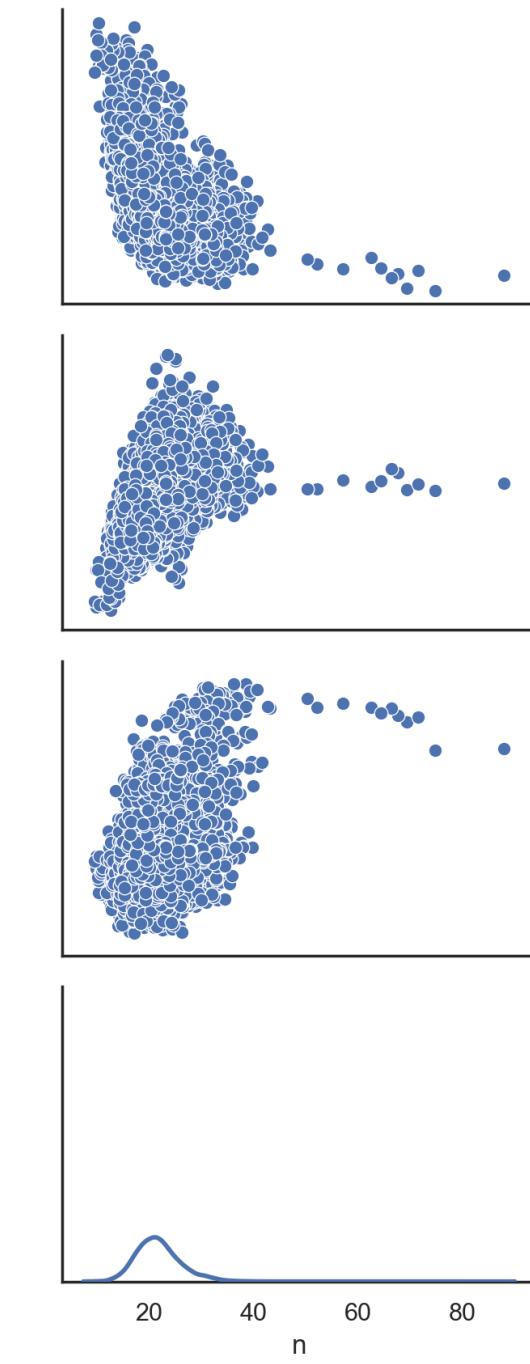
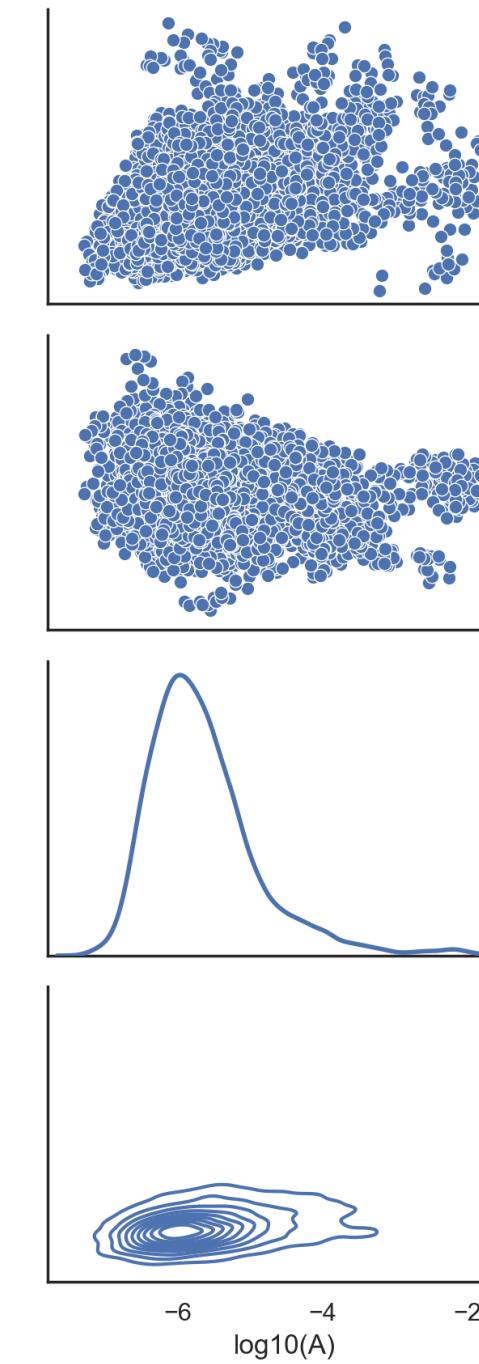
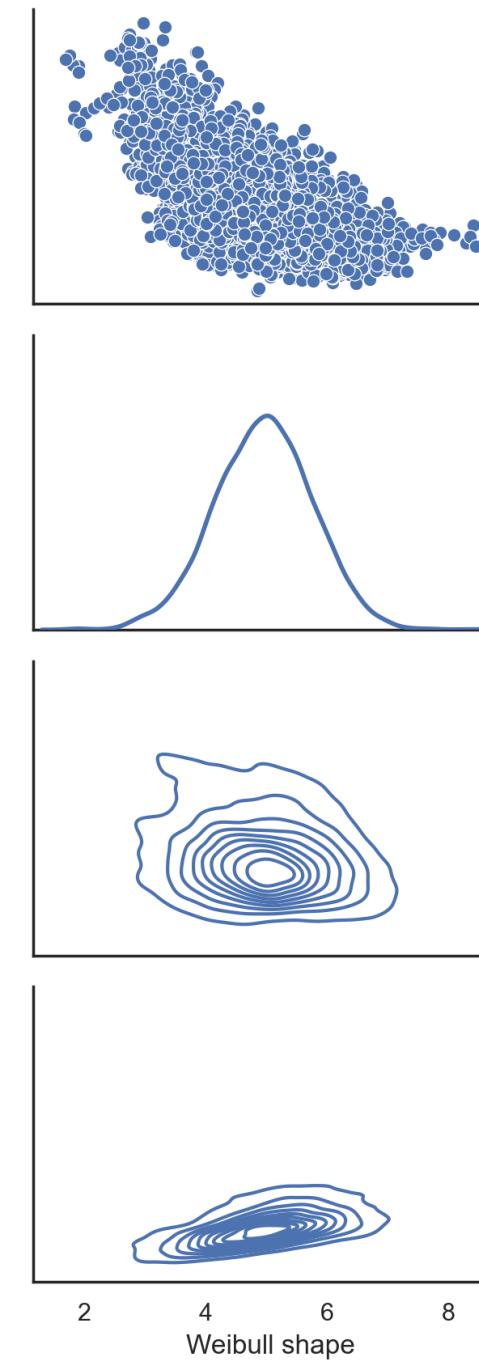
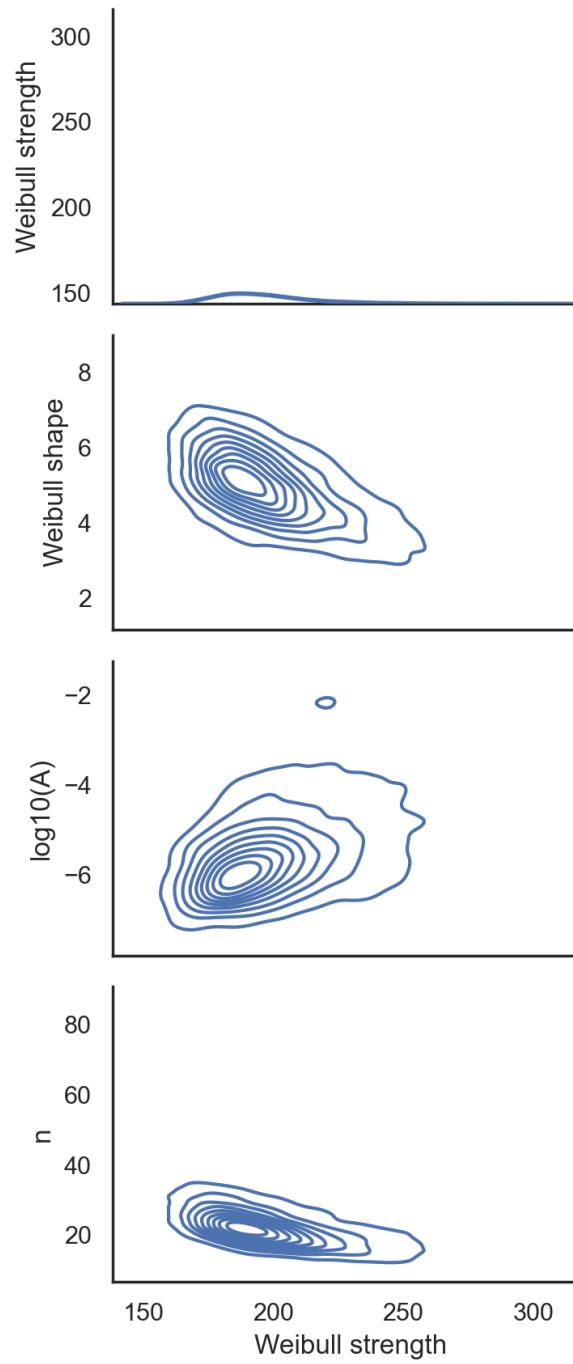


Marginal probability, $= p_{\sigma_f} = \frac{\partial P_f}{\partial \sigma_f}$



Marginal probability, $= p_{t_f} = \frac{\partial P_f}{\partial (\log t)}$





Time-to-failure with glass specimens



Try tests instead with a material which shows more SCG behavior: Schott S8061 glass

We have thus far been unable to measure any SCG in un-notched specimens held at approximately 50% of inert Weibull strength

What could be happening here?

Maybe threshold effects are important?

We will consider threshold through viscoelastic crack tip stress relaxation

Recent results (doi.org/10.1016/j.nocx.2022.100134) show threshold can be calculated through viscoelastic relaxation, for long lifetimes it should be considered here too

Threshold effects in SCG time-to-failure



Take time derivative of $K_I = Y\sigma\sqrt{a}$ and combine with, $v = \dot{a} = A \left(\frac{K_I}{K_{Ic}} \right)^n$, add viscoelastic relaxation of K_I with time constant β

$$\dot{K}_I = \frac{AK_I}{2a} \left(\frac{K_I}{K_{Ic}} \right)^n - \beta K_I, \quad \dot{a} = A \left(\frac{K_I}{K_{Ic}} \right)^n$$

Non-dimensionalize to get

$$\kappa = \frac{K_I}{K_{Ic}}, \quad \alpha = \frac{a\beta}{A}, \quad \tau = \beta t$$

$$\frac{\partial \kappa}{\partial \tau} = \frac{\kappa^{n+1}}{2\alpha} - \kappa, \quad \frac{\partial \alpha}{\partial \tau} = \kappa^n$$

We can interpret $\frac{\partial \kappa}{\partial \tau} = 0$ as SCG threshold

$$\kappa_{th} = (2\alpha)^{1/n} \quad \rightarrow \quad K_{I,th} = \left(\frac{2a\beta}{A} \right)^{1/n} K_{Ic}$$

Probabilistic SCG with threshold effects



Same procedure as before (but somewhat messier):

Assume σ_f is measured at t_f

We use the initial conditions $\alpha(0) = \left(\frac{K_{Ic}}{Y\sigma_i}\right)^2 \frac{\beta}{A}$, $\kappa(0) = \frac{\sigma_f}{\sigma_i}$

Integrate from $\{\alpha(0), \kappa(0)\}$ to $\{\alpha(\tau_f), 1\}$

Express as function $\tau_f = f(\sigma_i, \sigma_f, A, n, \beta)$

Invert to get function $\sigma_i = g(\tau_f, \sigma_f, A, n, \beta)$

Substitute into beginning-of-life Weibull distribution, $P_f = 1 - \exp\left[-\left(\frac{g(\beta\tau_f, \sigma_f, A, n, \beta)}{\sigma_0}\right)^\rho\right]$

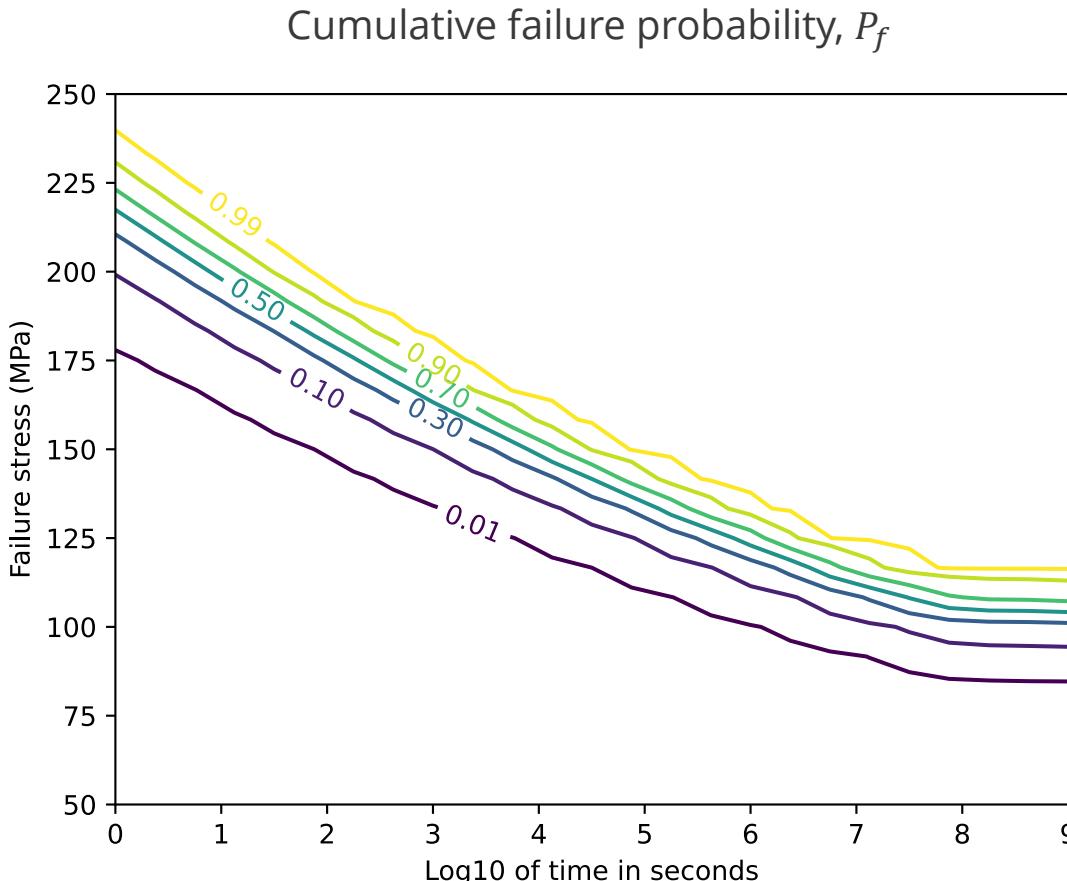
If $\kappa < \kappa_{th}$ then $\tau_f = \infty$ and $\sigma_i = \sigma_f$

Time-to-failure predictions for S8061 glass



Parameters for S8061 glass, $\sigma_0 = 252$ MPa, $\rho = 10.3$, $A = 0.325$ m/s, $n = 24$

Assume $\kappa_{th} \approx 0.5$ for 1 mm crack, estimate $\beta \approx 10^{-9}$ 1/s



For simplicity, here we assume $Y(a) = \text{CONSTANT}$, this can be relaxed and in some cases can significantly affect threshold prediction

We can also allow for time-evolving stress state

Given assumptions stated here, minimal flaw population aging occurs after $t \approx 1/(10\beta)$

Even with a threshold stress intensity, there is no threshold for applied load

Questions?

Scott Grutzik

sjgrutz@sandia.gov

Threshold calculation



Threshold is dependent on crack size, larger threshold for larger cracks

$$\kappa_{th} = (2\alpha)^{1/n} \rightarrow K_{I,th} = \left(\frac{2a\beta}{A} \right)^{1/n} K_{Ic}$$

Can an initially super-threshold crack become sub-threshold as it grows?

Yes, but this regime is small and we can neglect it

