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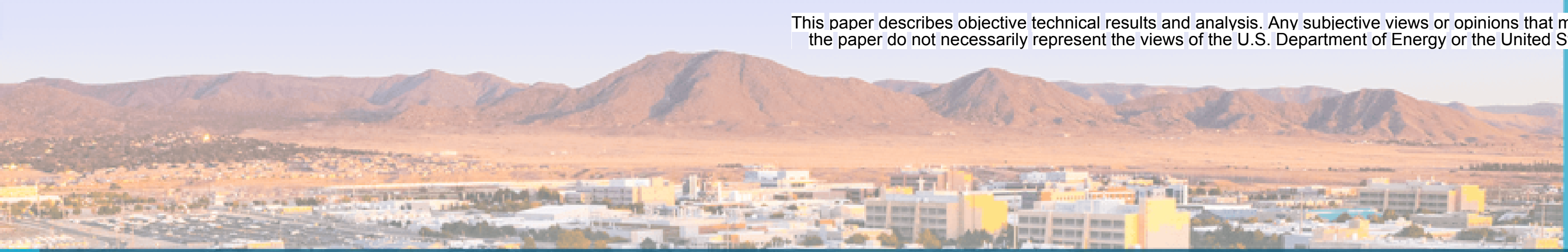

Kinetic model for environmentally assisted crack growth threshold

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Motivation for kinetic model of static fatigue threshold

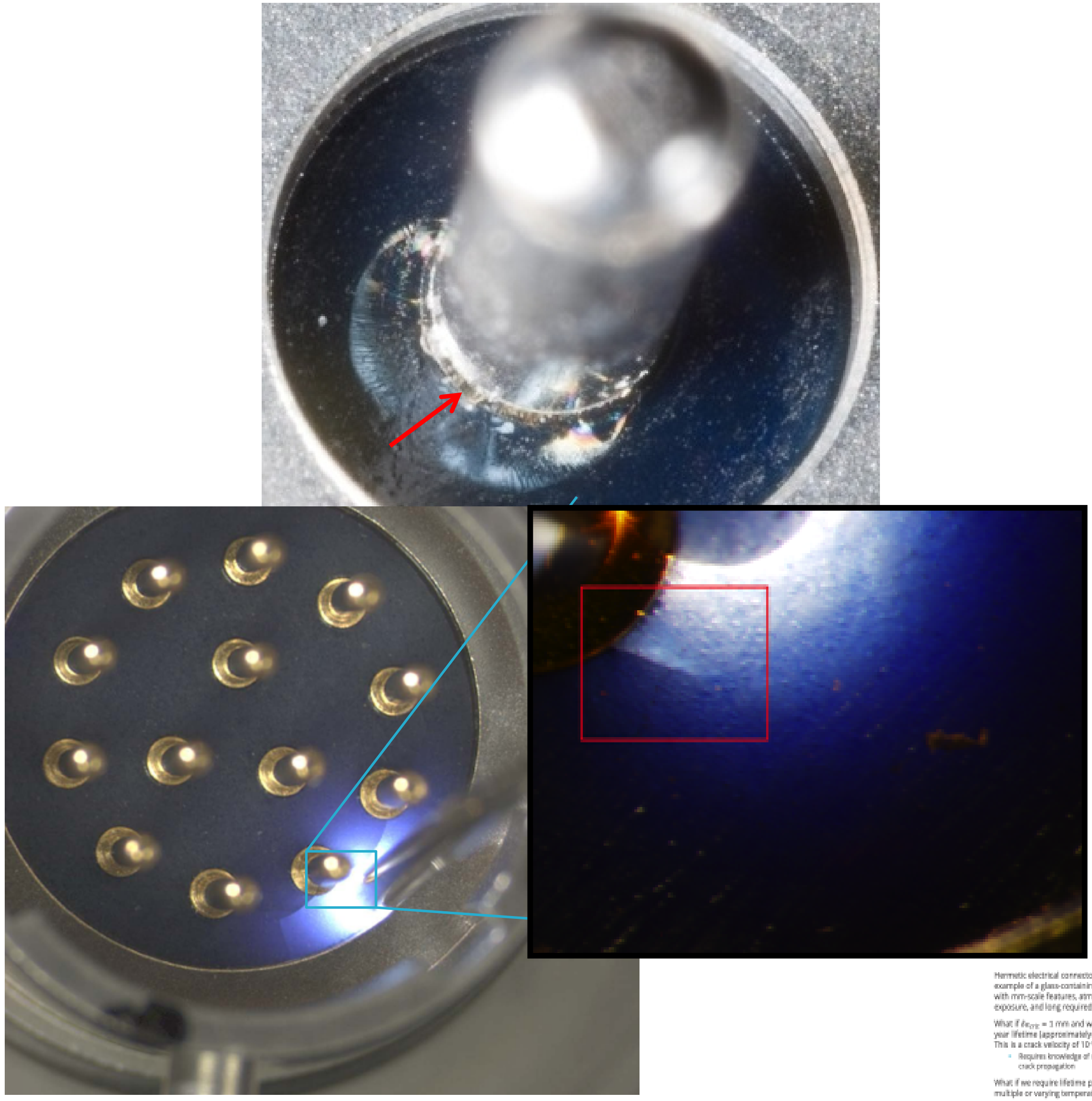
Hermetic electrical connectors are an example of a glass-containing component with mm-scale features, atmospheric exposure, and long required life.

What if $\delta a_{crit} \approx 1$ mm and we require 30 year lifetime (approximately 10^9 seconds)? This is a crack velocity of 10^{-12} m/s.

- Requires knowledge of near-threshold crack propagation

What if we require lifetime prediction at multiple or varying temperature?

- Requires temperature to be a variable in the model

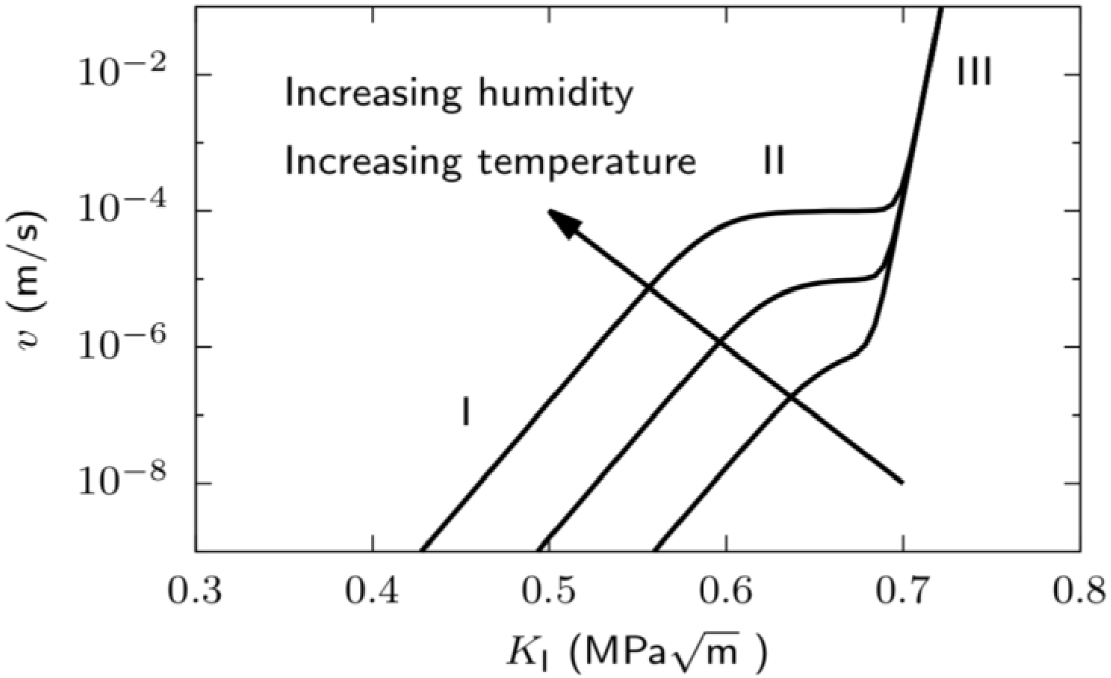


Three regimes of subcritical crack growth in glass

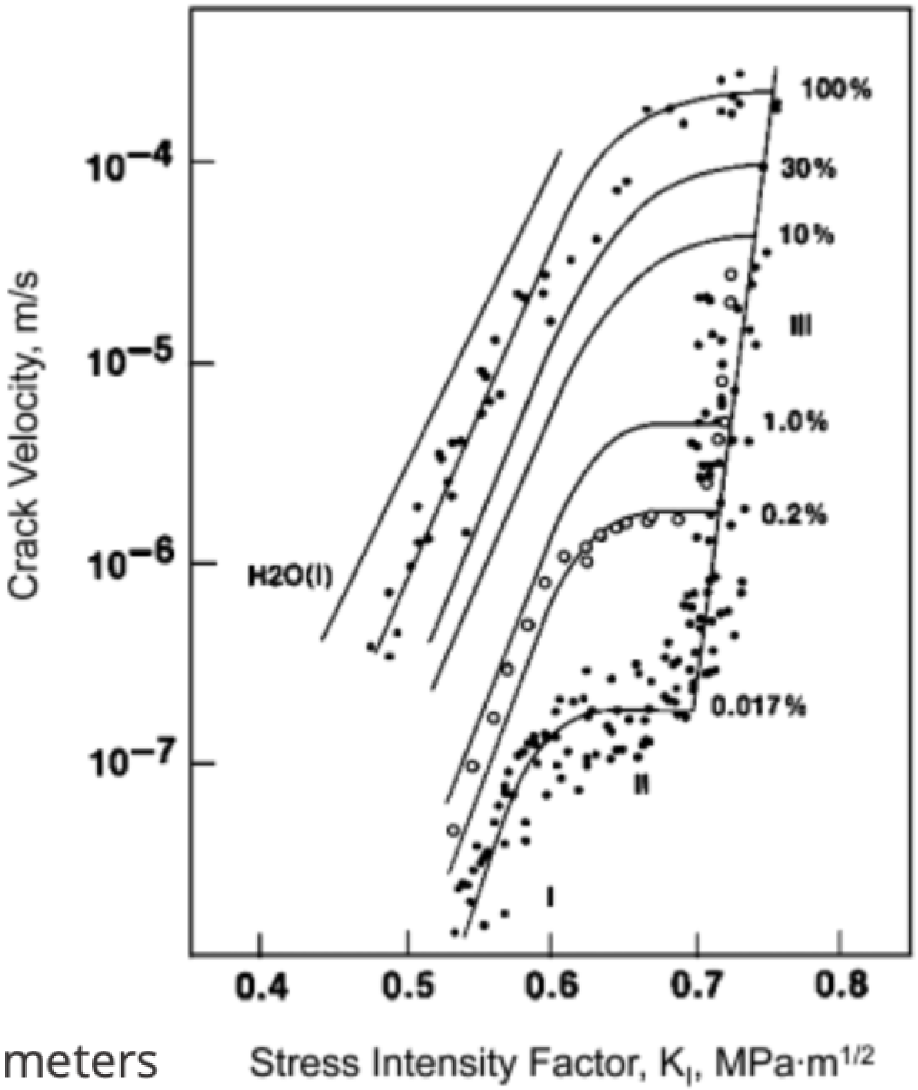
Regime I: Reaction limited, water assisted

Regime II: Transport limited, water assisted

Regime III: Reaction limited, not water assisted



Most work assumes a power law form $v = AK_I^n$ where parameters are implicitly dependent on temperature and humidity.

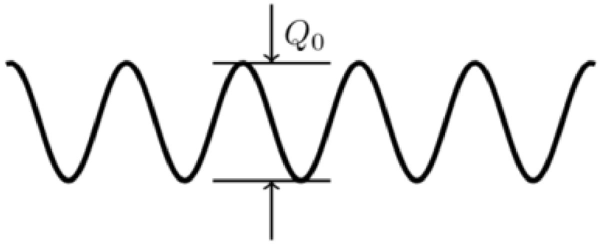


Freiman, S. W., Wiederhorn, S. M., & Mecholsky, Jr, J. J. (2009). Environmentally enhanced fracture of glass: a historical perspective. *Journal of the American Ceramic Society*, *92*(7), 1371-1382.

Thermally activated crack growth model

We model a crack as a system with crack length as a single degree of freedom. Assume a crack at rest is in a local energy minimum with energy barriers to forward (propagation) and backward (healing) events.

Assume regimes I and II are both water-assisted but have competing limiting behavior, I+II and III act independently.



Potential shape at zero crack driving force

Single transition

$$f = \frac{kT}{h} \exp\left(-\frac{Q}{kT}\right)$$

Net forward velocity

$$v_{\mathrm{I}} = \frac{2\delta_w kT}{h} \exp\left[-g(H)\frac{Q_w}{kT}\right] \sinh\left(\frac{K_{\mathrm{I}}^2 \delta_w^2}{2EkT}\right)$$

Cook, R. F. (2019). Thermal activation effects in crack propagation and reliability of fused silica. *Journal of the American Ceramic Society*, *102*(12), 7575-7583.

Potential shape with positive crack driving force

All three regimes

$$v = v_{\mathrm{I,II}} + v_{\mathrm{III}} = \frac{1}{\frac{1}{v_{\mathrm{I}}} + \frac{1}{v_{\mathrm{II}}}} + v_{\mathrm{III}}$$

$$= \left[\frac{h}{2\delta_w kT} \exp\left(g(H)\frac{Q_w}{kT}\right) \operatorname{csch}\left(\frac{K_{\mathrm{I}}^2 \delta_w^2}{2EkT}\right) + \frac{1}{B(T)H^{-2/3}}\right]^{-1}$$

$$+ \frac{2\delta_v kT}{h} \exp\left(-\frac{Q_v}{kT}\right) \sinh\left(\frac{K_{\mathrm{I}}^2 \delta_v^2}{2EkT}\right)$$

Model fit to data and interpretation

Wiederhorn, S. M. (1967). Influence of water vapor on crack propagation in soda- lime glass. *Journal of the American Ceramic Society*, *50*(8), 407-414.

Wiederhorn, S., & Bolz, L. H. (1970). Stress corrosion and static fatigue of glass. *Journal of the American ceramic society*, *53*(10), 543-548.

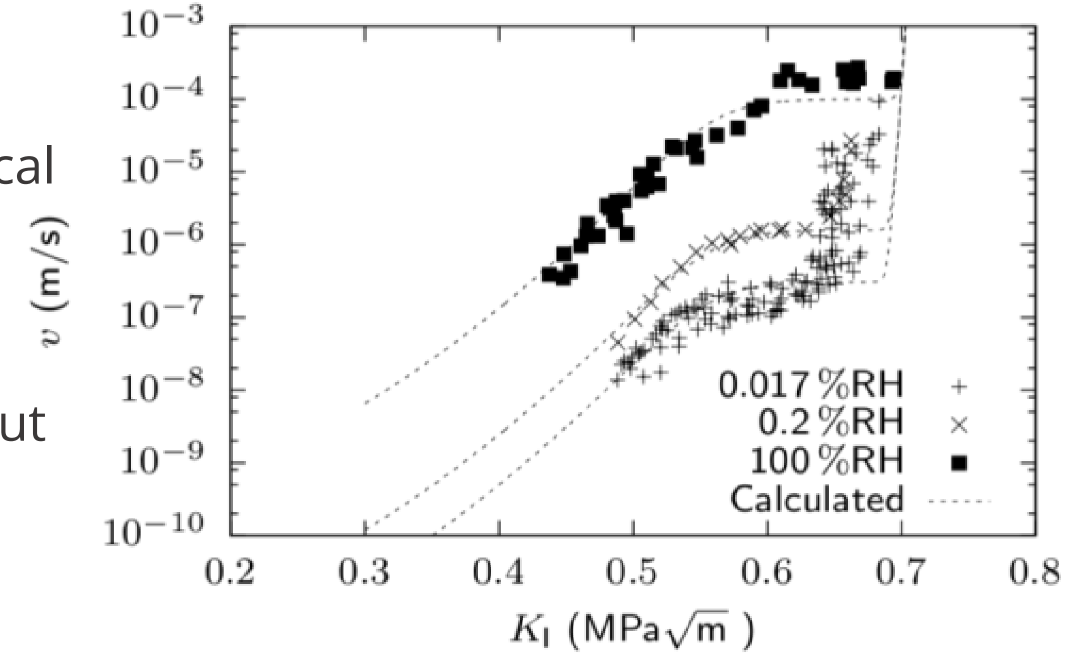
Wiederhorn, S. M., Johnson, H., Diness, A. M., & Heuer, A. H. (1974). Fracture of glass in vacuum. *Journal of the American Ceramic Society*, *57*(8), 336-341.

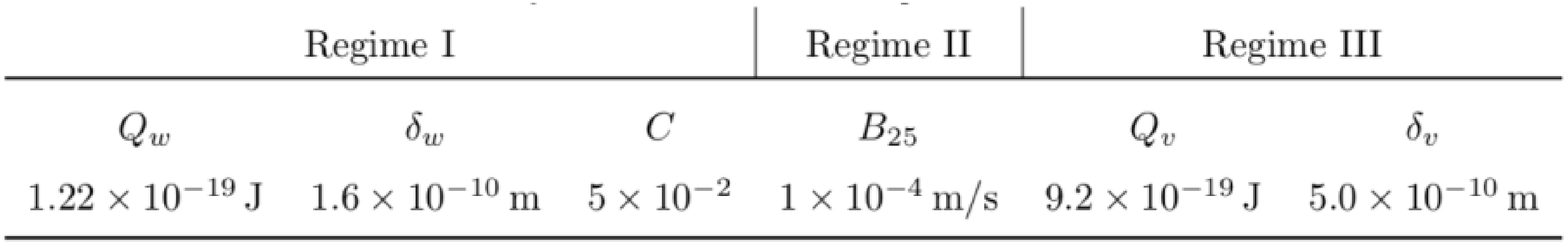
As a demonstration we fit to data from 3 Wiederhorn papers for SLS glass at different temperature and humidity.

NOTE: We assume that regime III is the same as subcritical propagation in vacuum

- Both regime III and vacuum are unassisted by water
- We assume both are thermally activated processes but different mechanisms so activation energy and characteristic length are different
- Water acts as a catalyst for propagation in regime I

For comparison, Si-O bond energy is around 1.5 ▪ 10^{-19} J





Regime I			Regime II	Regime III	
Q_w	δ_w	C	B_{25}	Q_v	δ_v
1.22×10^{-19} J	1.6×10^{-10} m	5×10^{-2}	1×10^{-4} m/s	9.2×10^{-19} J	5.0×10^{-10} m

Threshold via viscoelasticity

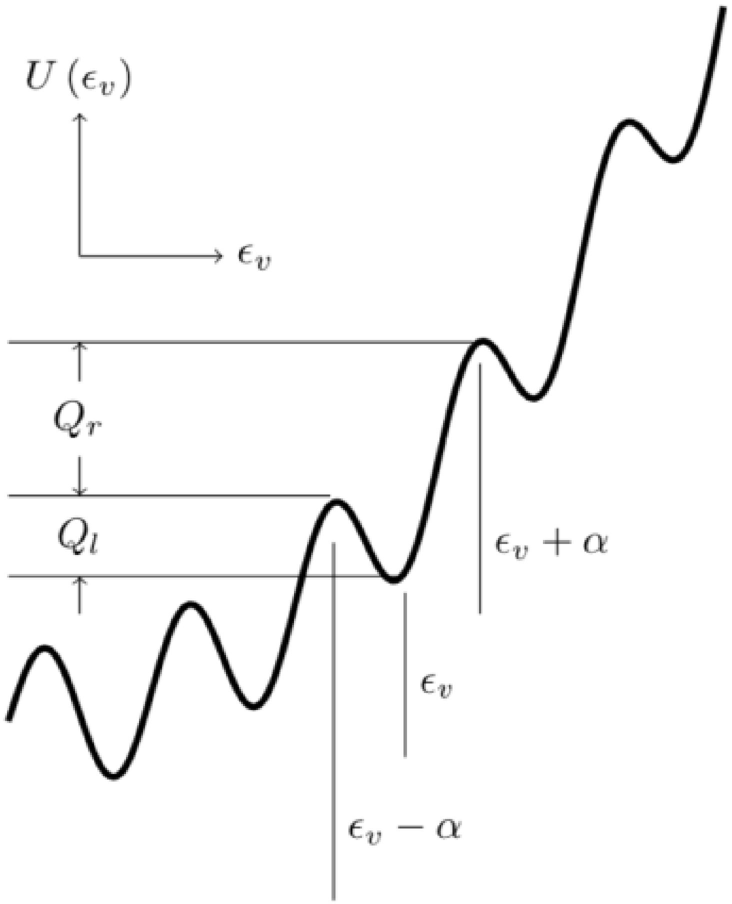
PROPOSITION: Cracks will not growth at $K_I < K_{thresh}$ where K_{thresh} is such that the crack tip stresses relax due to viscoelastic effects faster than it propagates

PROPOSITION: Fracture is bond breaking and viscoelasticity is bond re-arranging. However, broken bonds will re-form, so fracture is also bond re-arranging

PROPOSITION: Thermally activated fracture and thermally activated stress relaxation should be related.

Thermally activated stress relaxation model

Model a system with strain as a single degree of freedom. Assume an underlying quadratic elastic potential superposed with local variations.



Frequency for left (relaxation) and right (anti-relaxation) events

$$f_l = \frac{k_b T}{h} \exp\left[-\frac{q_e - \frac{1}{2}E_R\epsilon_v^2 + \frac{1}{2}E_R\left(\epsilon_v - \alpha\right)^2}{k_b T \rho_A}\right]$$

$$f_r = \frac{k_b T}{h} \exp\left[-\frac{q_e + \frac{1}{2}E_R\left(\epsilon_v + \alpha\right)^2 - \frac{1}{2}E_R\epsilon_v^2}{k_b T \rho_A}\right]$$

Net strain rate

$$\dot{\epsilon_v} = -\frac{kT\alpha}{h} \exp\left(-\frac{q_e + \frac{1}{2}E_R\alpha^2}{k_b T \rho_A}\right) \sinh\left(\frac{E_R\epsilon_v\alpha}{k_b T \rho_A}\right)$$

Linearized relaxation time scale

$$1/\tau_v = \frac{E_R\alpha^2}{hN_A\rho_A} \exp\left(-\frac{q_e + \frac{1}{2}E_R\alpha^2}{k_b T \rho_A}\right)$$

The big assumption (also some definitions)

ASSUME regime III fracture (no water) and bulk viscoelasticity are the same mechanism

$$\delta_v = \delta_e, Q_v = Q_e = q_e \delta_e^3$$

DEFINE glassy modulus is given by local potential function, rubbery modulus by underlying quadratic potential

$$E_G = \frac{1}{2}\frac{d^2U(\epsilon)}{d\epsilon^2} \text{ at metastable state,} \qquad U(\epsilon) = \frac{1}{2}E_R\epsilon^2 + \{local\ variations\}$$

DEFINE fictive temperature is related to well depth at zero strain, $kT_f = Q_e = q_e\delta_v^3$

DEFINE ρ_a is the atom spatial density and $n_v = \rho_a \delta_v^3$ atoms are involved in a relaxation mechanism

Then, we have relaxation time:

$$\begin{aligned} 1/\tau_v &= \frac{E_R\alpha^2}{h\rho_a}\exp\left(-\frac{Q_v/\delta_v^3 + \frac{1}{2}E_R\alpha^2}{k_b T\rho_A}\right) \\ &= \frac{\pi^2 kT_f}{2h\delta_v^3\rho_a}\frac{E_R}{E_G - E_R}\exp\left(-\frac{Q_v}{kT\rho_a\delta_v^3} - \frac{\pi^2 T_f}{4\rho_a T\delta_v^3}\frac{E_R}{E_G - E_R}\right) \end{aligned}$$

$$1/\tau_v = \frac{\pi^2 kT_f}{2hn_v}\frac{E_R}{E_G - E_R}\exp\left(-\frac{Q_v}{kTn_v} - \frac{\pi^2 T_f}{4Tn_v}\frac{E_R}{E_G - E_R}\right)$$

Evolution of K_I and prediction of threshold

So, $K_I = Y\sigma\sqrt{a}$ increases from crack propagation but decreases from stress relaxation

$$\dot{K}_{\mathrm{I}} = \frac{Y\sigma\dot{a}a^{-1/2}}{2} - \frac{1}{\tau_v}K_{\mathrm{I}} = \frac{K_{\mathrm{I}}\dot{a}}{2a} - \frac{1}{\tau_v}K_{\mathrm{I}}$$

$$\dot{a} = \frac{2\delta_w kT}{h}\exp\left(-g(H)\frac{Q_w}{kT}\right)\sinh\left(\frac{K_{\mathrm{I}}^2\delta_w^2}{2E_G kT}\right)$$

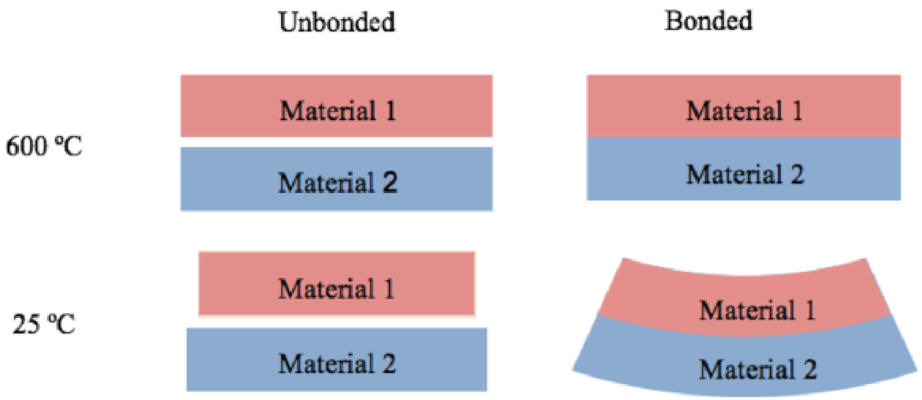
Find $K_{I,thresh}$ by setting $\dot{K}_I = 0$ with $K_I \neq 0$, this gives the transition between K_I increasing or decreasing in time

$$K_{\mathrm{I,thresh}} = \left[\frac{2E_G kT}{\delta_w^2}\sinh^{-1}\left[\frac{\pi^2 a T_f}{2\delta_w\delta_v^3\rho_a T}\frac{E_R}{E_G - E_R}\cdot \exp\left(g(H)\frac{Q_w}{kT} - \frac{Q_v}{kT\rho_a\delta_v^3} - \frac{\pi^2 T_f}{4\rho_a\delta_v^3 T}\frac{E_R}{E_G - E_R}\right)\right]\right]^{1/2}$$

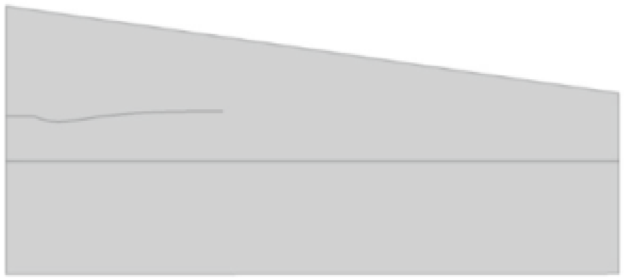
This PREDICTS threshold from regimes I and III subcritical fracture parameters, macroscale parameters, and atom spatial density ρ_a

Threshold measurement with residually stressed bibeams

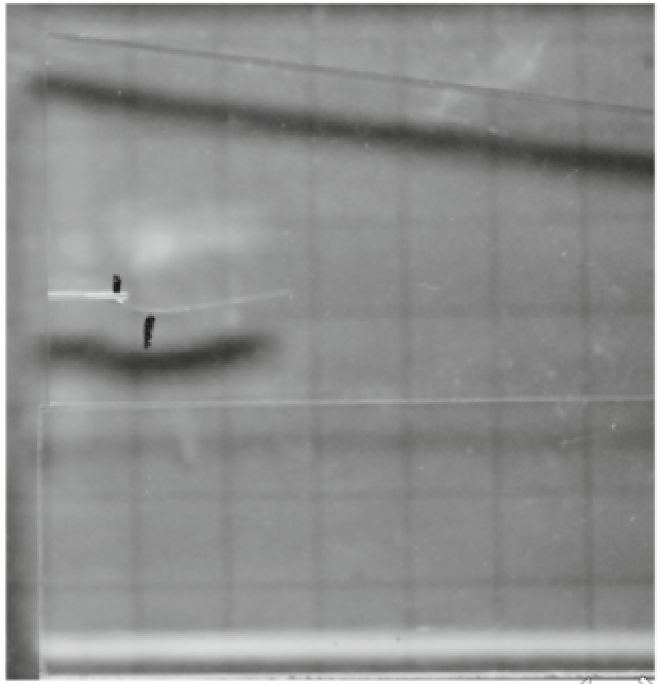
We diffusion bonded 2 SLS glass variants with slightly different CTE, after cooling residual stress puts the specimen in bending. A crack was initiated with a notch and aged until it stopped propagating (about 2 years for the low humidity case). We calculate K_I in this final state and assume it is $K_{I,thresh}$. This has been done at 3 humidity levels.



Grutzik, S. J., Aduloju, S., Truster, T., & Reedy, E. D. (2021). Residually Stressed Bimaterial Beam Specimen for Measuring Environmentally Assisted Crack Growth. *Experimental Mechanics*, *61*(2), 411-418.



(a) Crack path in tapered specimen predicted by FRANC3D



(b) Experimentally observed cra path in tapered specimen

Comparison of measured and predicted threshold

If we use SLS subcritical fracture parameters fit to Wiederhorn data, let T_f=600 °C, and assume ρ_a is calculated using mass density and a weighted average molar mass assuming nominal SLS chemical composition. We then get $K_{I,thresh}$= 0.64 MPa $m^{1/2}$ at 100% RH.

If we reduce ρ_a by 30% we get $K_{I,thresh}$= 0.34 MPa $m^{1/2}$. Measured threshold is 0.31-0.33 MPa $m^{1/2}$ and literature value of 0.34 MPa $m^{1/2}$.

Treating ρ_a as a fitting parameter we then predict threshold of 0.36 at 35%RH and 0.4 MPa $m^{1/2}$ at 10% RH.

We measure threshold values of 0.35 at 35%RH and 0.38 MPa $m^{1/2}$ in lab air.

RH	0.1	0.35	1.0
Measured (MPa $m^{1/2}$)	0.38	0.35	0.31-0.33, 0.34
Predicted (MPa $m^{1/2}$)	0.40	0.36	0.34

Concluding comments

Model shows only slight dependence on fictive temperature and activation energy but strong dependence on ρ_a.

This model assumes only a single mechanism for both regime I and regime III (where regime III is also stress relaxation).

We know that glass is not well described by single mechanism models. Prony series are needed for viscoelastic accuracy and fictive temperature arrays are commonly calculated.

In the special case of a highly confined, highly stressed, localized region around a crack it is not unreasonable that a single (or small number) of mechanisms dominate.

Current work is investigating an alternate formulation based on nonequilibrium statistical mechanics, generalization to non-sharp crack geometry, and how to include multiple mechanism effects.

Questions?

Watch for our upcoming paper!

Please contact me at:

- Scott Grutzik
- sjgrutz@sandia.gov

See also:

“Investigation of Slow Crack Growth of Sodium Silicates with AFM”, Kevin Strong

”Atomistic Fracture Mechanisms in Sodium Silicates”, Jessica Rimsza