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Title: Coupled experimental-numerical investigations of polymer deformation and failure

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Coupled experimental-numerical investigations of polymer deformation and failure

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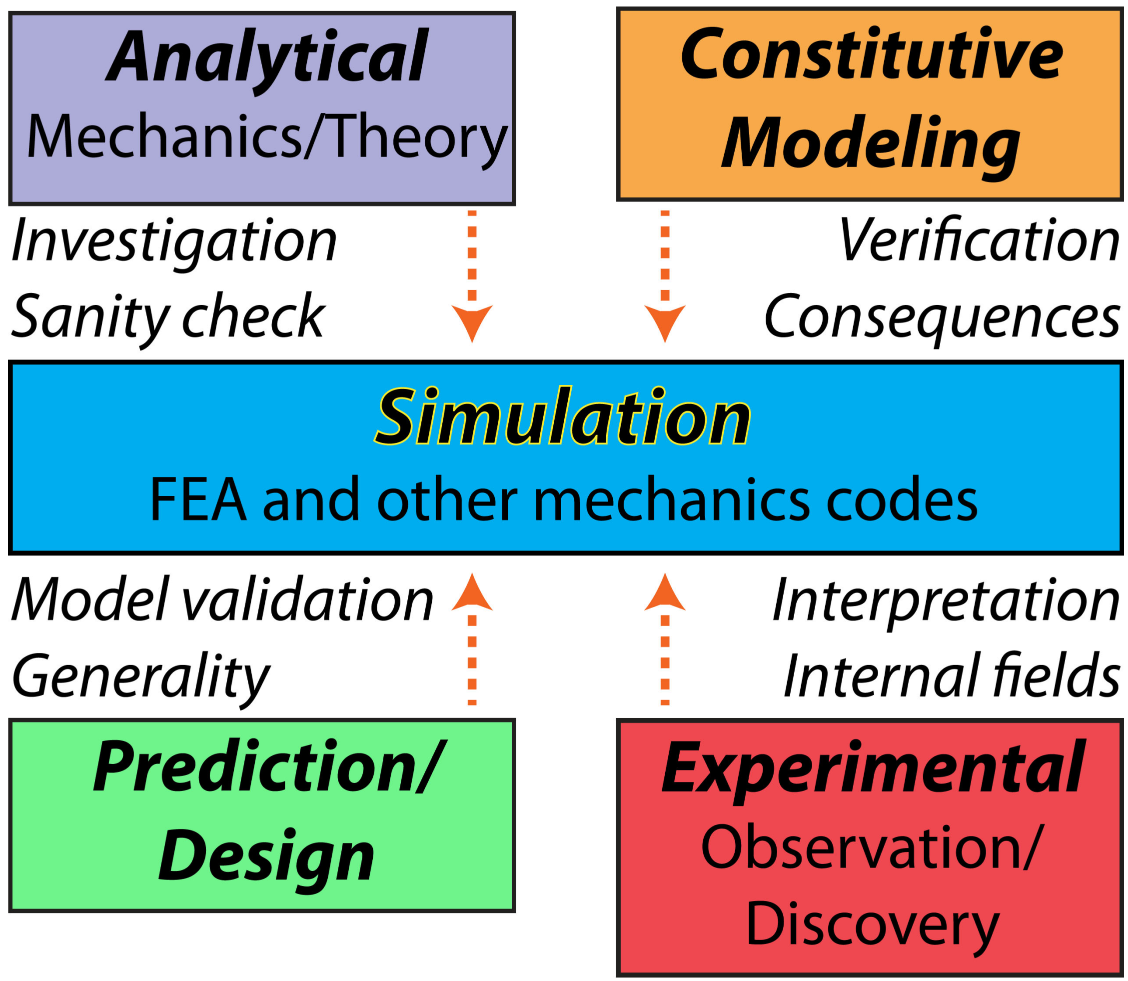
Simulation is at the heart of engineering efforts



Materials research for polymers at extremes

Research at interfaces of Analytical/Experimental/Numerical

- **Analytical theory validation**

  Viscoplastic fracture mechanics and J(t) integral

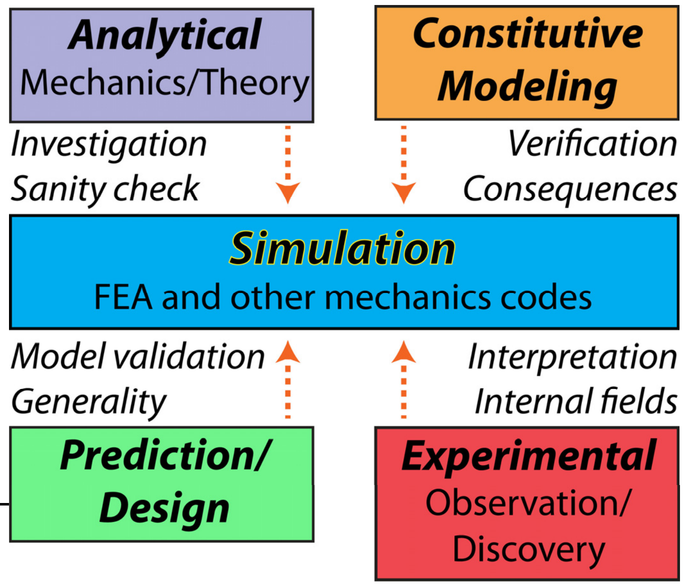
- **Experimental mechanism discovery**

  High-rate stable tensile failure in PE during Dynamic-Tensile-Extrusion

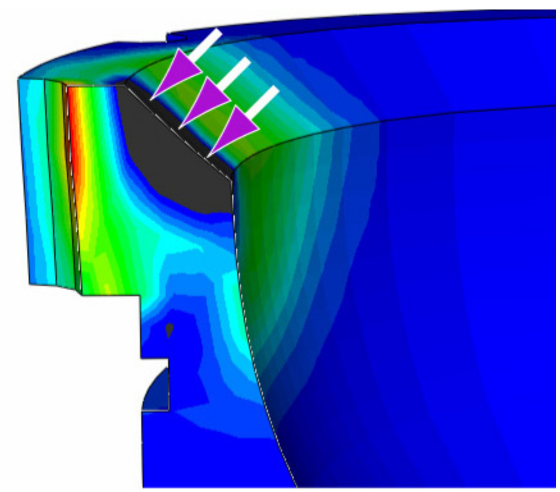
- **Internal fields w/o explicit constitutive model**

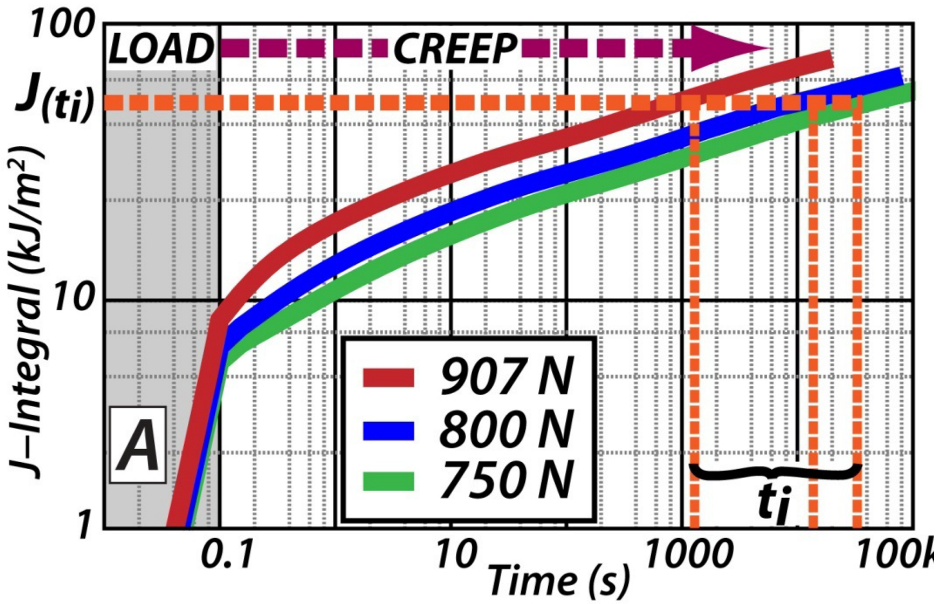
  Large strain time-temperature equivalence

  Infer physics of internal failure during DTE

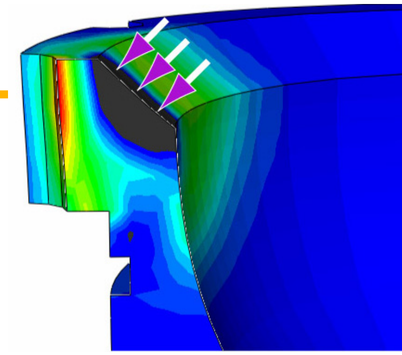


Coupled experimental-numerical validation of viscoplastic fracture mechanics

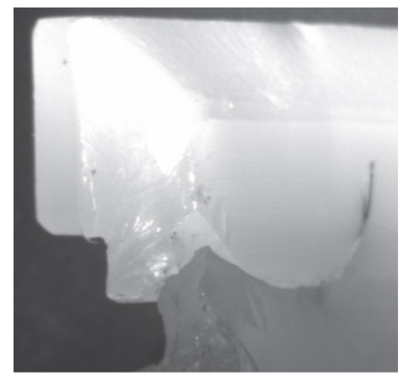


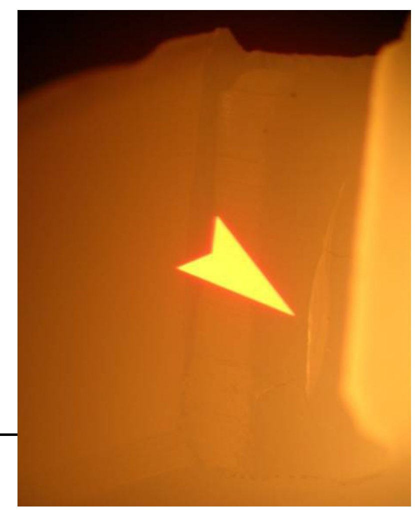


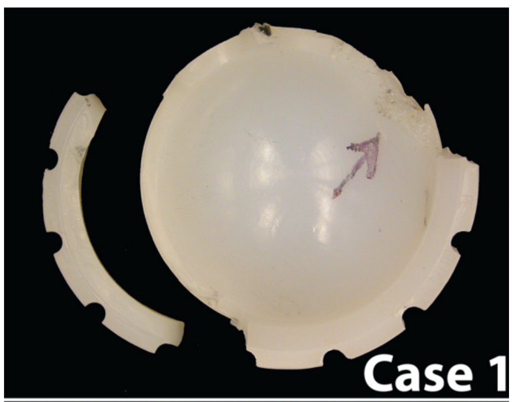
Motivation: Clinical fracture of UHMWPE hip replacement bearings

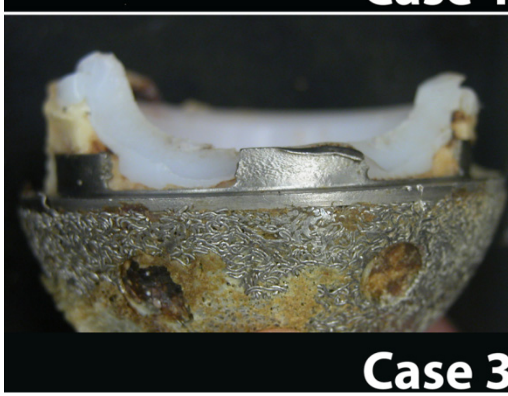


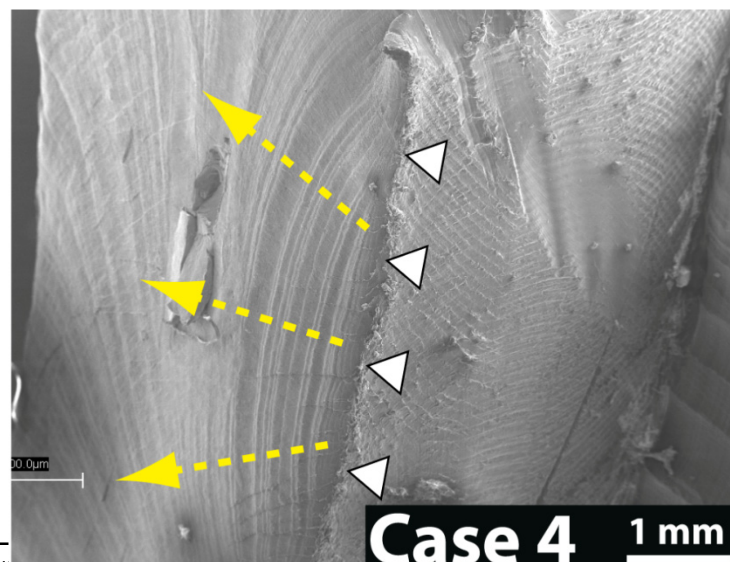
- **Four designs, all initiated a crack from a designed notch and fractured without trauma**
- **No failure theory or design criteria for fracture**
- **Cracks can initiate long before failure**





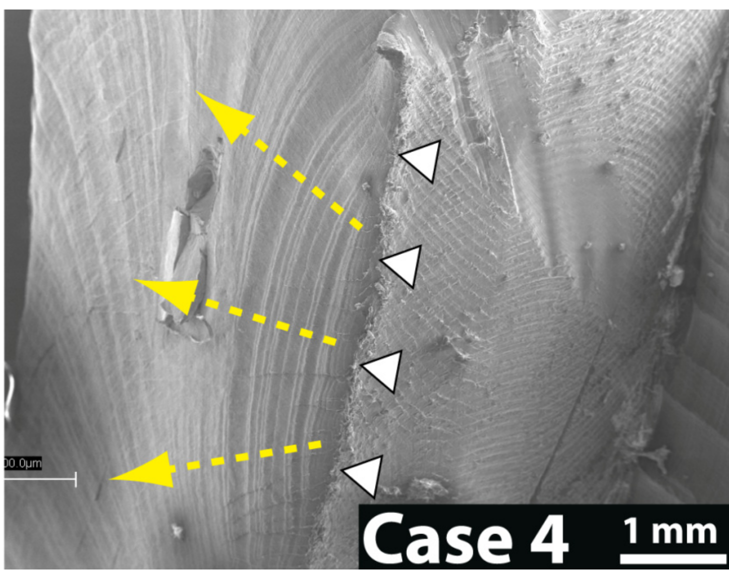


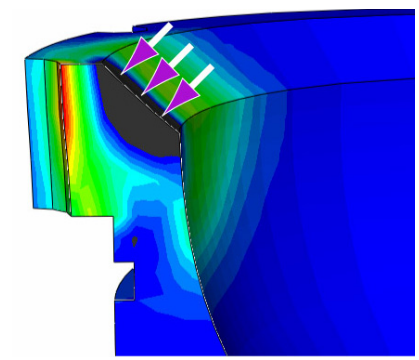


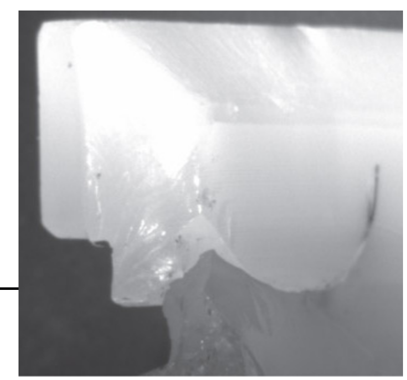


DoD Analog: Controlled fragmentation of a UHMWPE slip-obturator in Excalibur

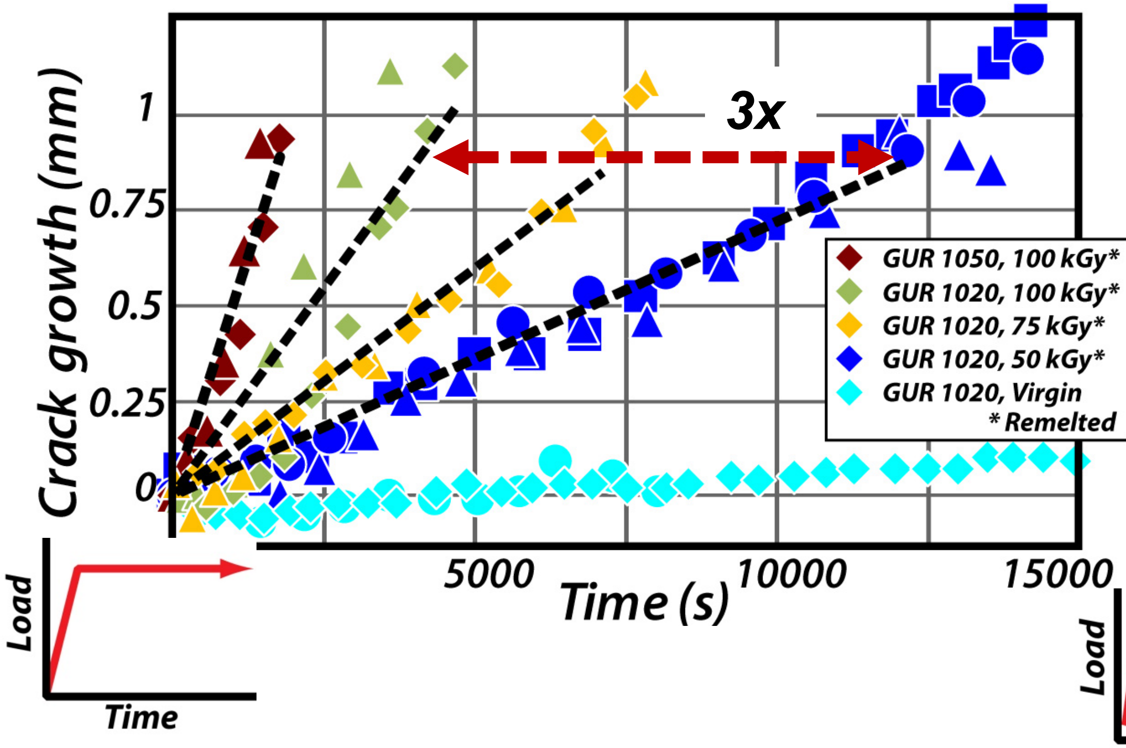
- **Failure at designed notches under tension**
- **Fracture time and path critical to performance: *Design***

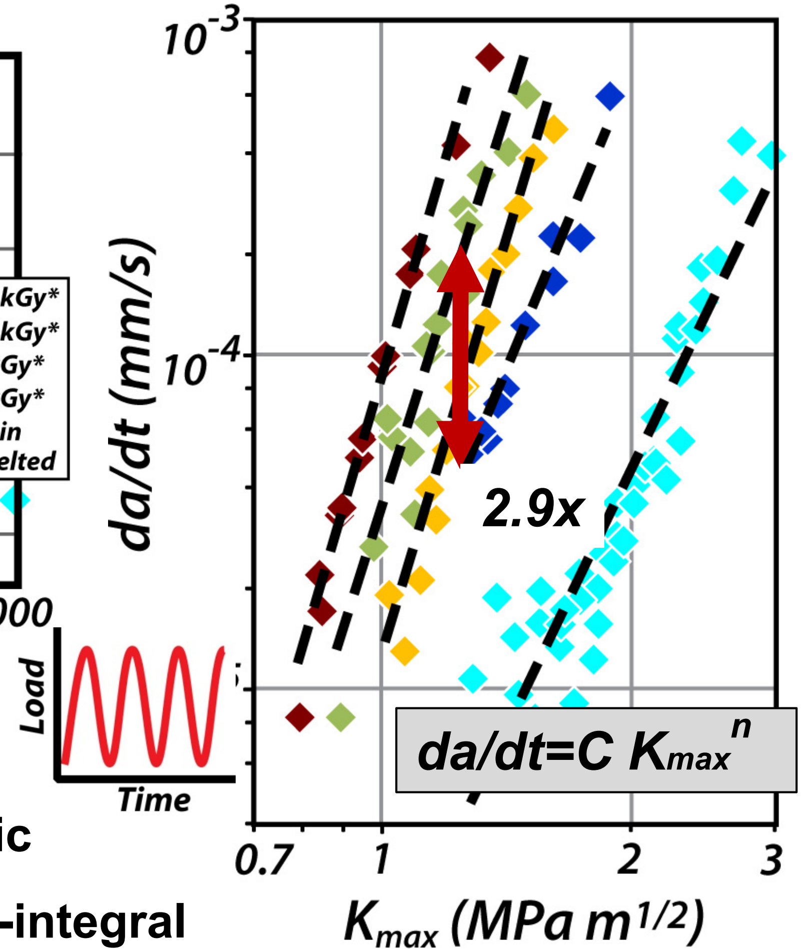






Crack behavior in UHMWPE is *non-cyclic*

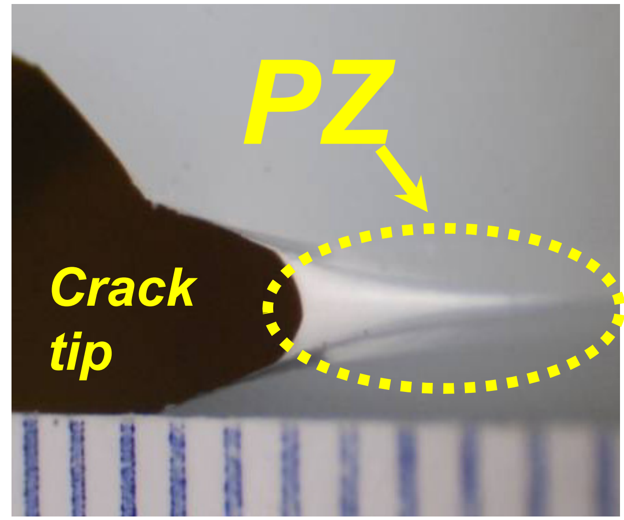


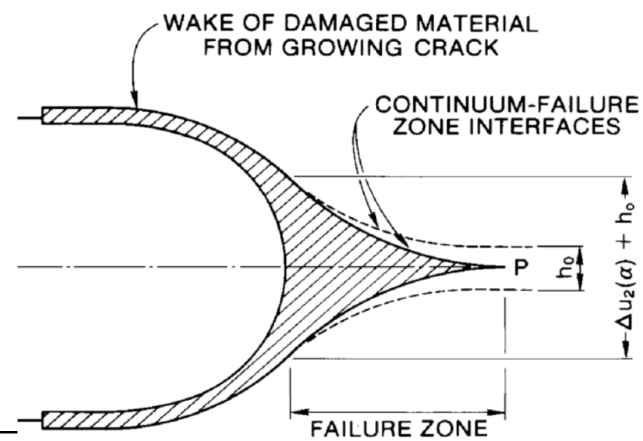


- **Crack propagation is stable, quasi-static**
- **Growth is predictable from simple time-integral**

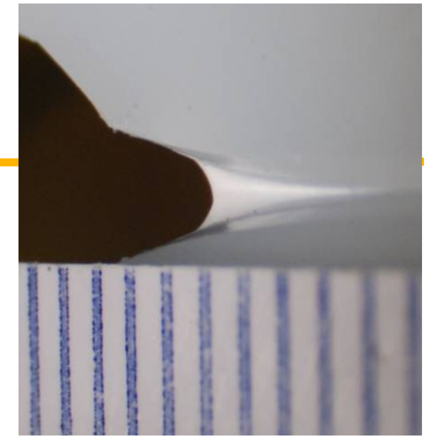
Why static mode crack behavior?

- **Overall crack phenomena are determined by behavior in the fracture process zone (PZ)**
- **Crack tip deformation is principally quasi-static**
  - Viscous flow
  - Time-dependent fracture
- **Intrinsic cyclic damage mechanisms appear absent**
  - Crazing, crack tip resharpening





A “new” approach to viscous fracture

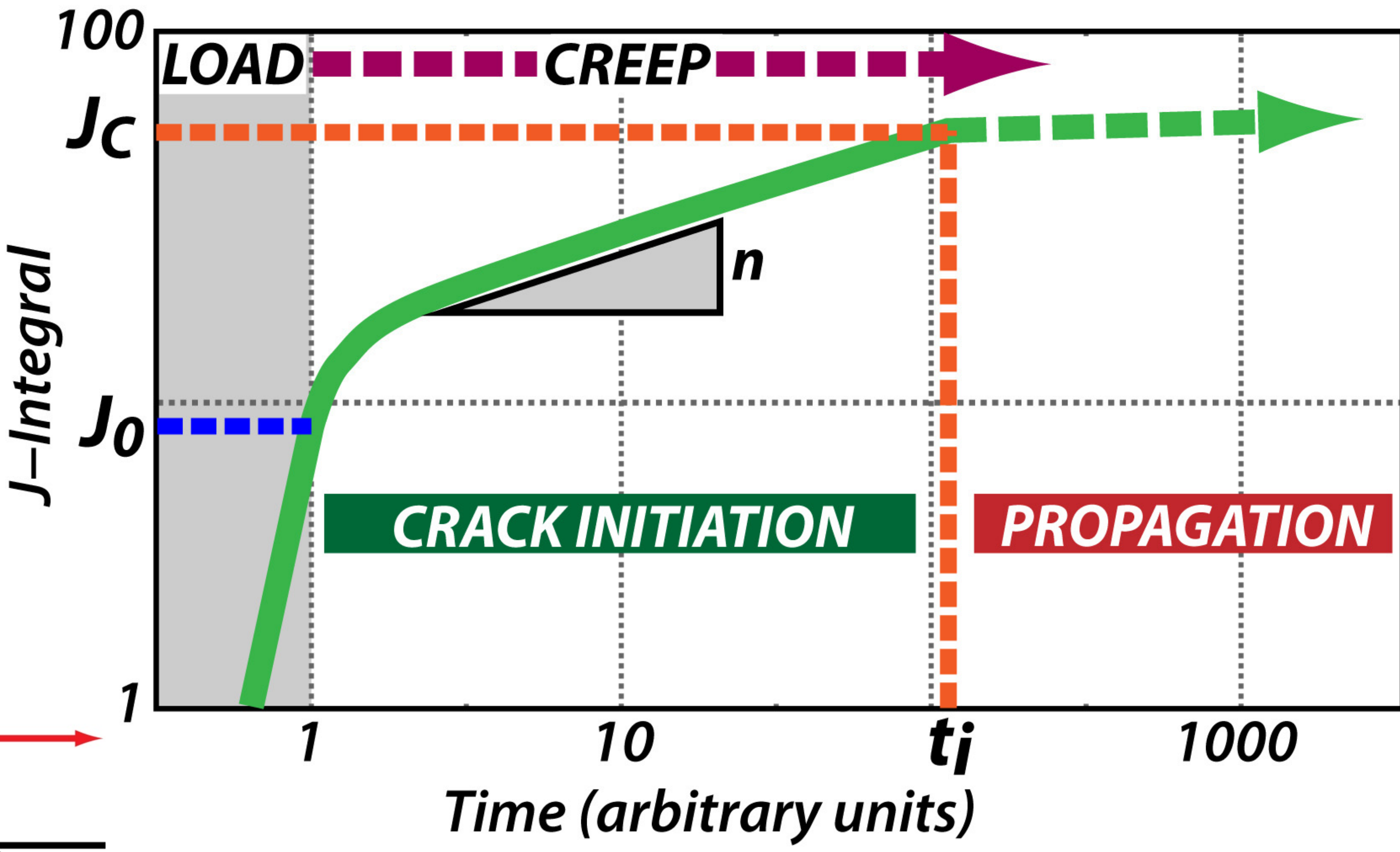


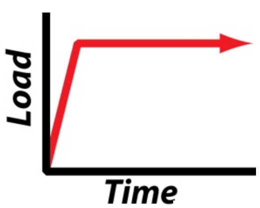
- **JG Williams model of viscous crack initiation and propagation**
  - Power law ***time dependent*** J-integral
  - ***J0*** is applied (instantaneous) J-integral
  - Exponent ***n*** *(related to creep resistance, <u>unifying factor</u>)*
  - Similar to work by Schapery

$$\frac{J}{J_0} = \left(\frac{t}{t_0}\right)^n$$

$$\frac{t_i}{\tau_0} = \left(\frac{J_C}{J_0}\right)^{1/n}$$

$$\frac{da}{dt} = Q\left(\frac{J_0}{J_C}\right)^{\frac{1+n}{n}}$$





$$\frac{J}{J_0} = \left(\frac{t}{t_0}\right)^n \qquad \frac{t_i}{\tau_0} = \left(\frac{J_C}{J_0}\right)^{1/n}$$

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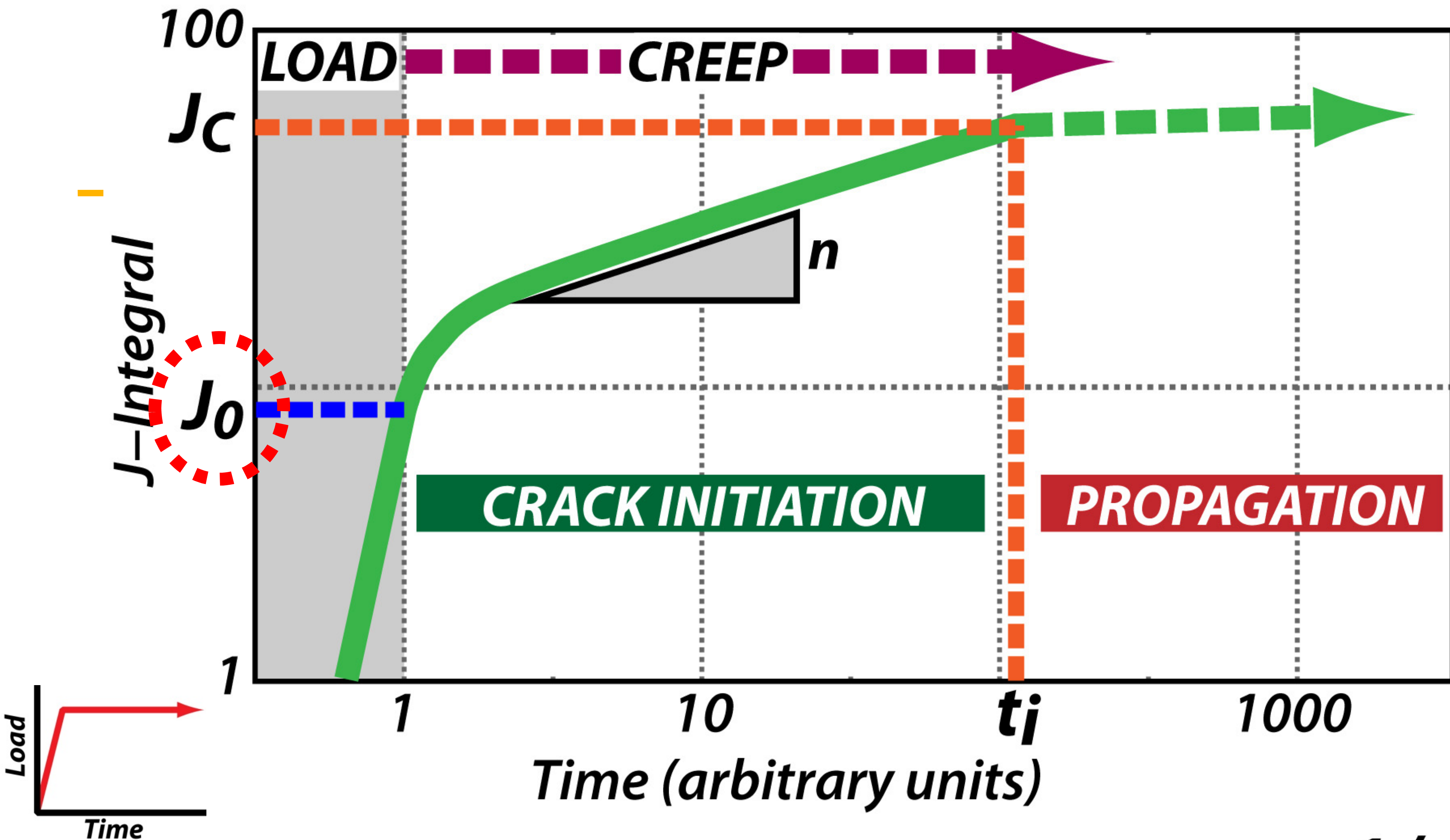

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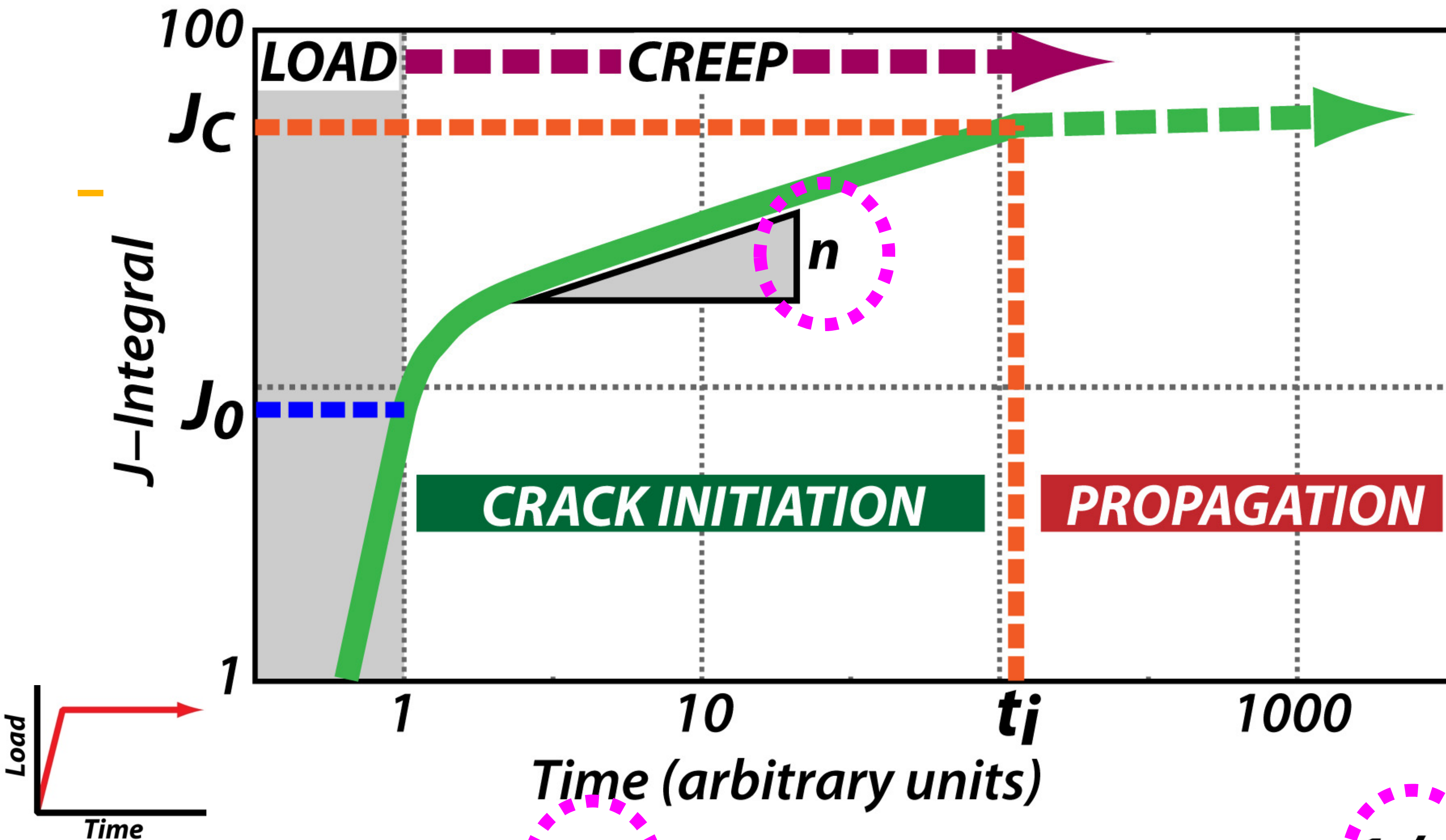

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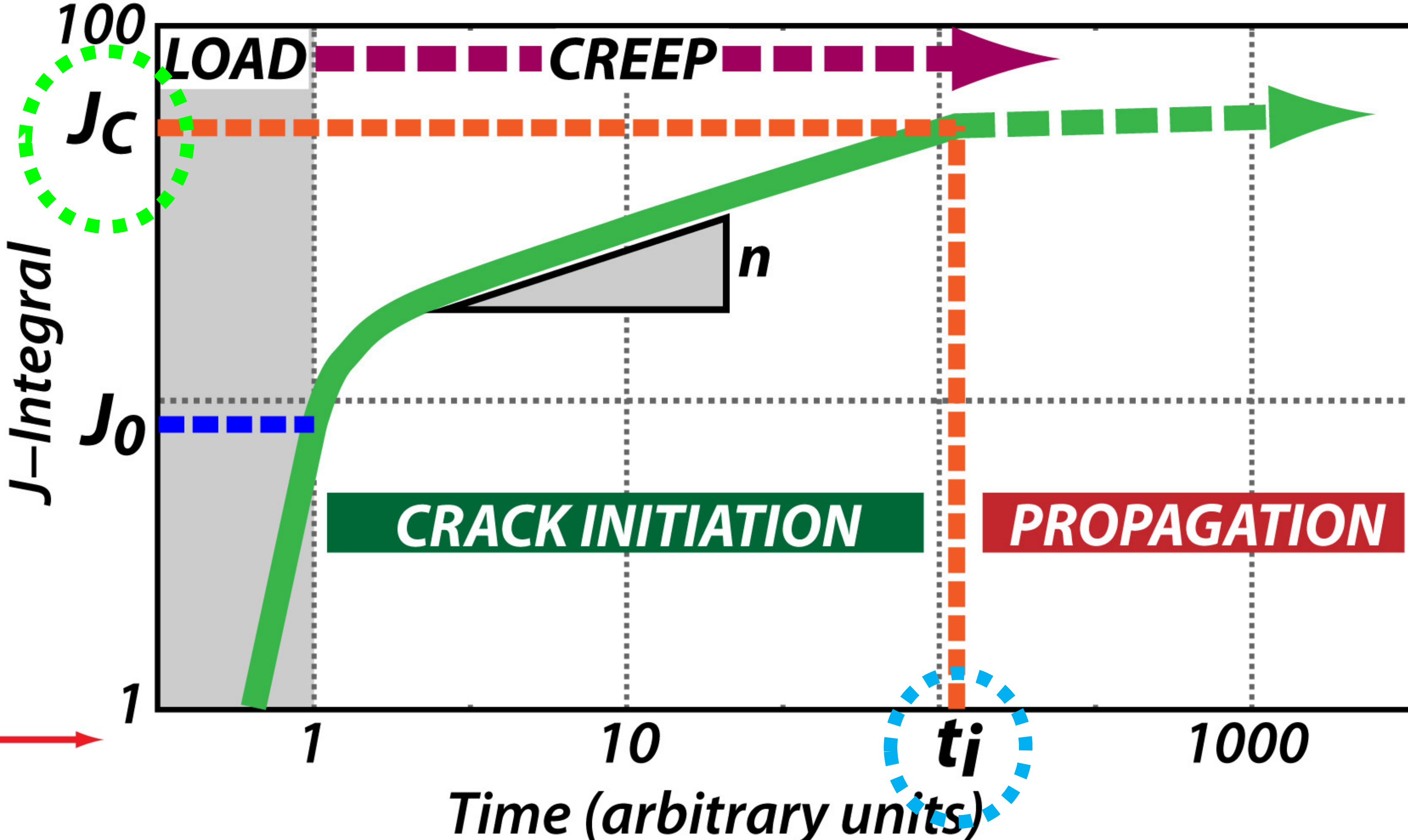
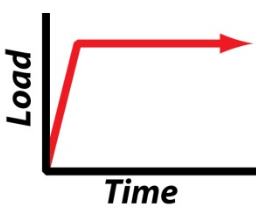


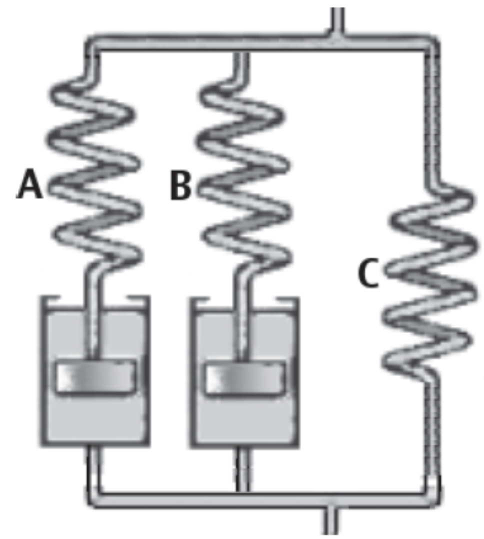


$$\frac{J}{J_0} = \left(\frac{t}{t_0}\right)^n$$

$$\frac{t_i}{\tau_0} = \left(\frac{J_C}{J_0}\right)^{1/n}$$

FEA: Constitutive model

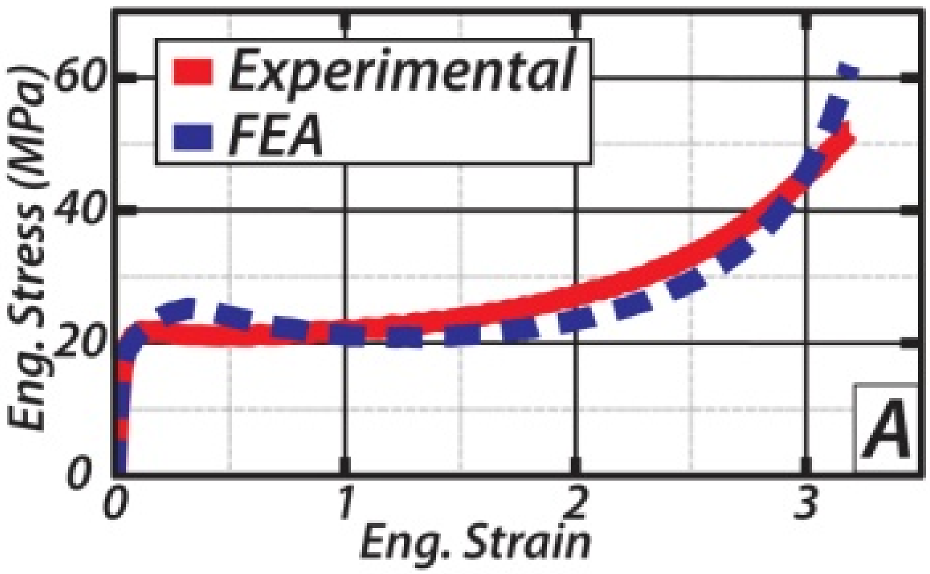
- **Hyperelastic-viscoplastic "Three Network Model"**
  - Arruda-Boyce 8-chain hyperelastic springs
  - Power law viscoplasticity
  - Yield stress distribution through parallel plastic elements, variable stiffness
- **Molecular chain stretch of hyperelastic element C is correlated to tensile failure (decohesion)**

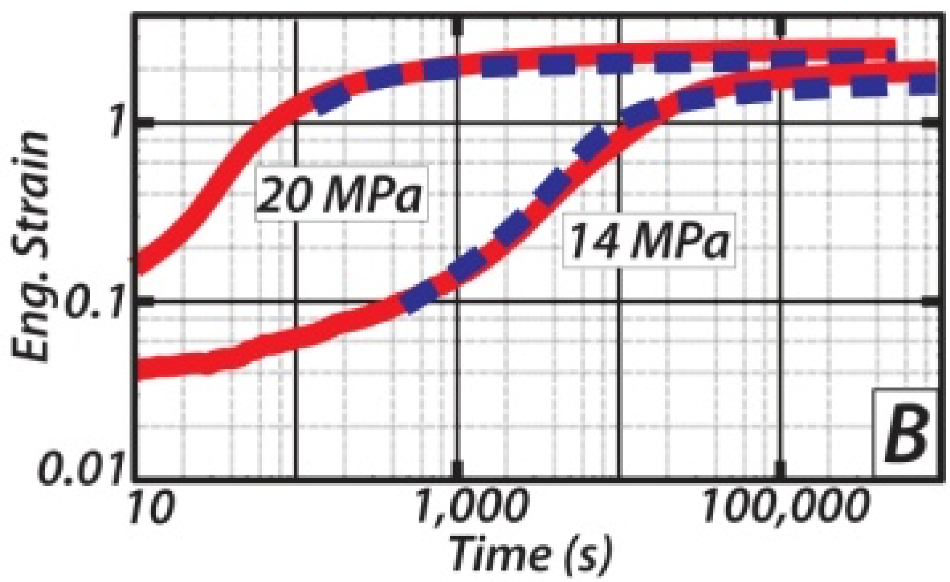


*J Bergstrom and Veryst Inc.
Update for Hybrid Model, i.e.,
Bergstrom et al., Biomat *25*
Bergstrom et al., J Ortho Res *23*

TNM calibration

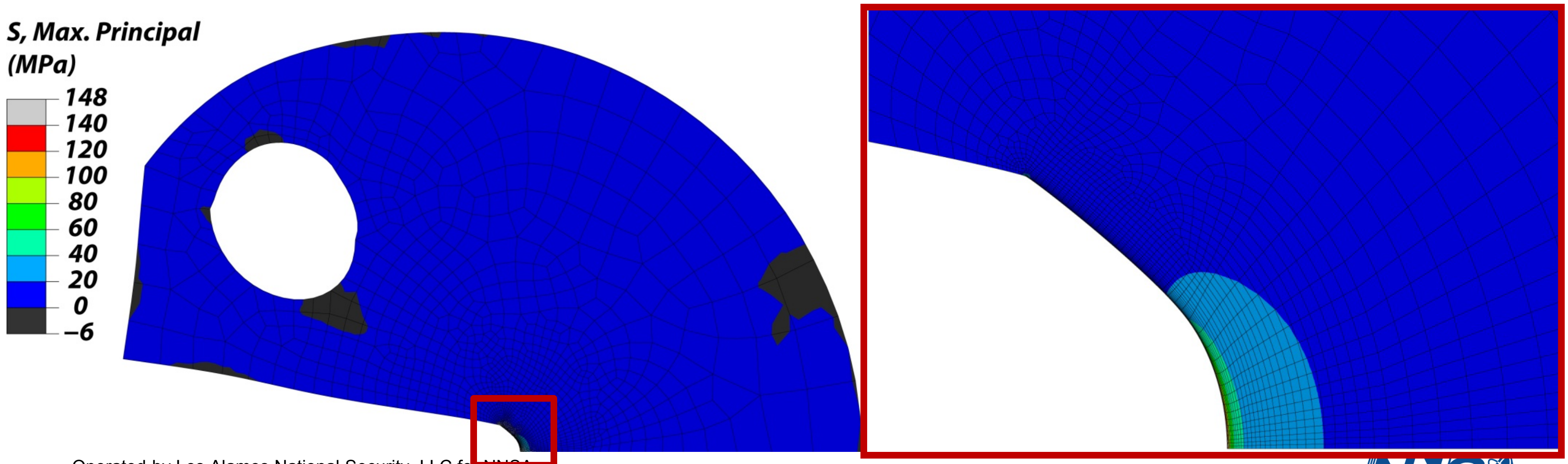
- **FEA modeling using hyperelastic-viscoplastic TNM**
  - Calibrated to 65 kGy remelted 1-D behavior
  - Monotonic to failure, post-yield creep at two loads





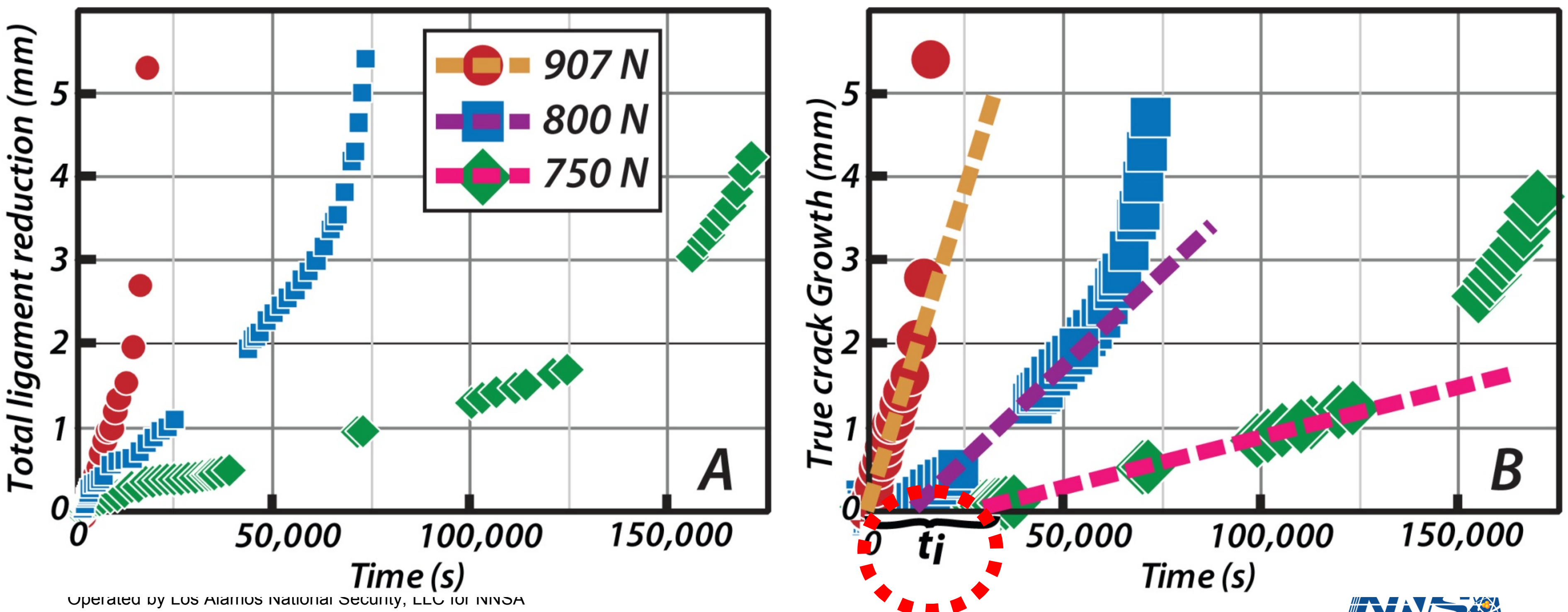
Finite element model

- **Abaqus CAE v6.8**
- **2450 CPS8 quadratic quadrilateral elements**
- **UMAT user material subroutine for TNM**
  - Licensed from Veryst Engineering (Cambridge, MA, USA)



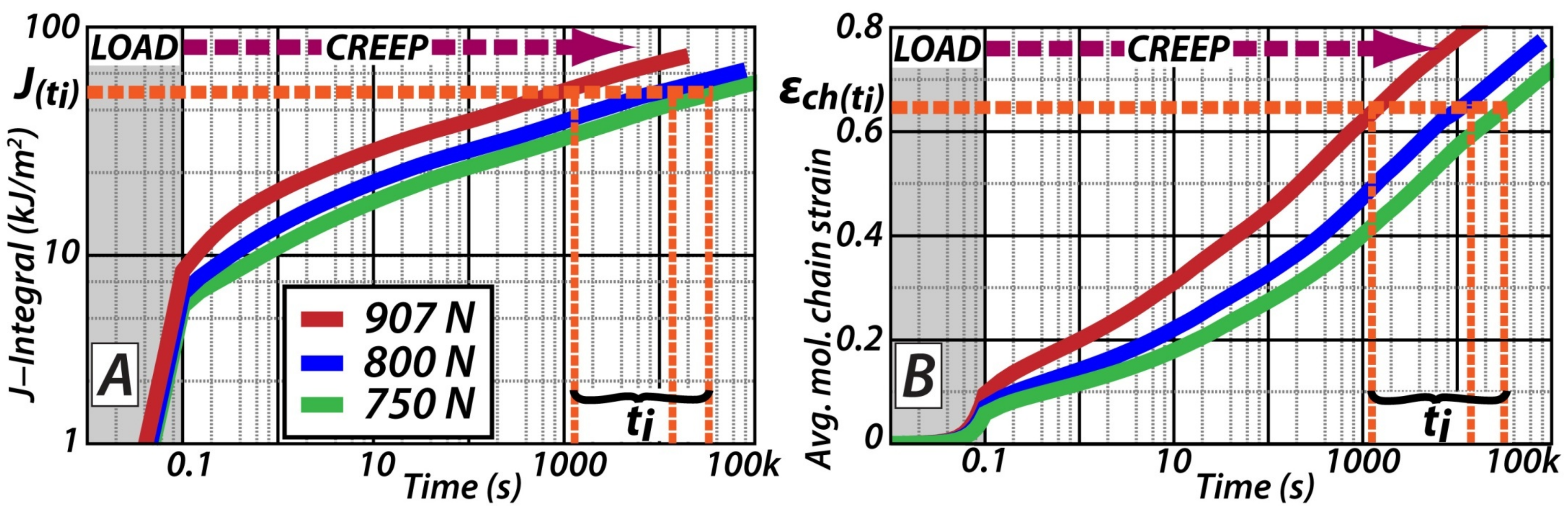
Experimental constant load crack growth

- Observed ligament reduction is initially logarithmic.
- With logarithmic contribution regression fitted and subtracted, crack growth is seen to initiate at time t_i



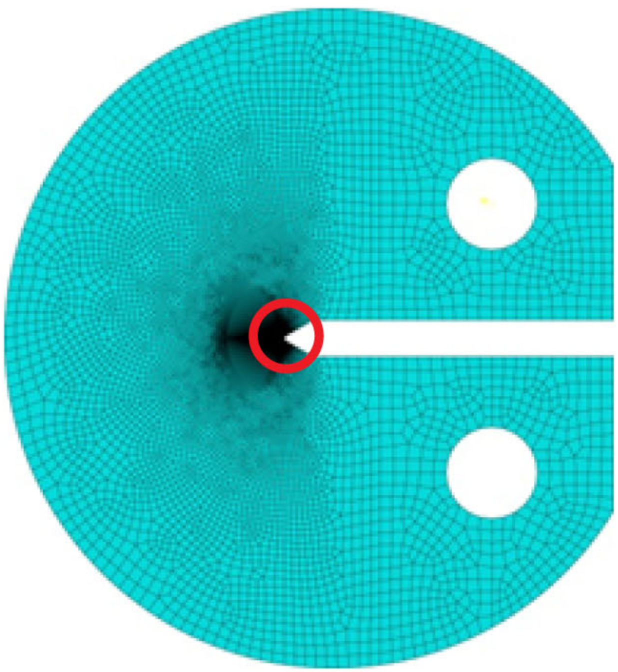
Crack initiation: FEA computation of critical quantities

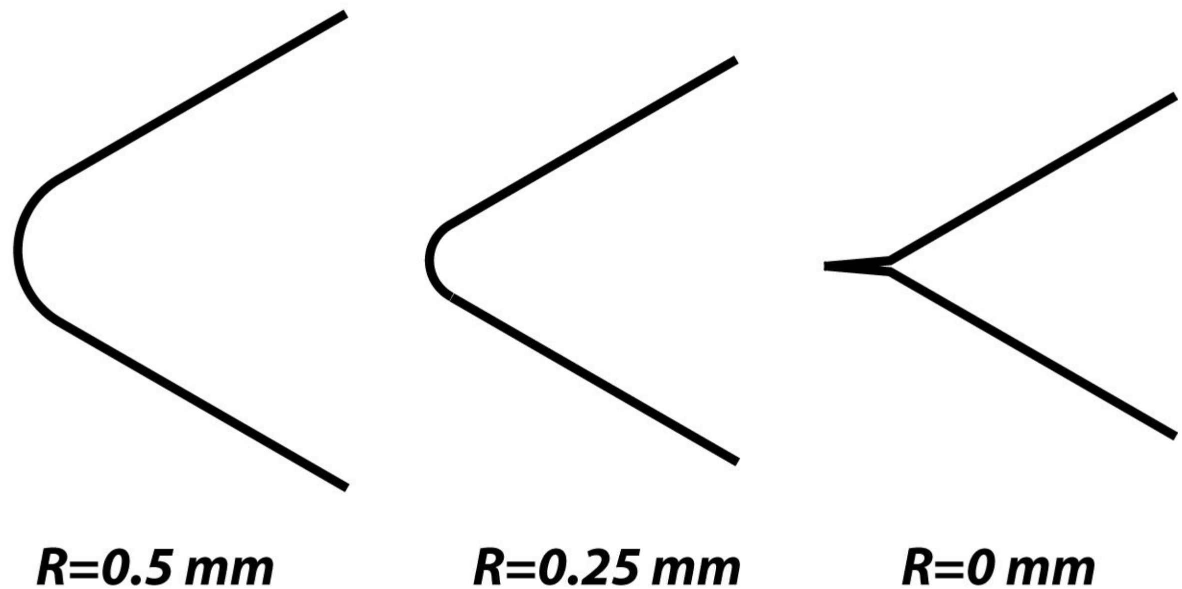
- **Calibrated FEA predictions of quasi-static crack initiation agree with analytical expectations**
  - J-integral is power-law time dependent
  - ***Experimental*** initiation times for 3 loads map to a single predicted values of ***$J(t_i)$*, *molecular chain strain $\varepsilon_{ch}(t_i)$***
  - ***Single-valued $J(t_i)$ and $\varepsilon_{ch}(t_i)$ implies legitimate failure criteria***



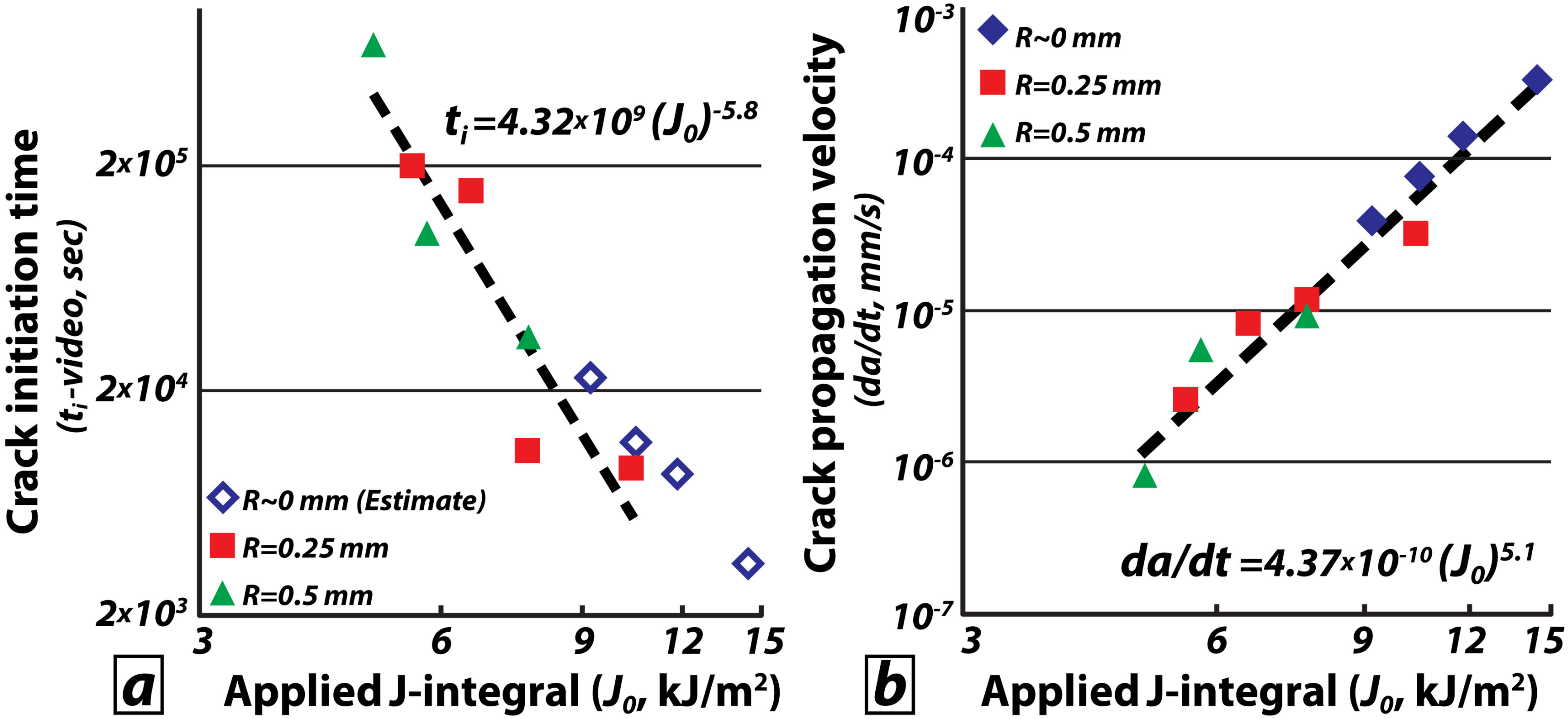
Generality: J-controlled initiation for design

- **Applied J_0 is an FEA computed quantity (design/service specific)**
- ***Experimentally verify J_0 controls initiation for arbitrary geometry***
- ***If J_0 is sufficient (general), then can use in design/ fracture control***





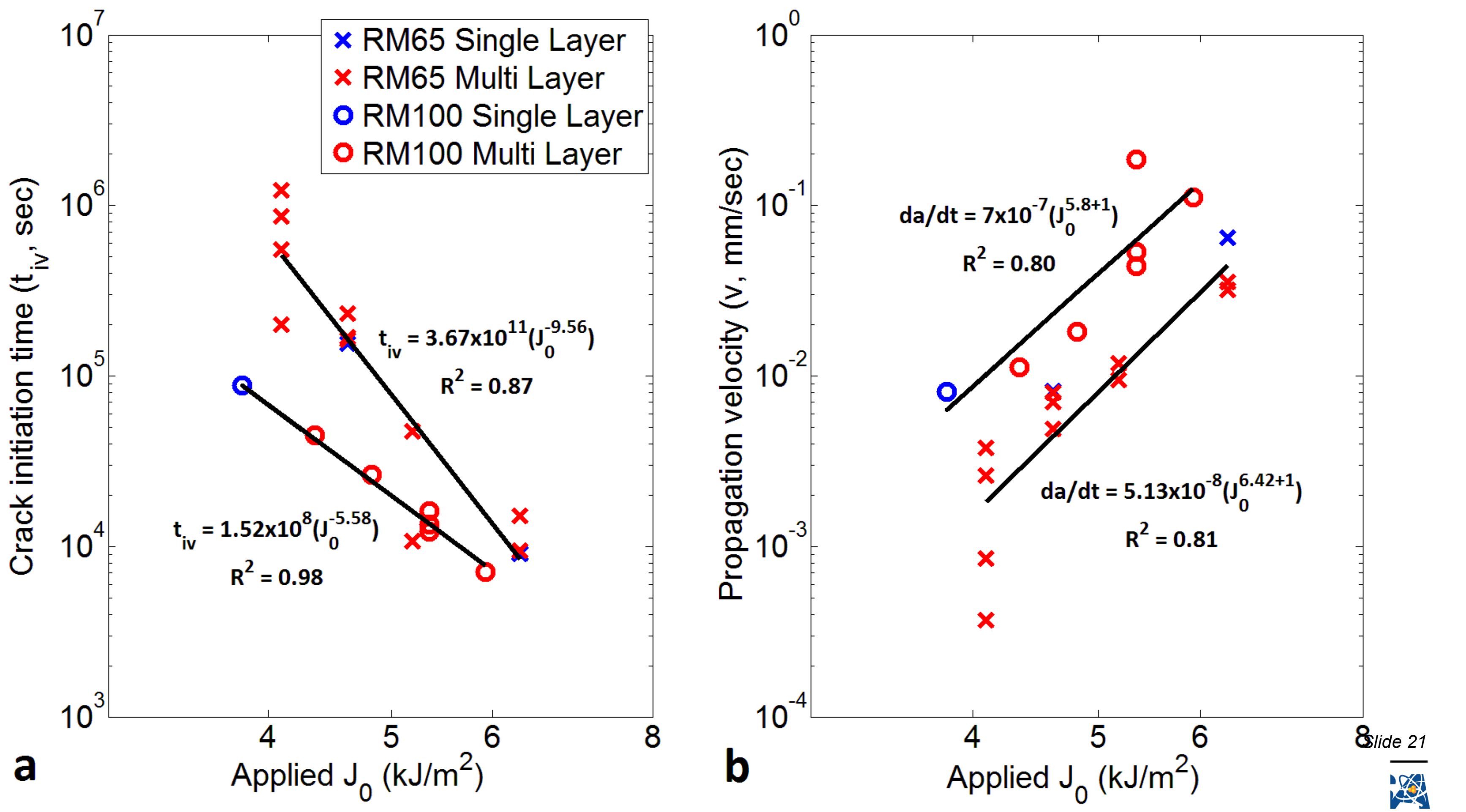
Crack initiation and propagation both correlate to *J0*



- Moderately crosslinked UHMWPE

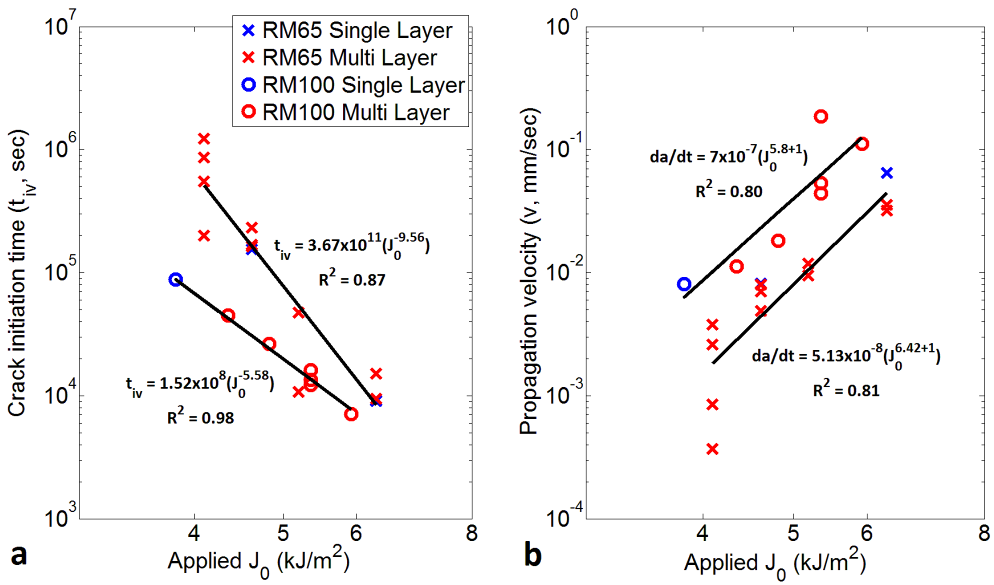
J_0 correlation holds for varying crosslink density

- **Highly crosslinked shows similar behavior, with lower initiation time and higher velocity. Some subtle differences.**

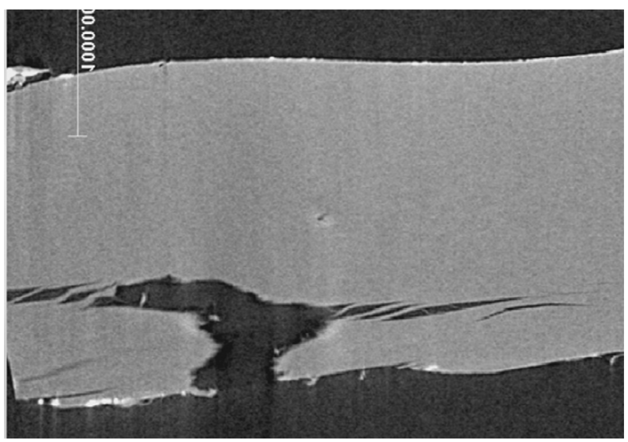


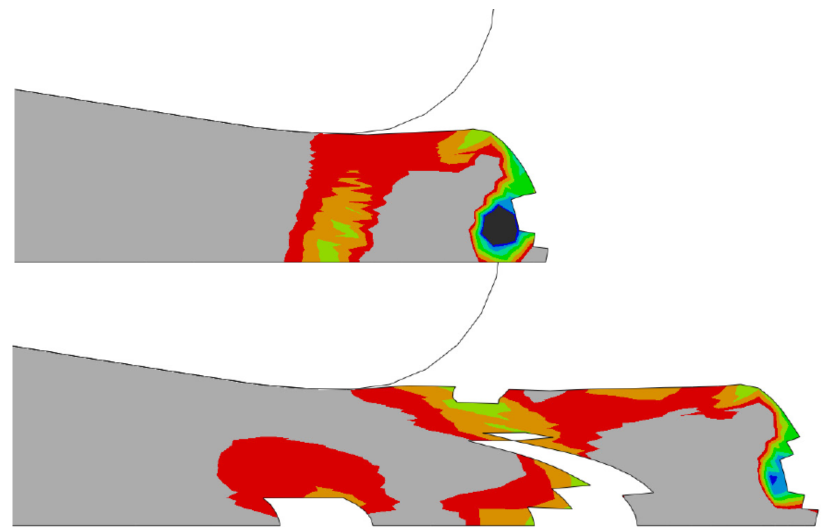
Williams theory is sound for design

- **First-of-its-kind safety metric for crack inception in UHMWPE structures**
- ***Initiation and propagation theory should hold even up to dynamic case, until kinetic effects become appreciable.***



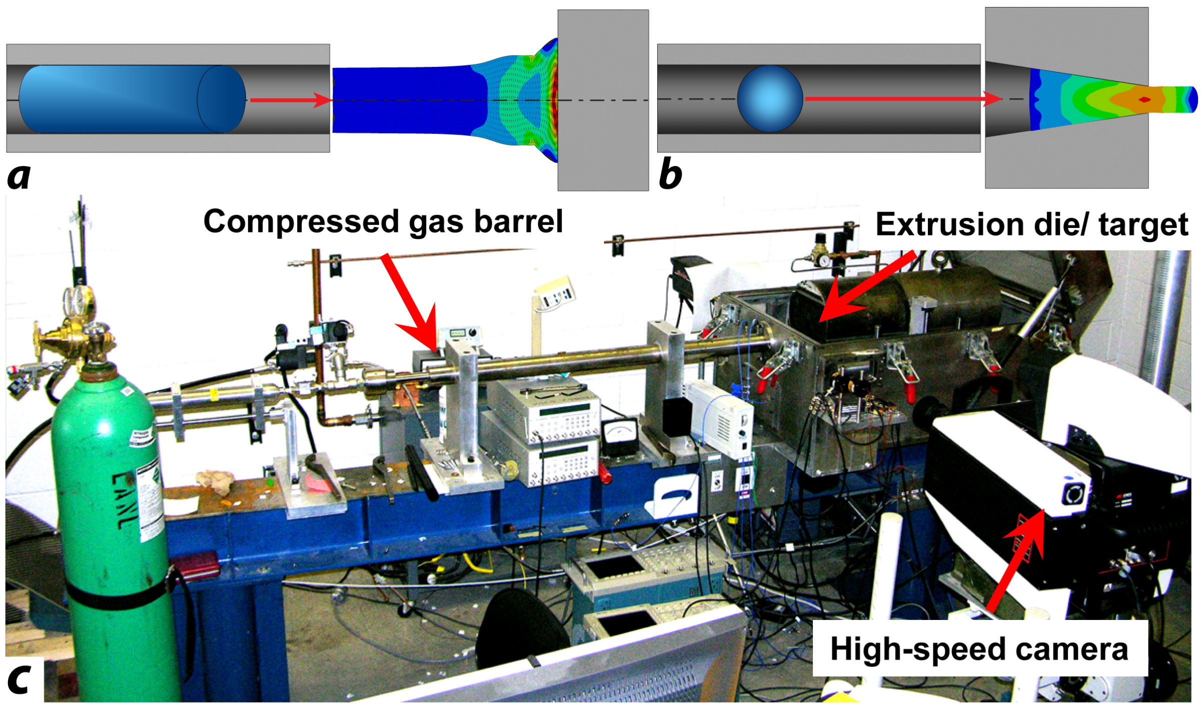
Mechanisms of failure in HDPE during extreme tensile deformation





Extreme deformation:
Taylor impact and Dynamic-Tensile-Extrusion

- *Extreme deformation*: Strain >1 with strain-rate>10,000/s
- Gradients in strain and strain-rate – rich data for validation
- Some damage may be suppressed under compression (pressure)



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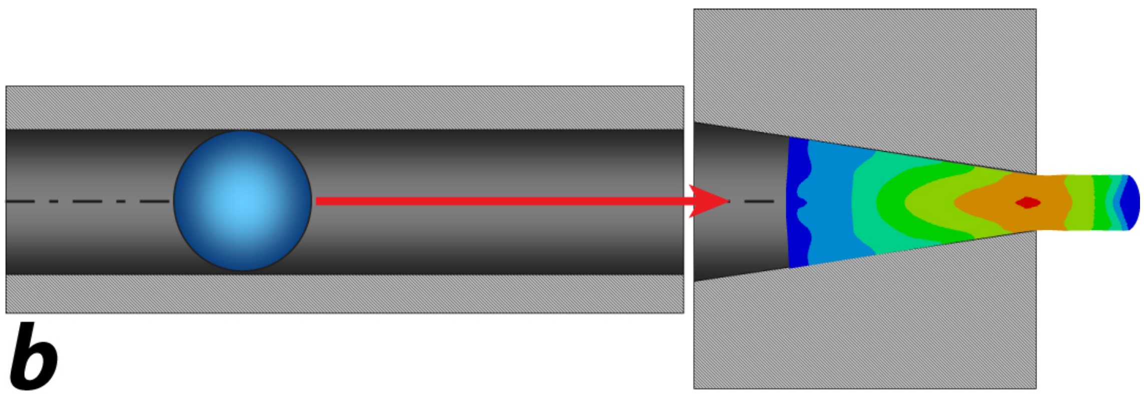
Dynamic-Tensile-Extrusion

- **He gas gun accelerated projectile to 300-600 m/s**
- **Conical extrusion – extrusion true strain 1-2**
- **Vary velocity and area reduction to focus on behavior of interest**
  - *Too severe: fragmentation*
  - *Too moderate: no extrusion or pass-through*



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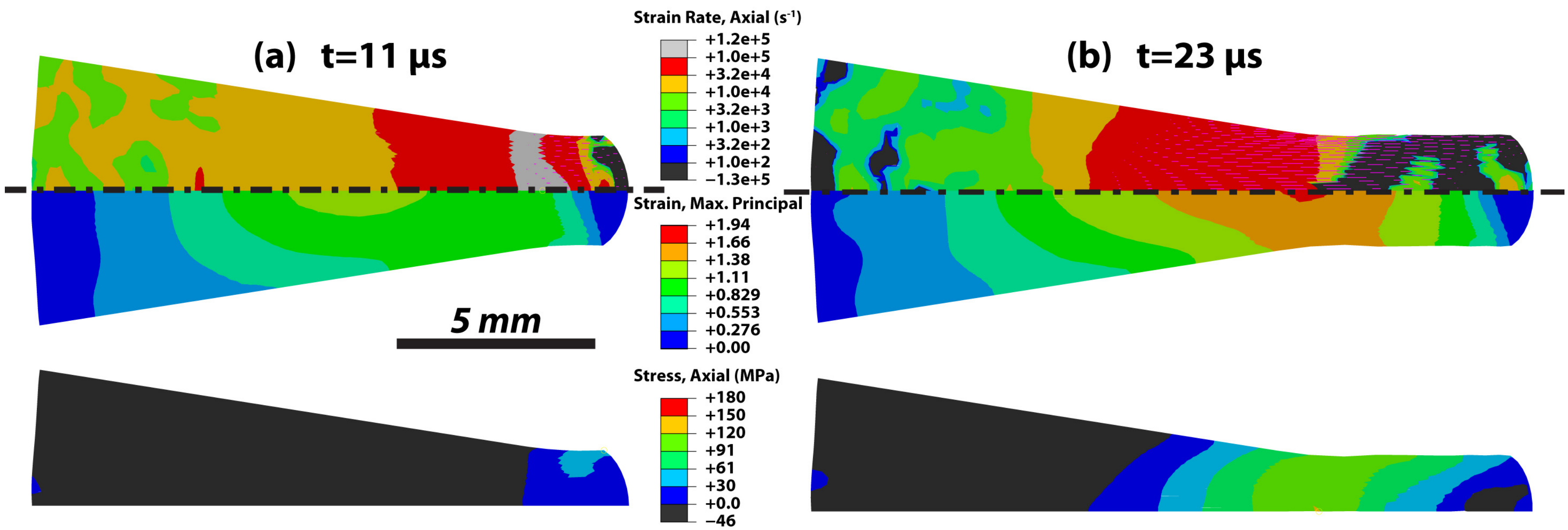
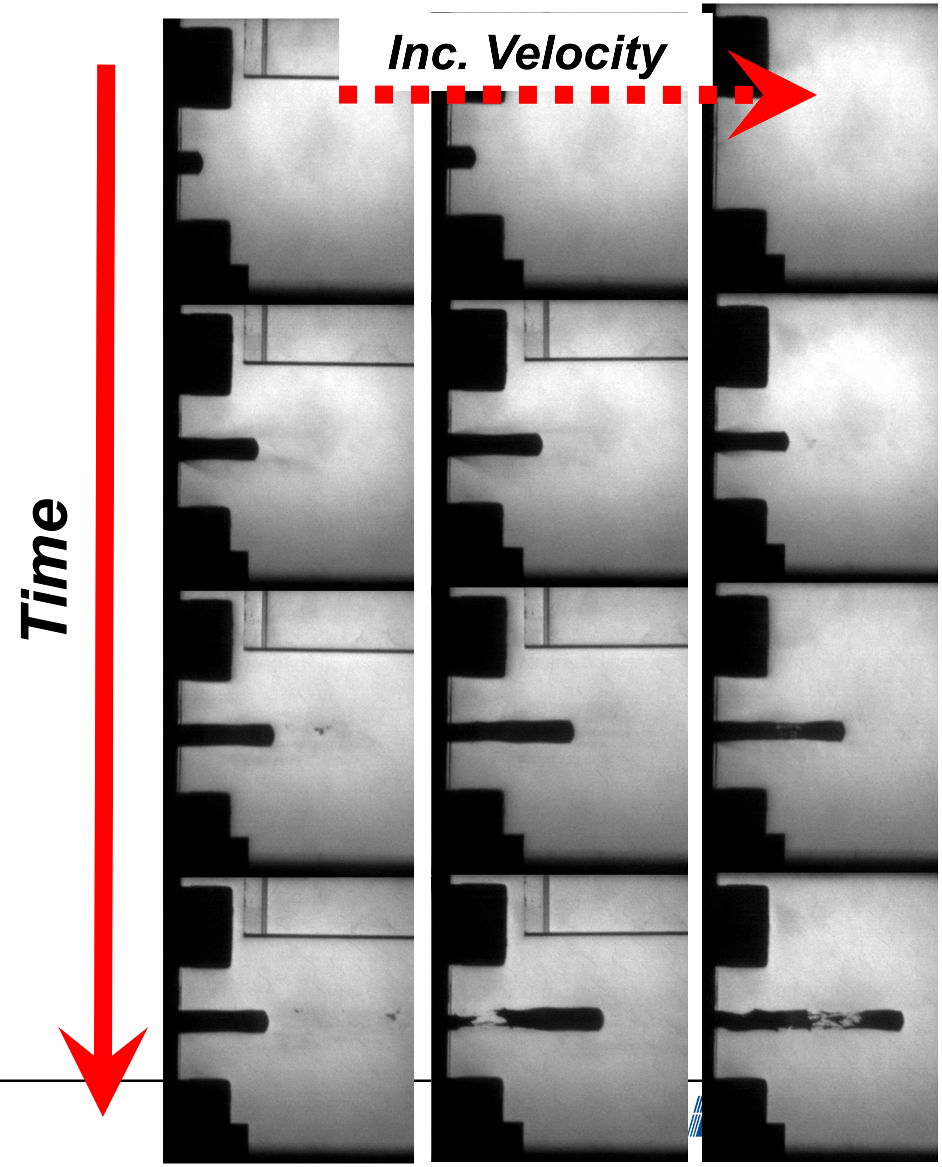
Dynamic-Tensile-Extrusion: Stress/Strain Fields

- *Taylor-validated* **constitutive model in ABAQUS/Explicit**
- **Simulations demonstrate extreme tensile behavior:**
  - *Strain>1, strain-rate>10,000, axial stress>0 (pressure<0)*



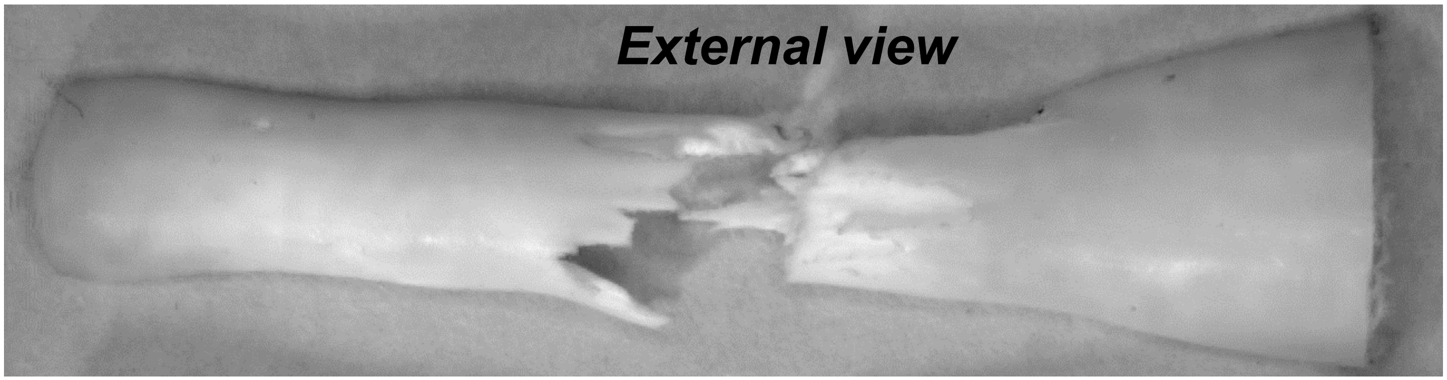
Results: Dyn-Ten-Ext of HDPE

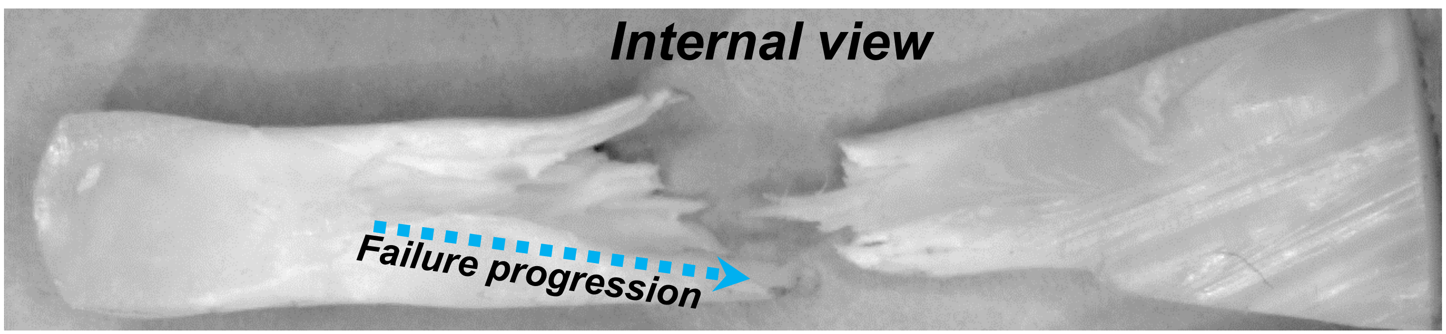
- ***At lower velocities (450 m/s)***, specimen survives and contains sub-critical damage
- ***Intermediate velocities (486 m/s)*** fail in a sequential tensile/shear manner
- ***High velocities (550 m/s)*** fragment at neck catastrophically



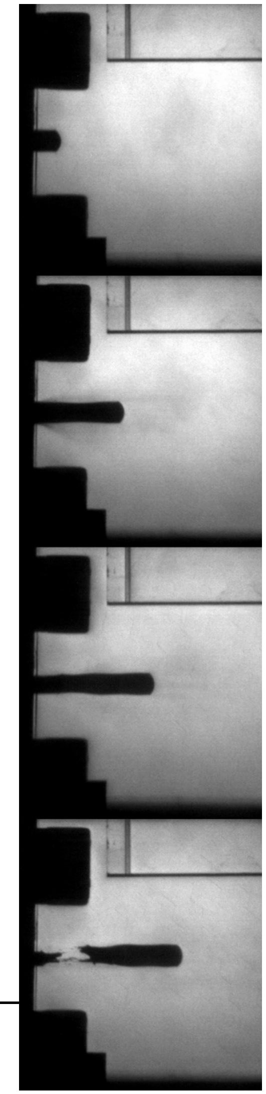
Intermediate velocity: Internal failure, external rupture

- Internal tensile failure, shear failure, rupture at die exit



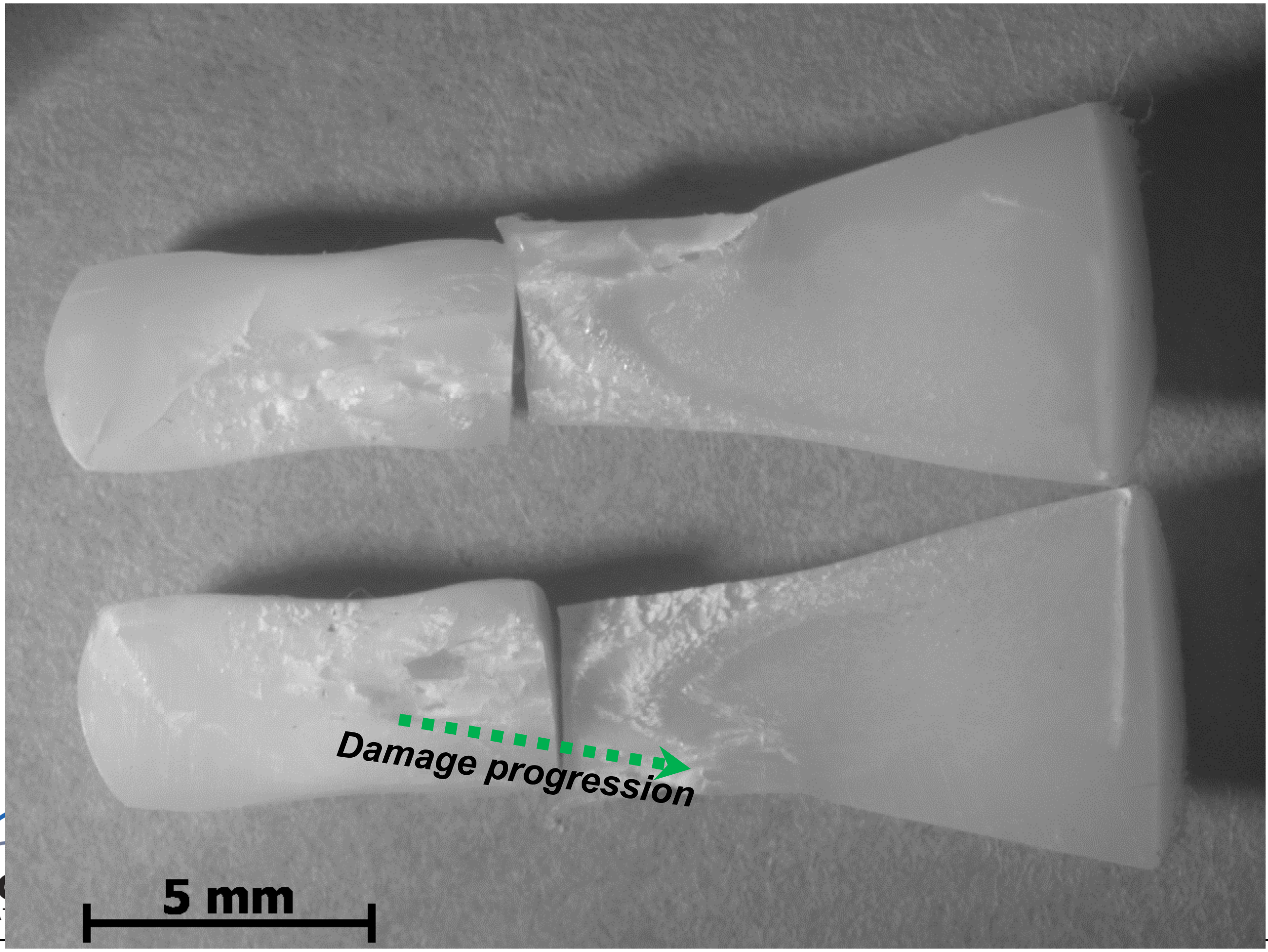


465 m/s

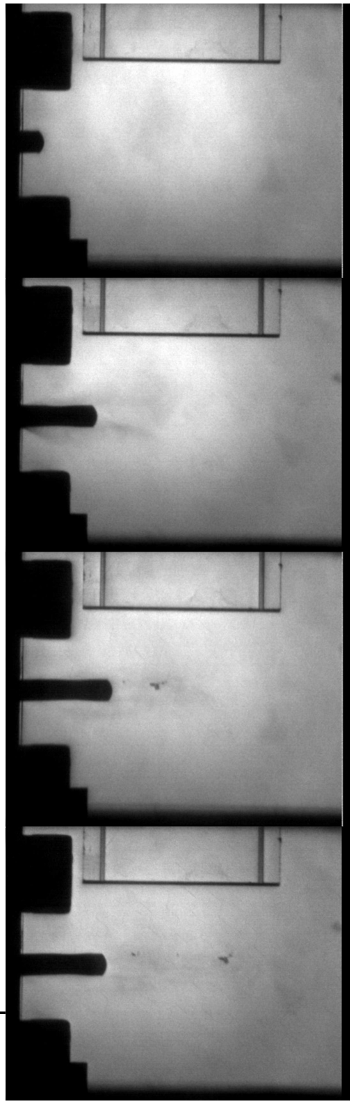


Low velocity: Incomplete failure; incipient damage

- Internal tensile failure, sheared damage region

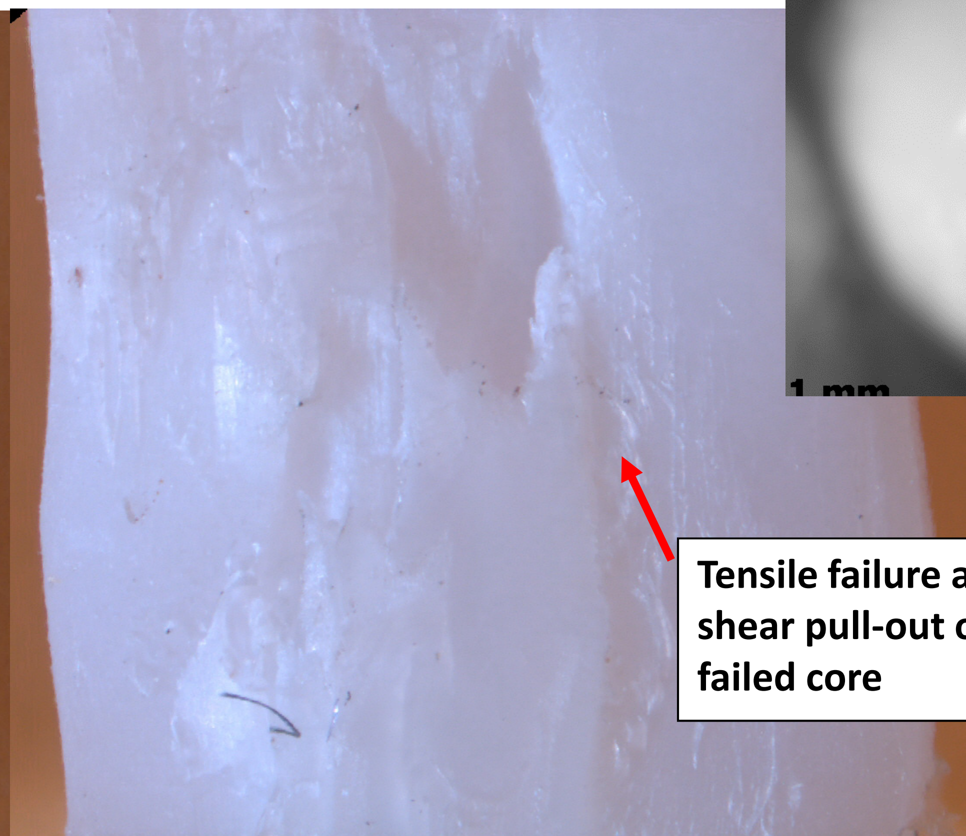


450 m/s



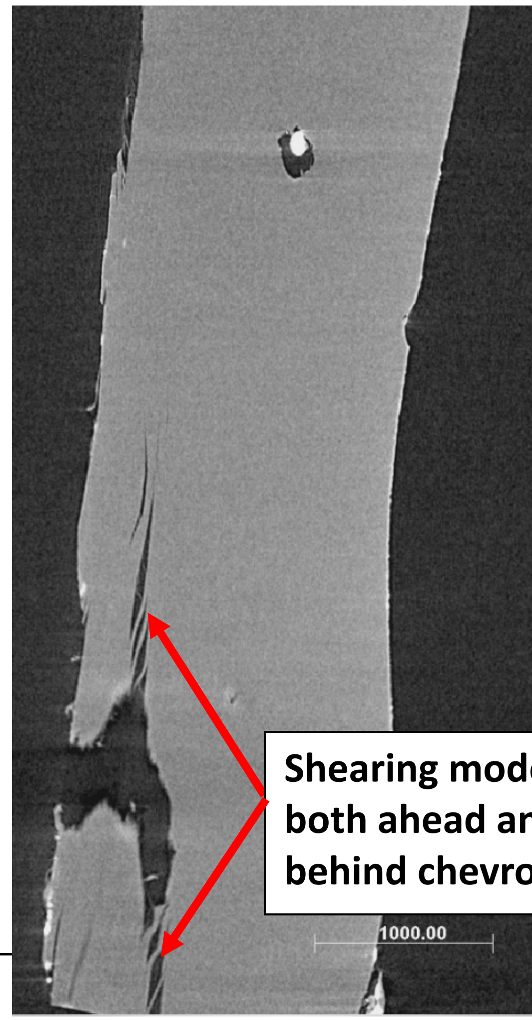
Low velocity: Internal failure; shear damage tube

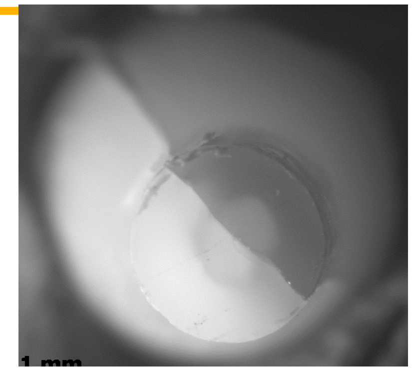
Chevron rupture, mode-II crack, transition to shear damage field in tube shape

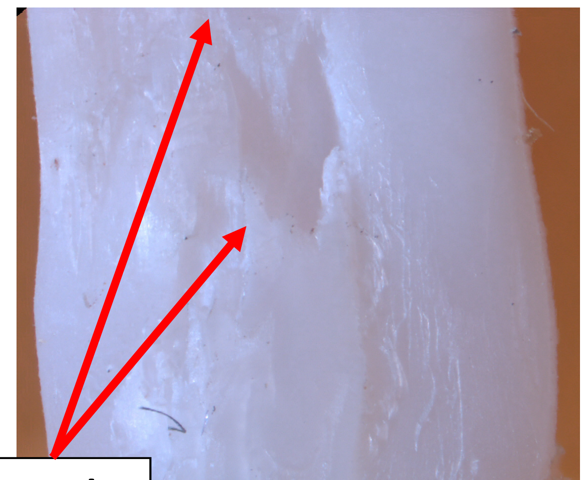


X-ray CT: Internal failure; shear damage tube

Damage tube is a crack surface bridged by ligaments



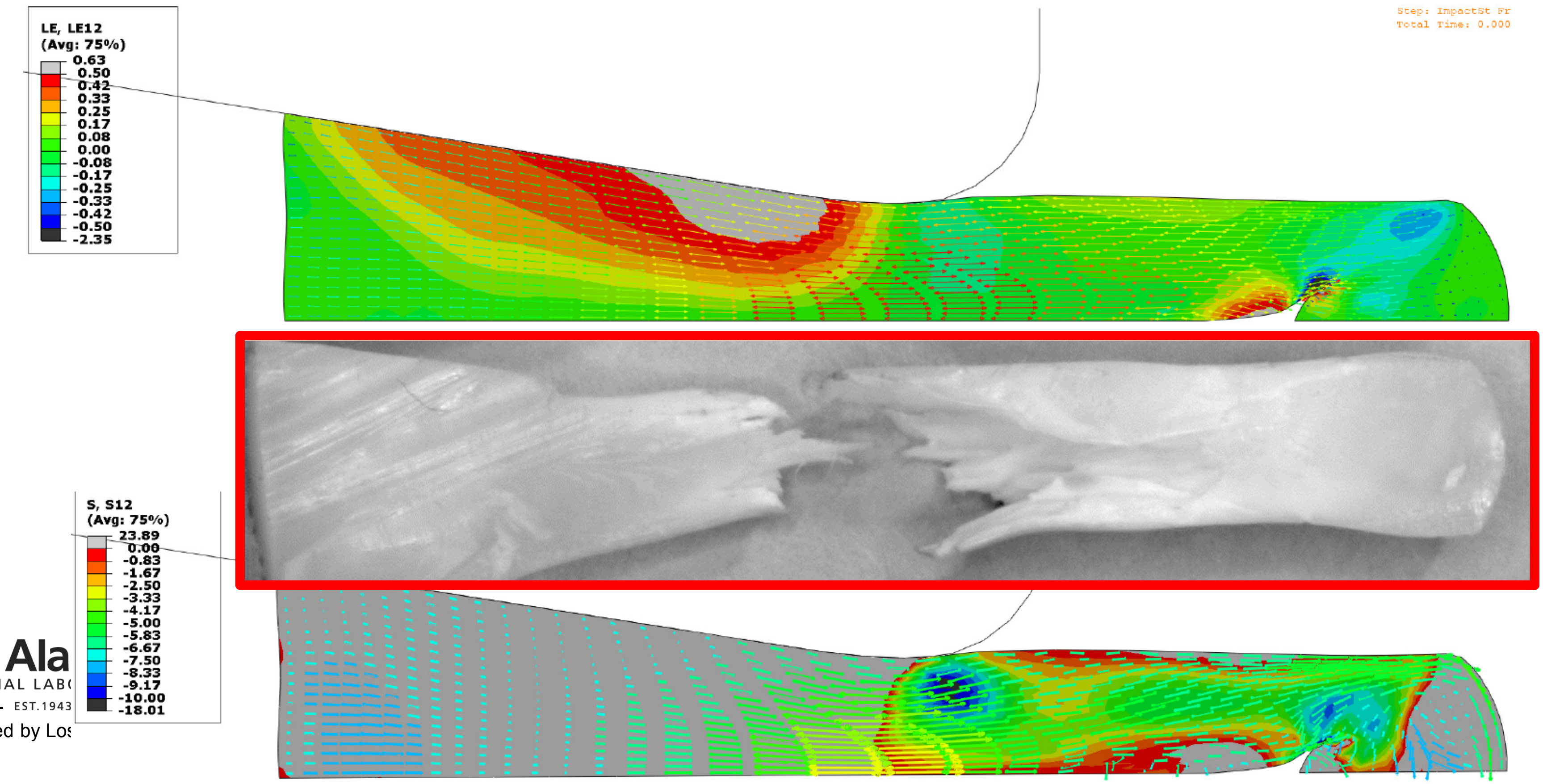




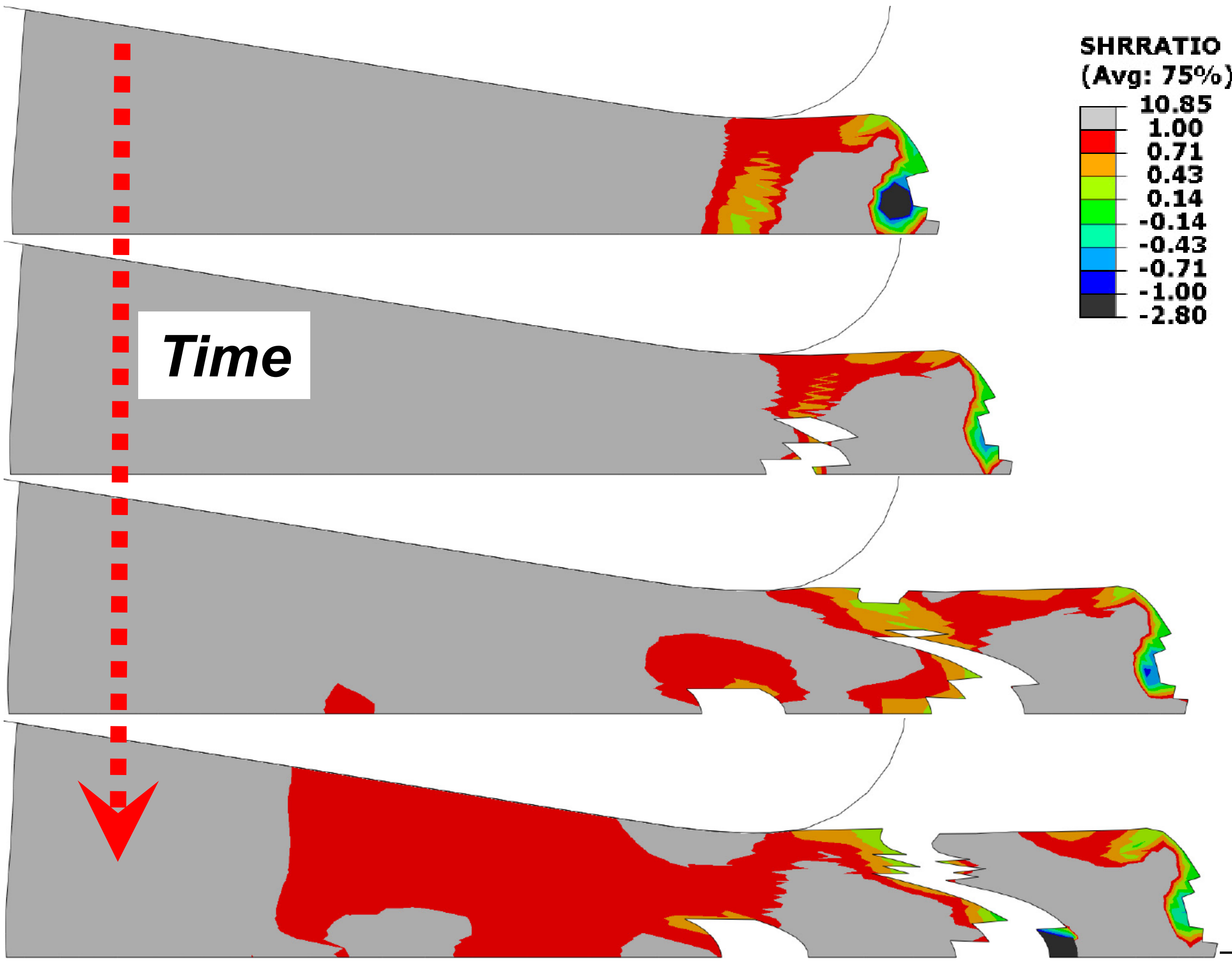
Shearing mode crack both ahead and behind chevron

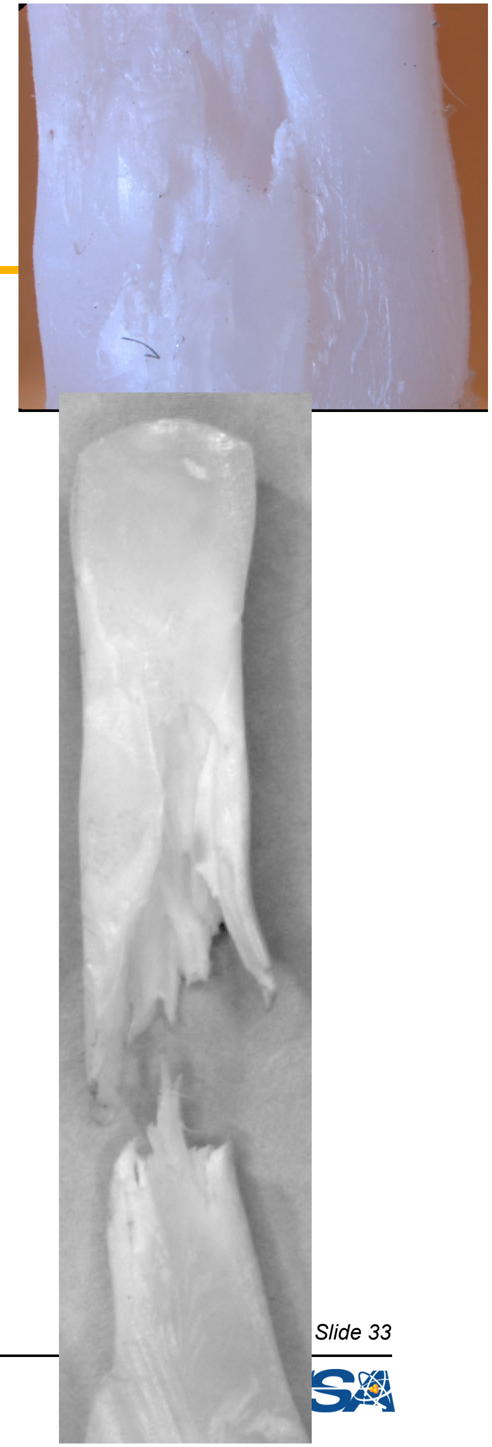
Low velocity FEA: Shear stress localization

- **Terminal strain field does not match damage due to model limitations**
- **Shear stress focus region maps to shear damage zone**
- ***A pressure-shear damage model could yield correct strain field***



Exploratory results with pressure-shear damage: Failure progression similar to observed path

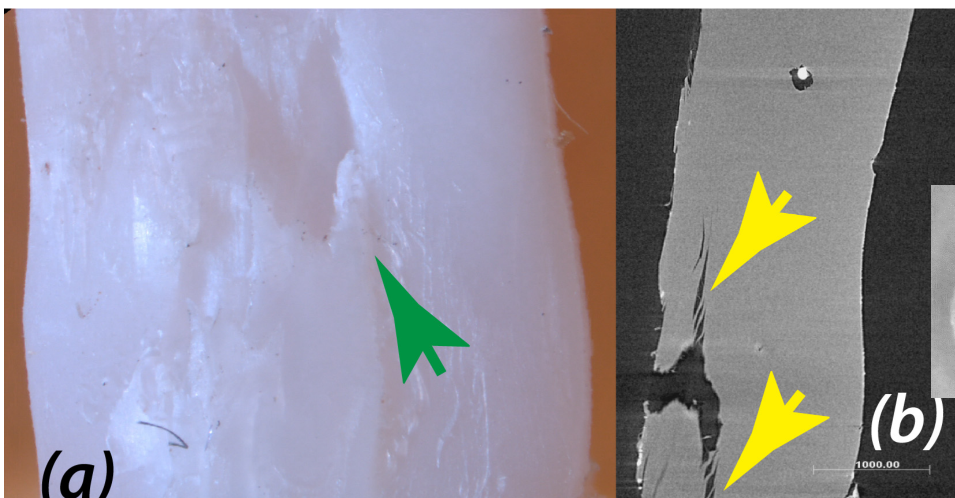


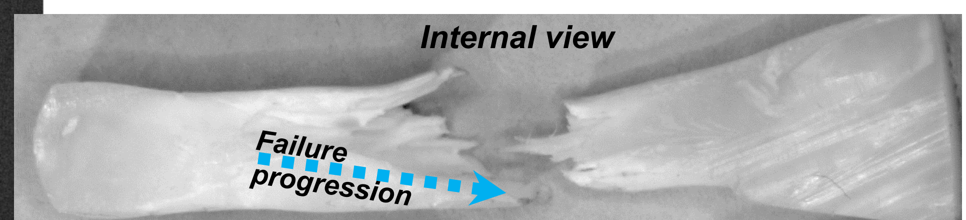


Conclusions

Dynamic-Tensile-Extrusion is an excellent tool for studying dynamic damage in polymers

- **Deformations not accessible by other means, yet simple BCs**
- **Next: map mechanisms with input KE and extrusion severity**

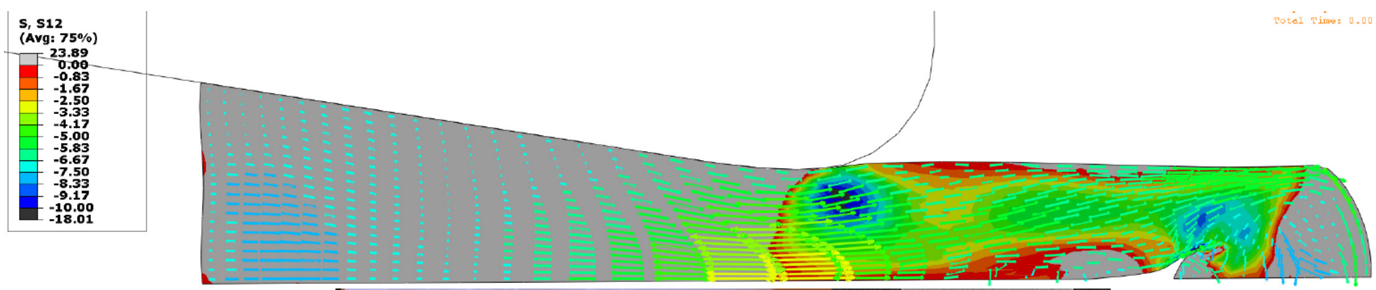


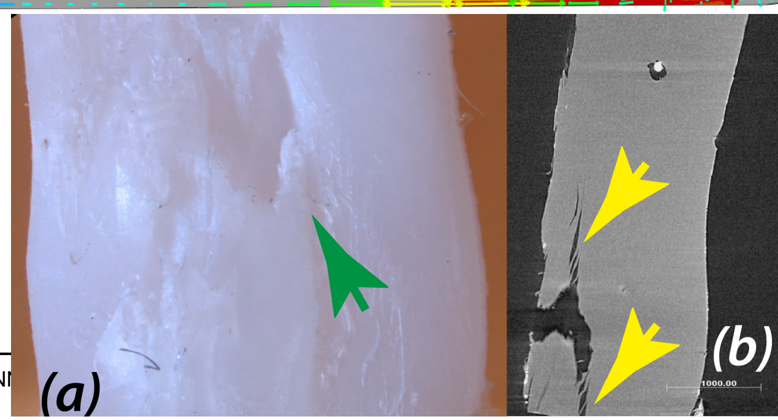


Conclusions

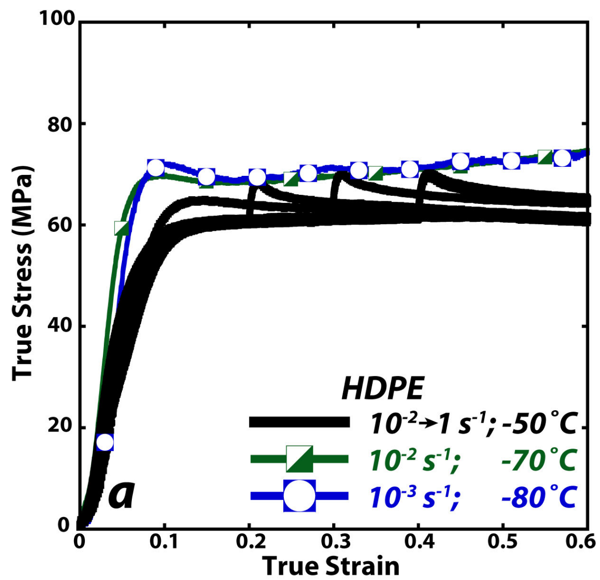
Modeling of continuum deformation in Dyn-Ten-Ext can elucidate mechanisms of damage and failure

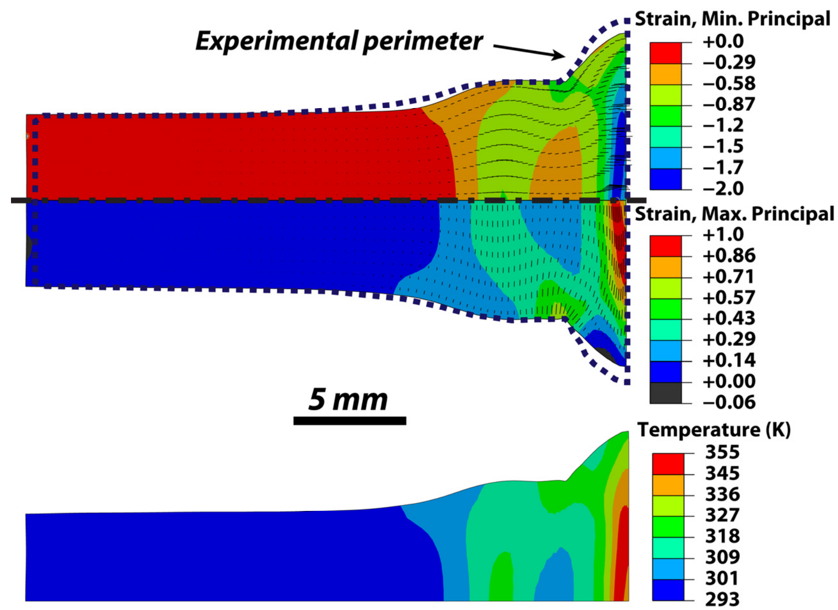
- **Infer damage mechanisms by matching path, field localizations**
- **Use to generate hypothetical damage mode and test**
- **Discovery tool, even with limited FEA (e.g., simple constitutive model)**



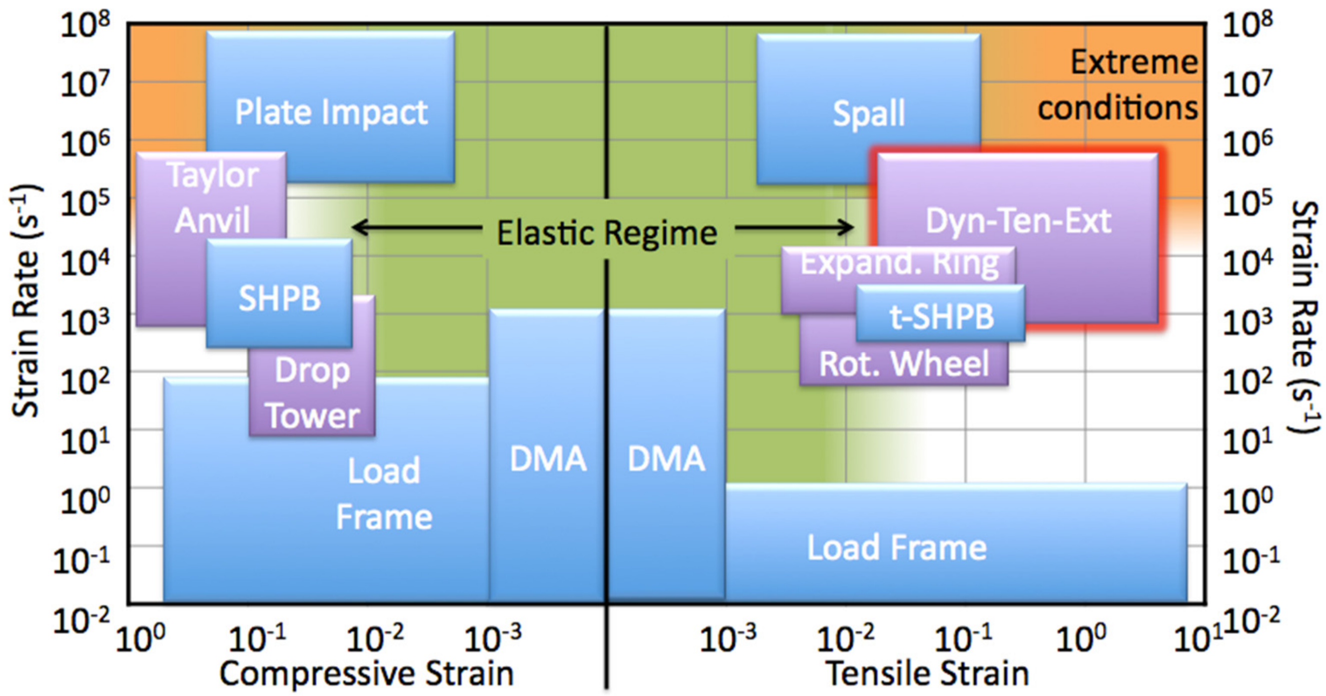


Large-strain time-temperature equivalence and adiabatic heating of HDPE





Material characterization is limited by strain and strain-rate

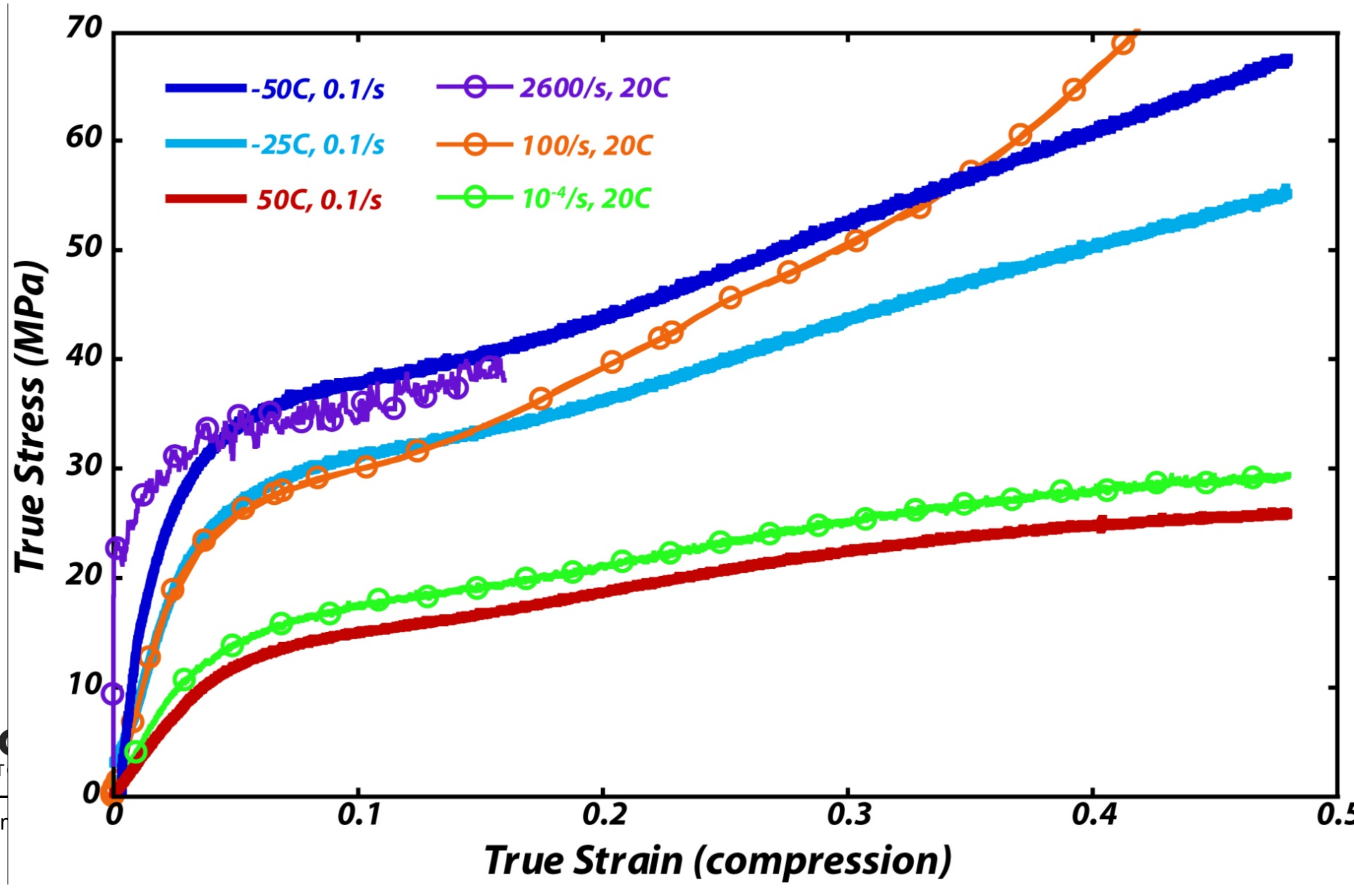


- Characterization with homogeneous 1-D stress/strain, *if possible*
- Extrapolate data with validated constitutive model (rigorous, expensive)
- ***Strain-rate limitations can be overcome with a rate-equivalence model***

Experimental time-temperature equivalence

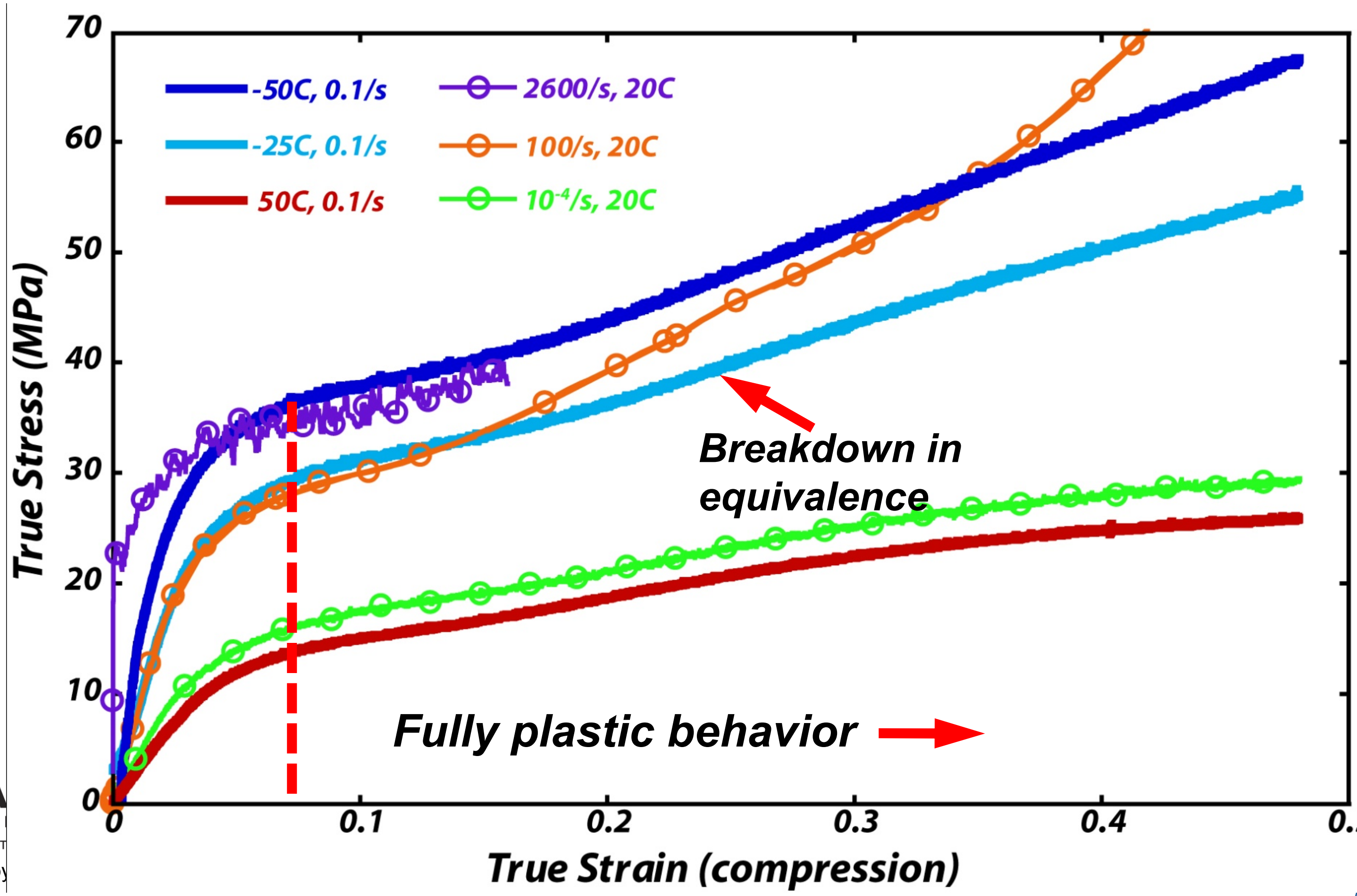
Stress-strain curves are seen to collapse to a common state over a large range of temperatures and rates

- *Breakdowns in equivalence are important to clarify*

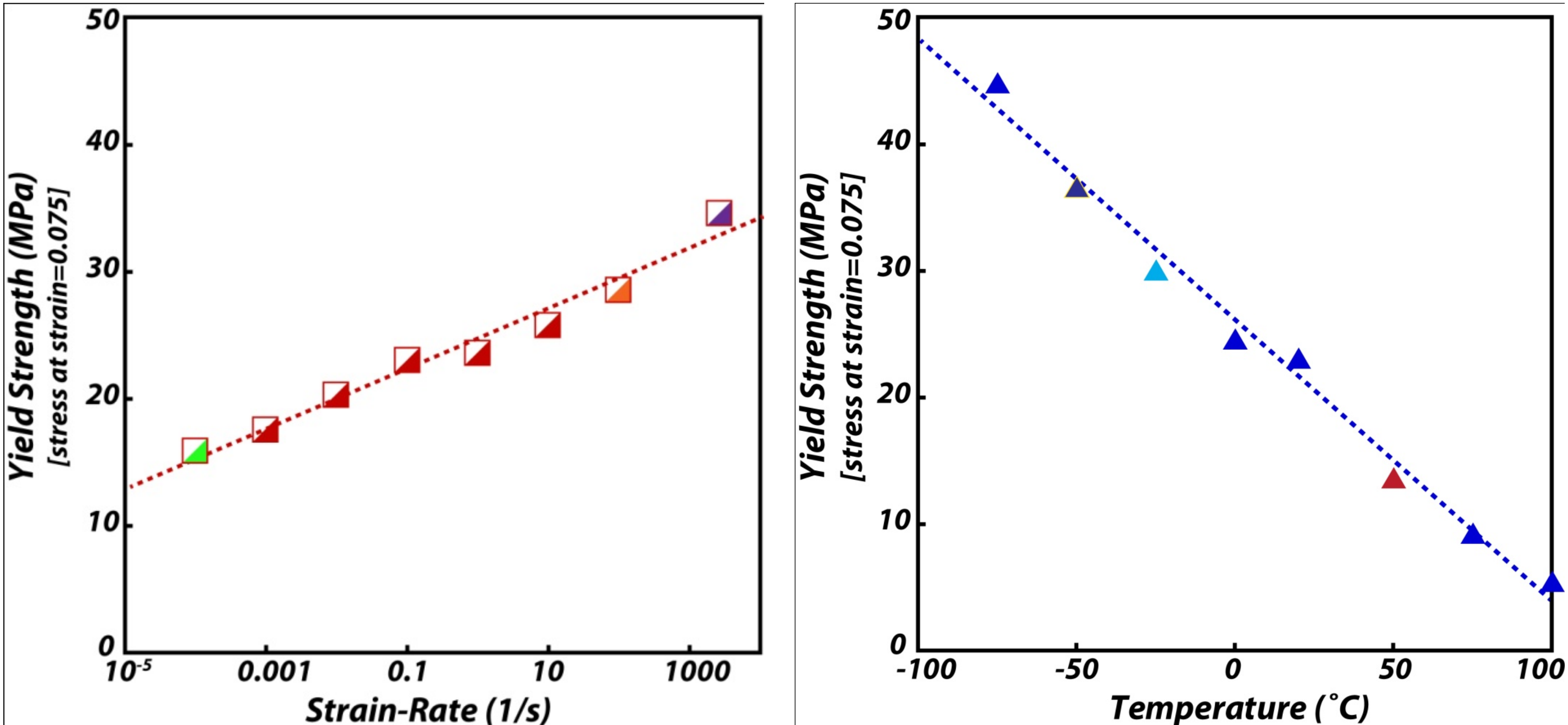


Experimental time-temperature equivalence

- **Extract a time-temperature equivalence relationship for onset of plasticity**



Temperature and rate dependence of yield (onset)

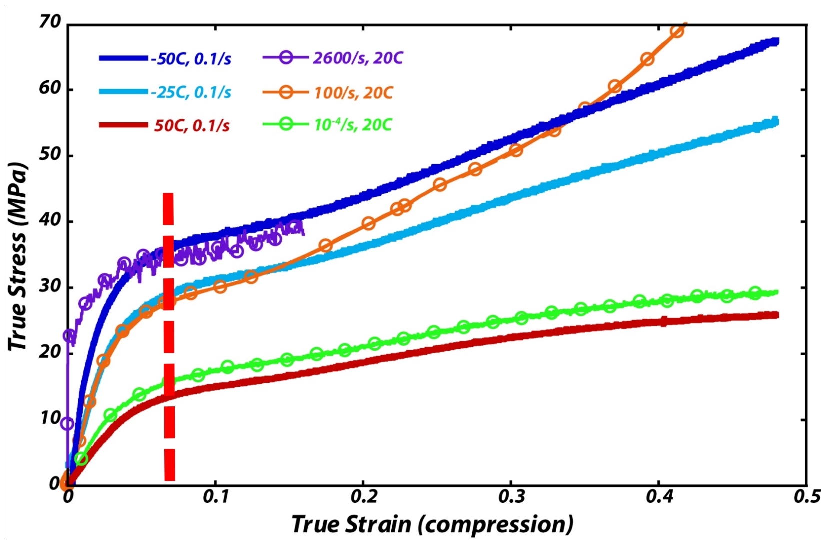


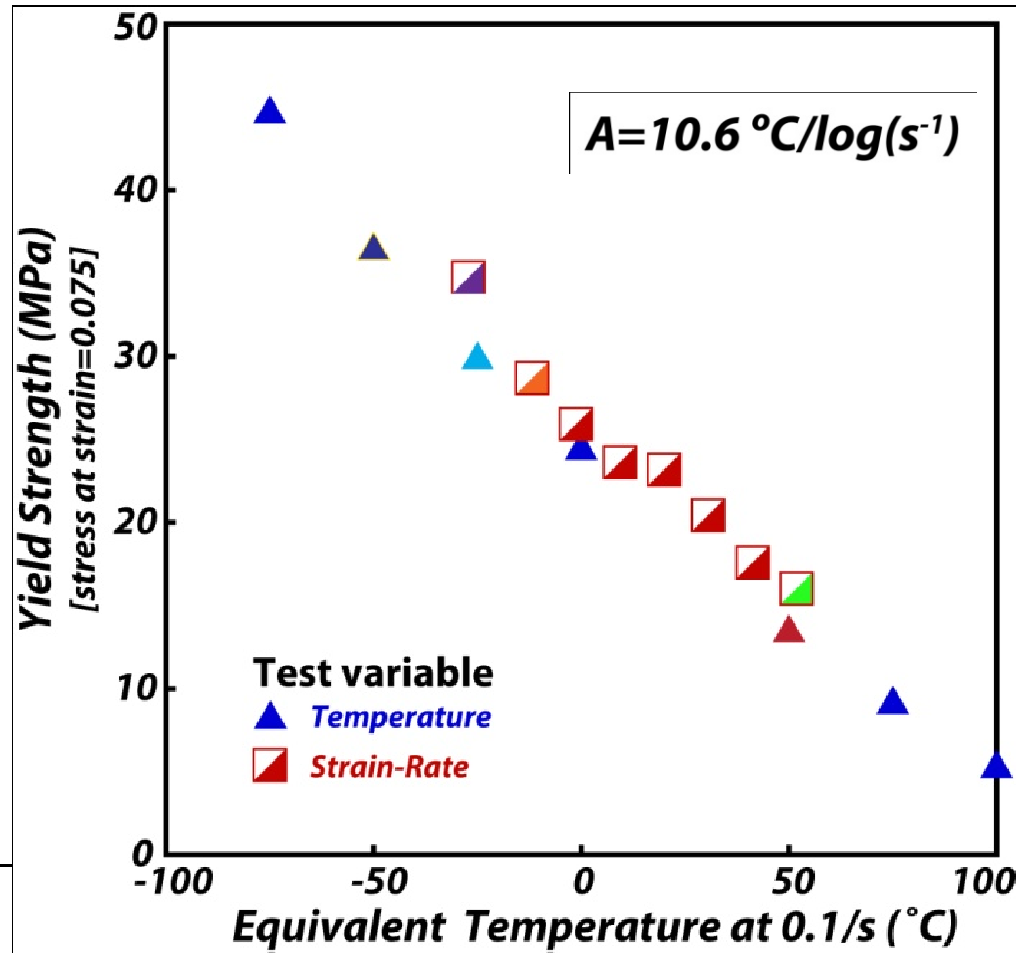
Time-temperature equivalence for nonlinear deformations

- **Plasticity onset maps well to simple logarithmic relation (1 Param.)**
- **Note that 100 K is equivalent to ~ 9 decades of strain rate**

Empirical time-temperature equivalence

$$T_{eq}=T_{exp}+A[\log(\dot{\varepsilon}_{eq})-\log(\dot{\varepsilon}_{exp})]$$

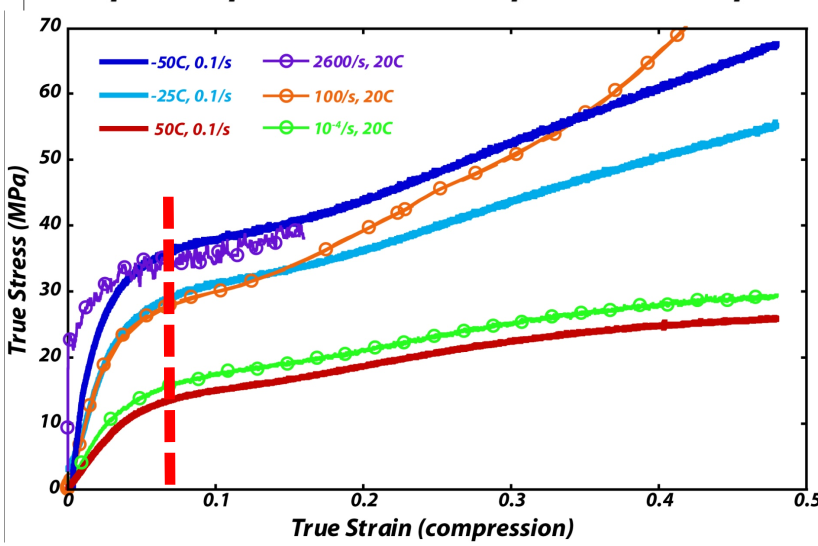


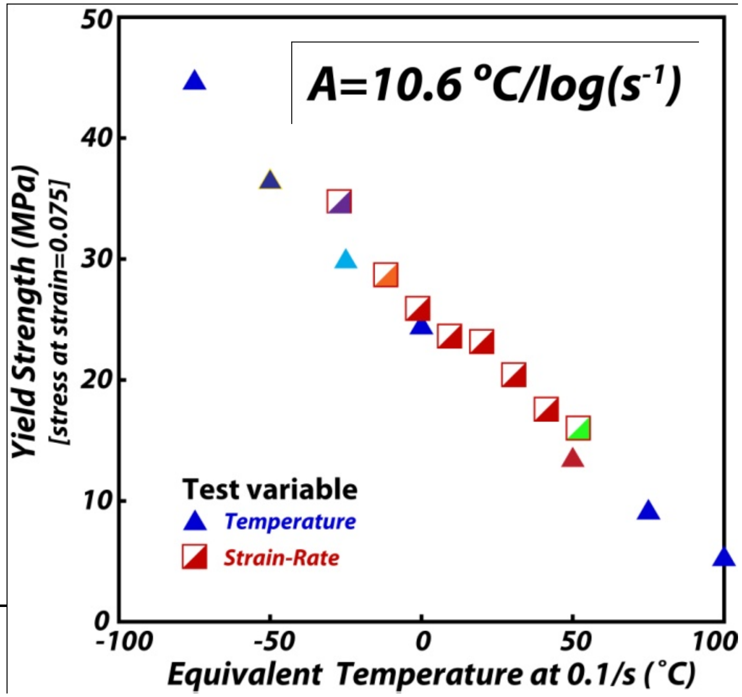


Equivalence locus at yield- *need continuous response*

- Equivalence may not hold for whole response
- Other issues: plastic work (adiabatic heating)
- *Continuous response needed for engineering solutions*

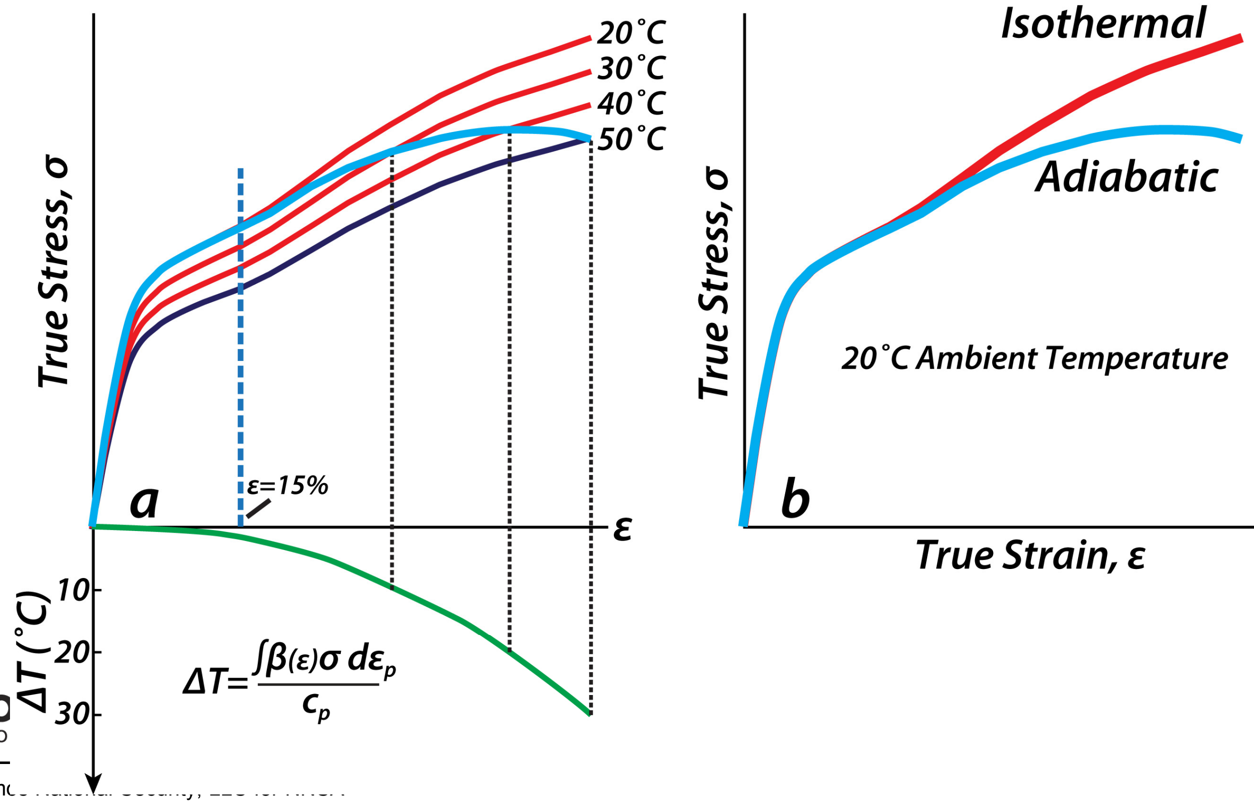
$$T_{eq}=T_{exp}+A[\log(\dot{\varepsilon}_{eq})-\log(\dot{\varepsilon}_{exp})]$$





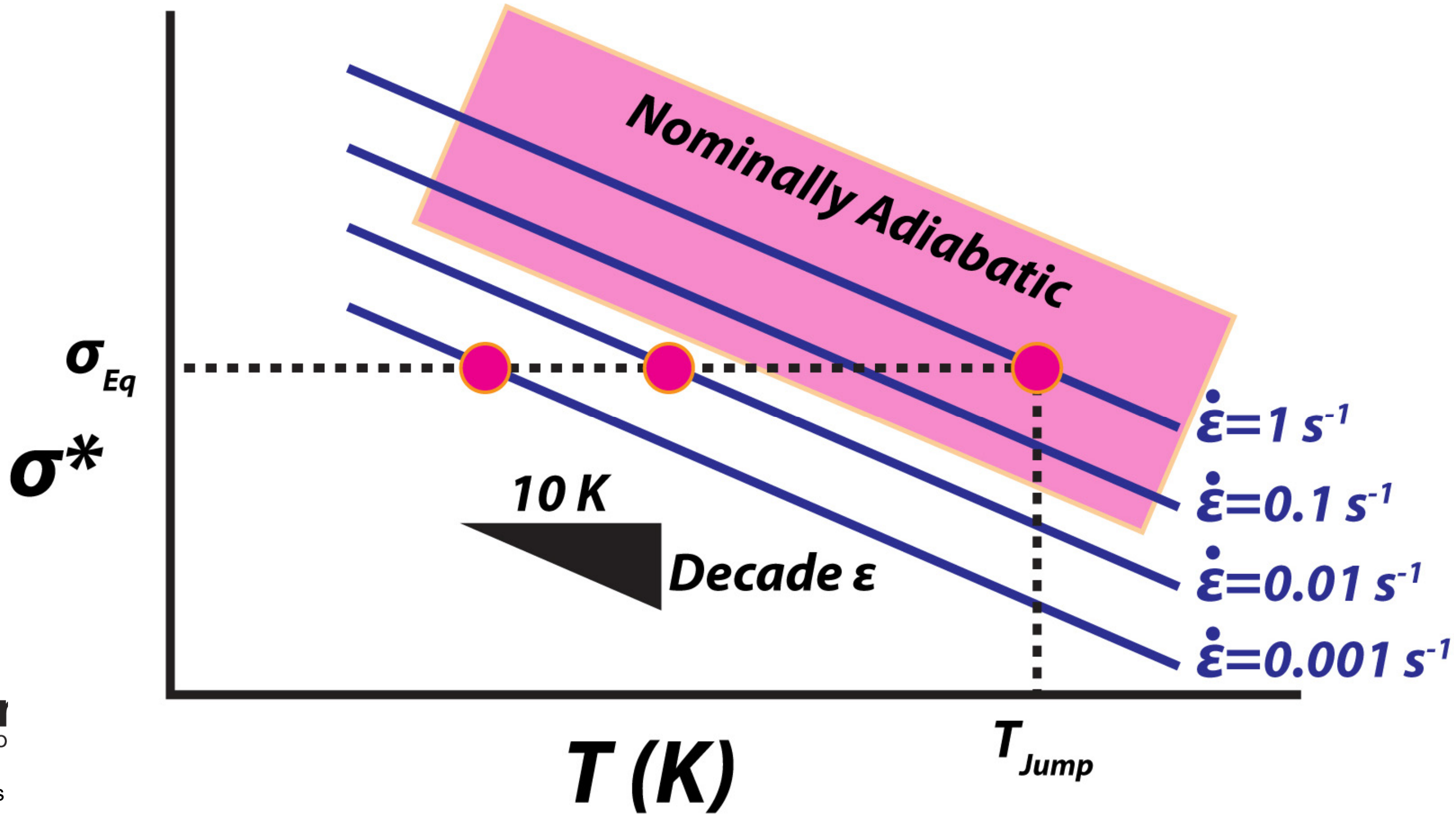
Adiabatic heating results in apparent thermal softening

- Stress-strain curves are presumed isothermal
- Plastic work substantially heats sample and breaks equivalence



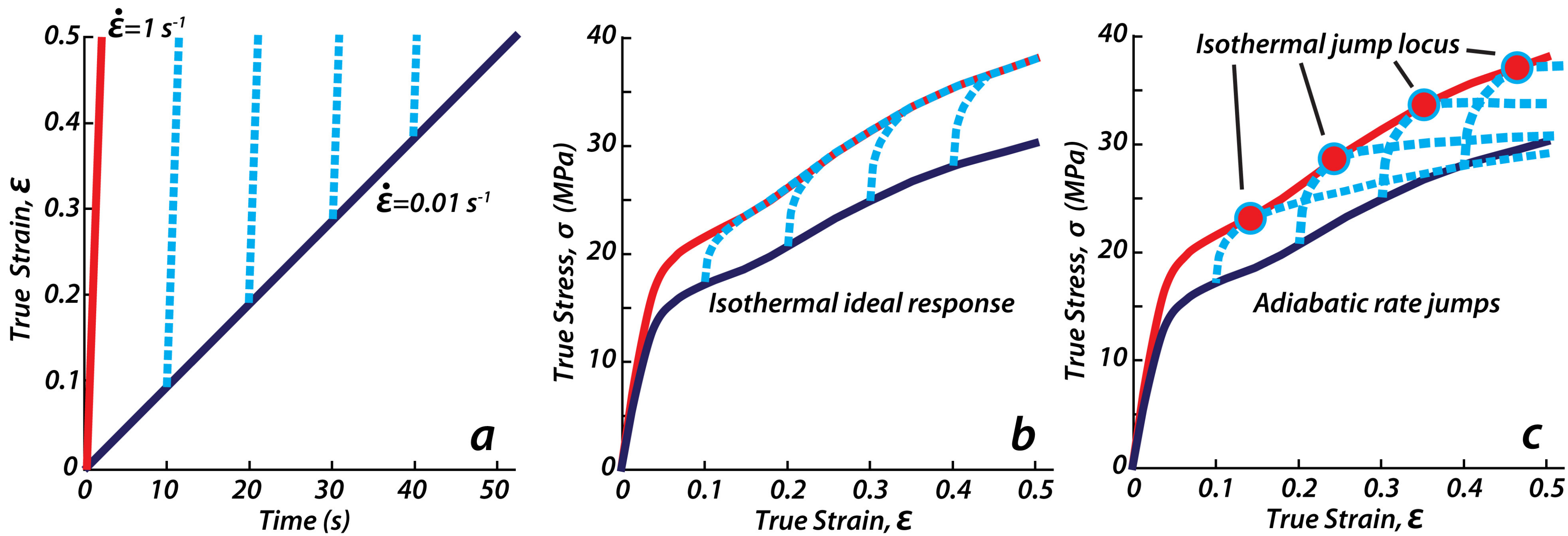
Establish equivalence including adiabatic states

- Equations are for isothermal data, insensitive to other physics
- Need a means to access higher strain-rates without heating
- Eq. stress is generally any stationary flow stress (pointwise)



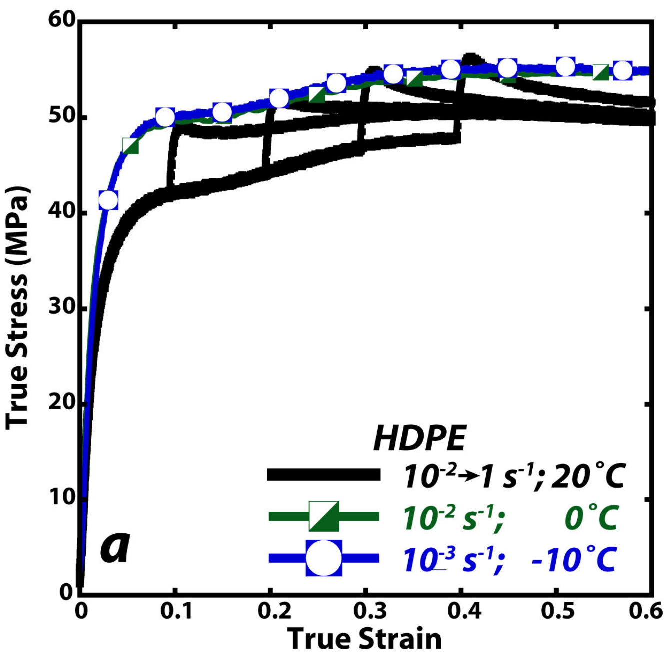
Isothermal Jump Locus

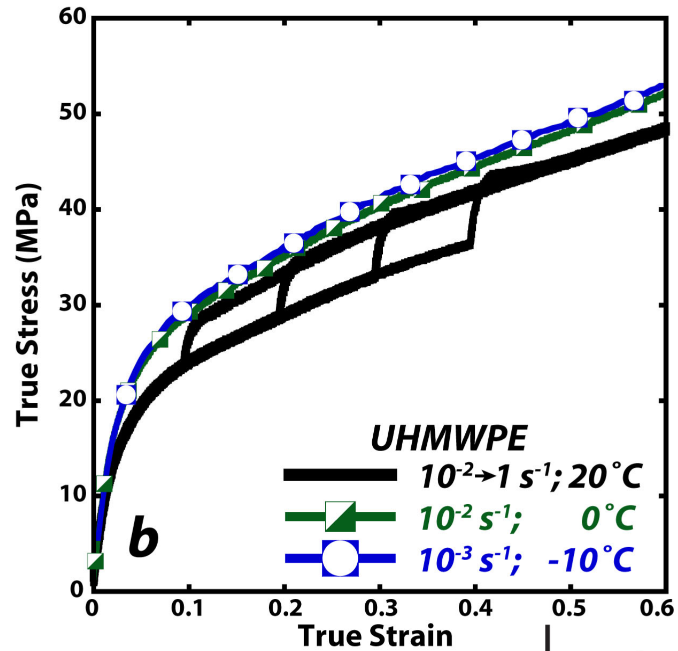
- First instant of high strain-rate deformation is still isothermal, as no plastic work has accumulated
- Assemble a locus of isothermal response from multiple jumps
- Uniaxial compression

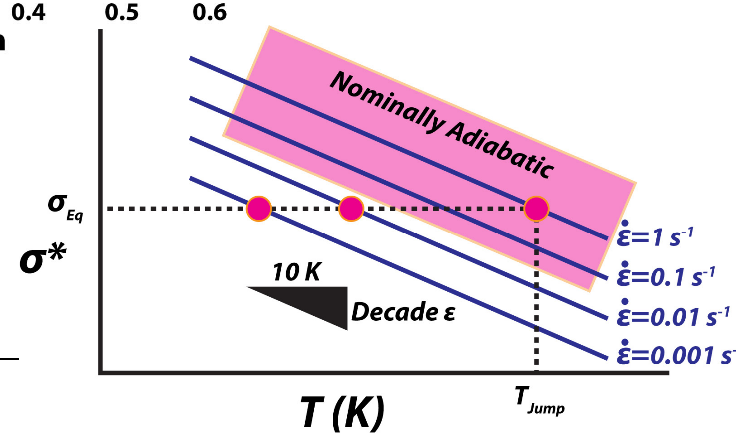


Jump Locus at 20ºC in HDPE and UHMWPE

- **Good agreement between jump locus and isothermal equivalent**







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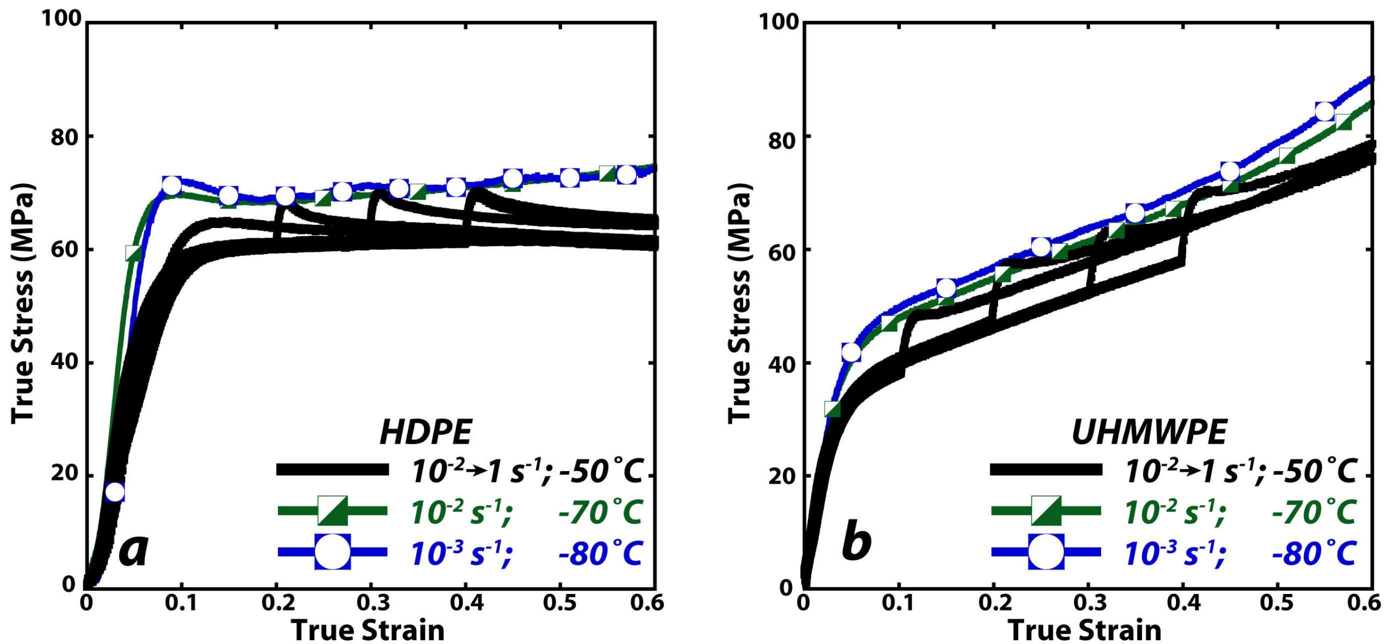
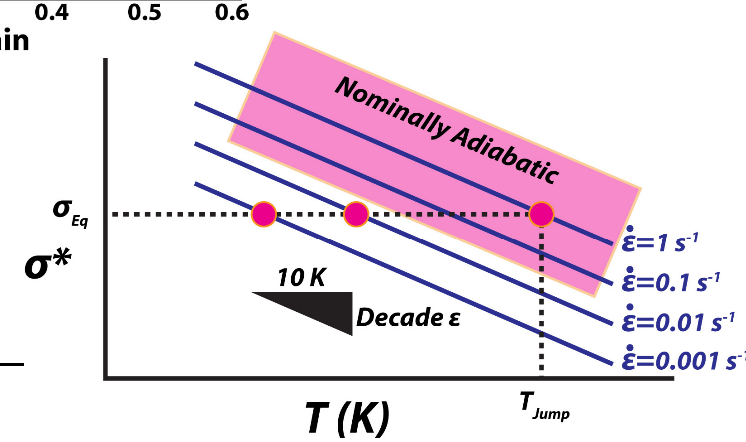
NATIONAL LABORATORY
EST.1943

Jump Locus at -50ºC

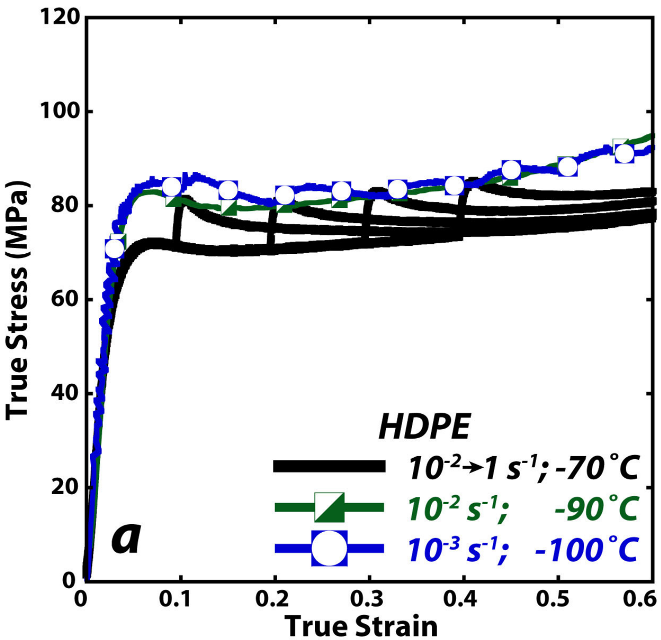
- Good agreement between jump locus and isothermal equivalent

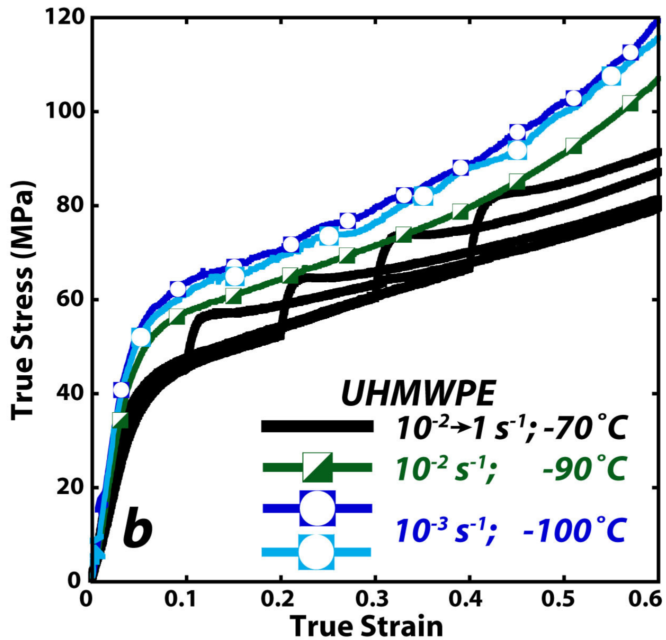


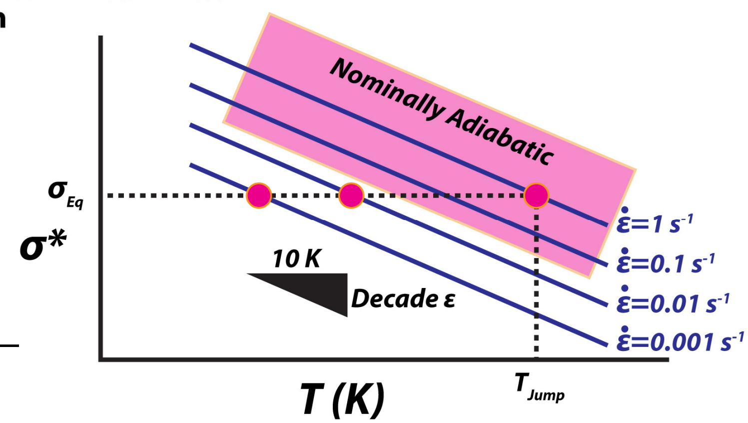


Jump Locus at -70ºC

- **Underpredicted response in UHMWPE at -100ºC & 0.001/s**

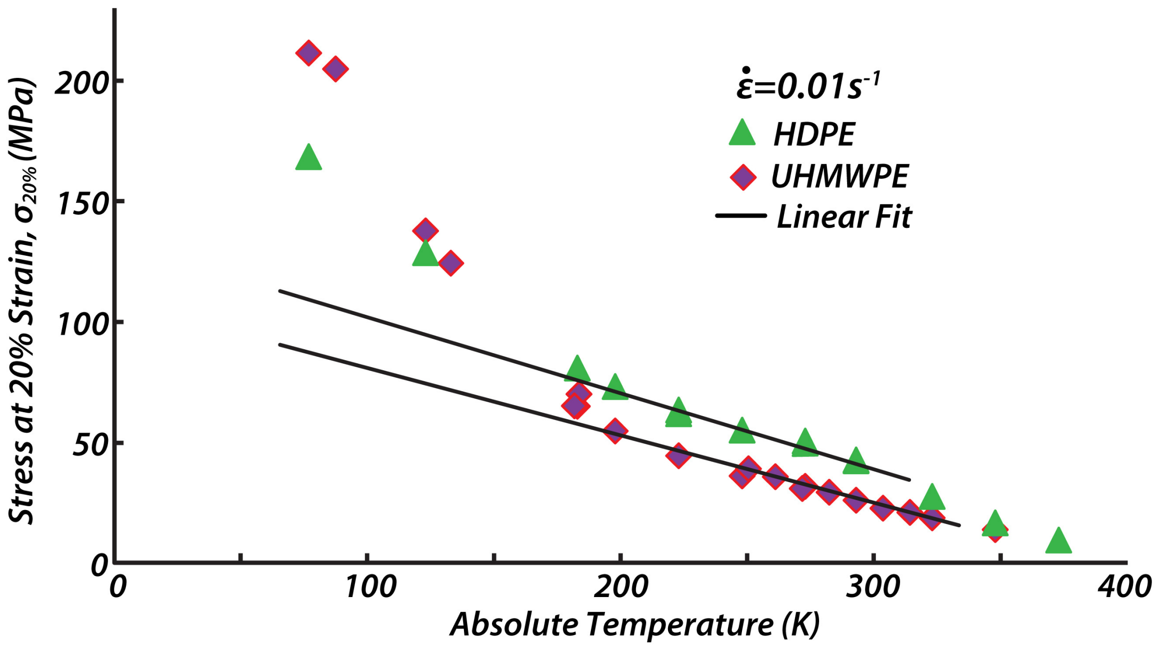


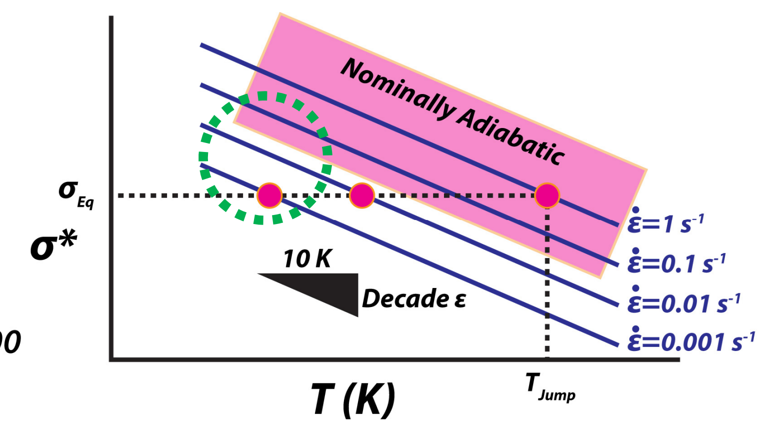




Flow stress is non-linear with temperature

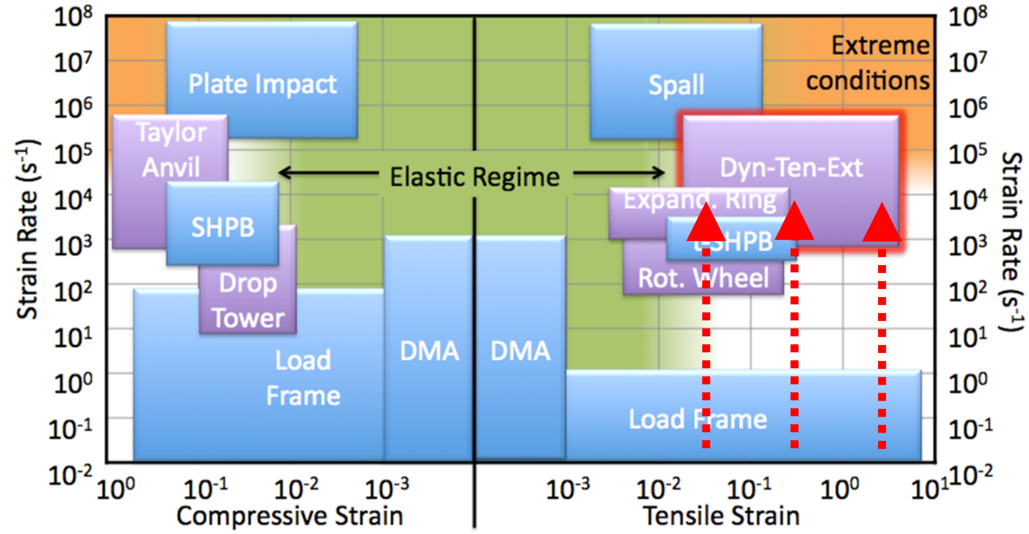
- Deviation from linear model assumption is at -90ºC at 0.01/s
- Valid linearized window: 0-130ºC & 10^6/s
- Melt transition at 130ºC appears to affect HDPE but not UHMWPE





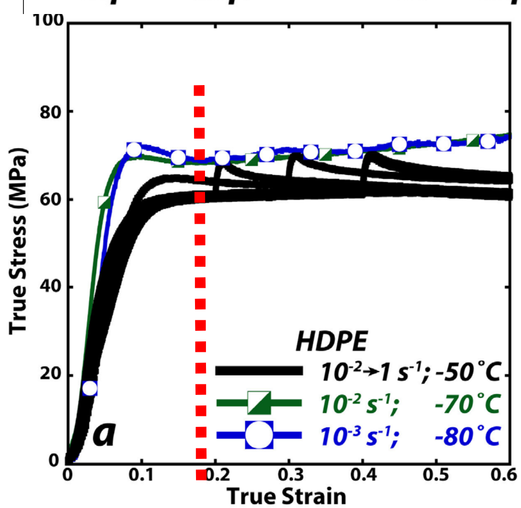
Application: Simulation of Dyn-Ten-Ext and Taylor Impact

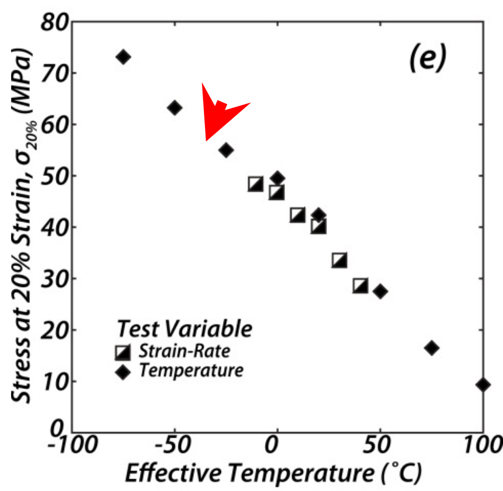
- Use ***rate-temperature equivalence*** to shift cold, low rate stress-strain data up to 10,000/s
- Temp: RT up to melt



Work by: Clive Siviour, Jennifer Jordan, Eric Brown

$$T_{eq}=T_{exp}+A[\log(\dot{\varepsilon}_{eq})-\log(\dot{\varepsilon}_{exp})]$$



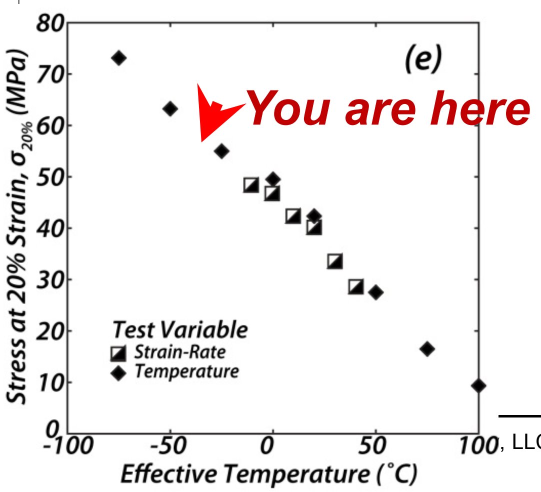


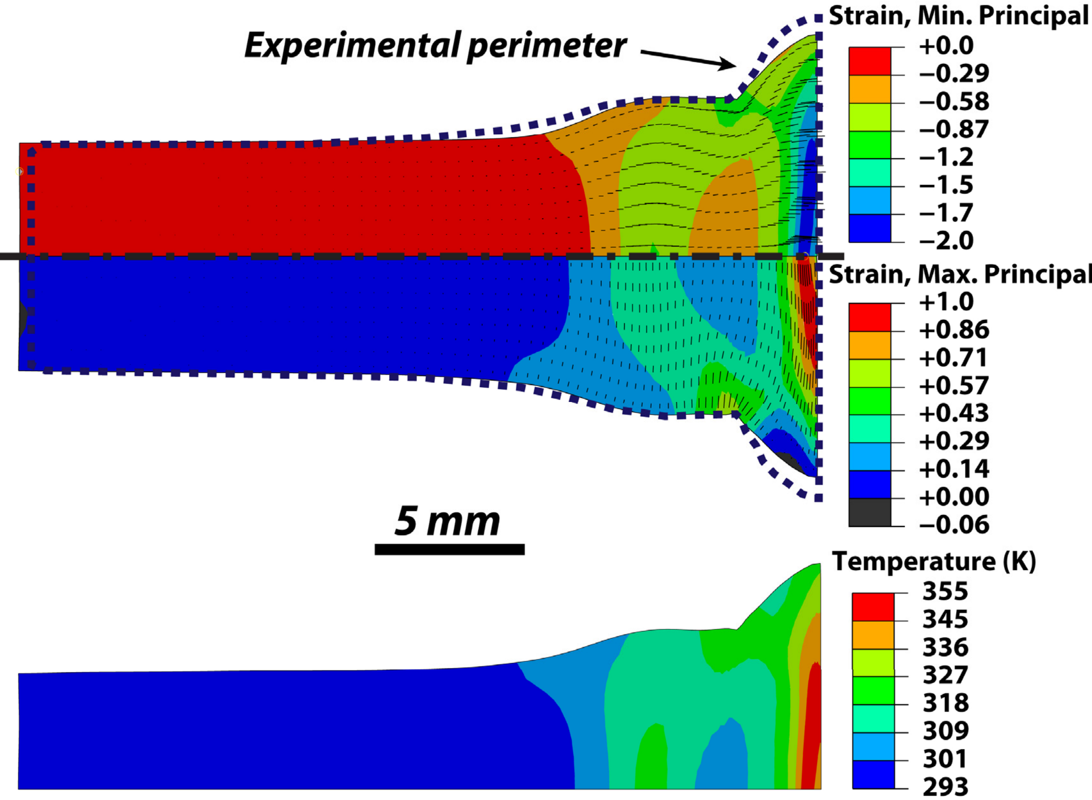
FEA simulation using t-T equivalent set

- ABAQUS/Explicit dynamic axisymmetric model of experimental case
- Metal plasticity, no damage, adiabatic (β=0.9)
- Validated scheme with Taylor impact results

Work by: Clive Siviour, Jennifer Jordan, Eric Brown

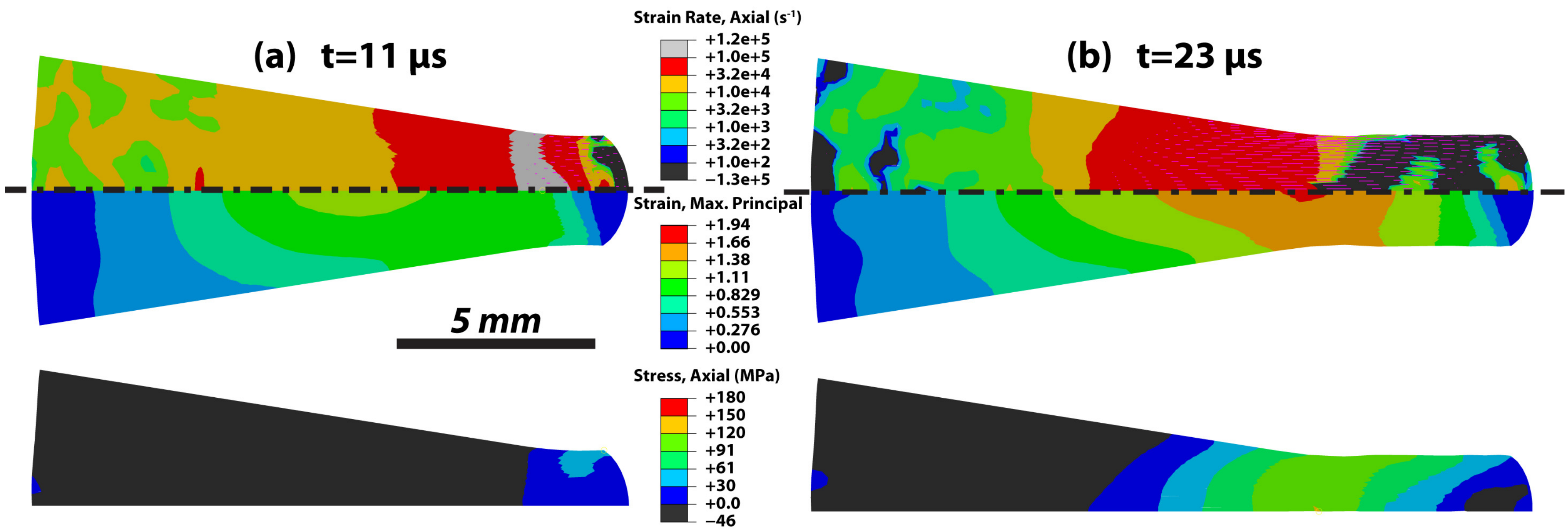
$$T_{eq}=T_{exp}+A[\log(\dot{\varepsilon}_{eq})-\log(\dot{\varepsilon}_{exp})]$$



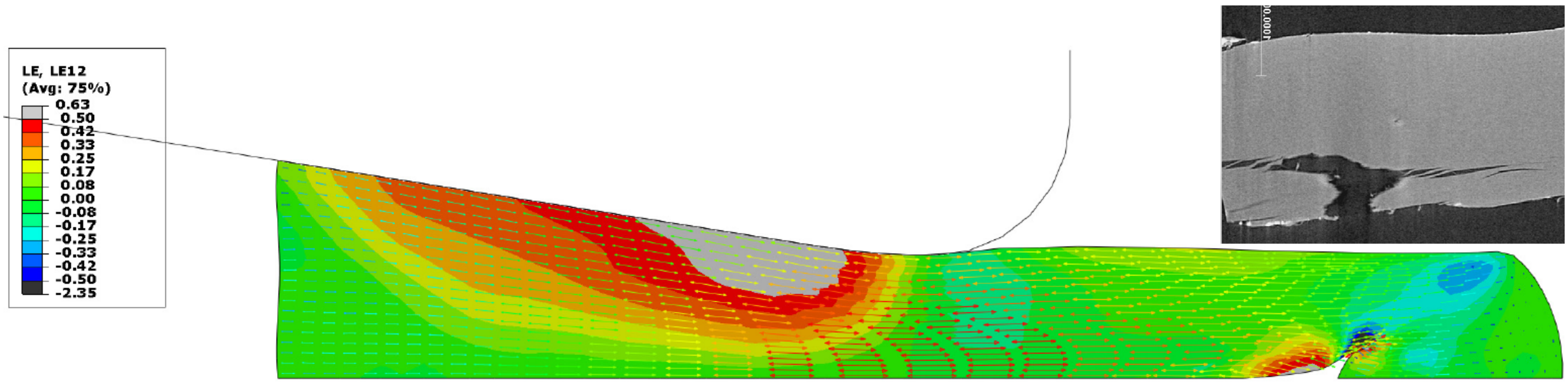


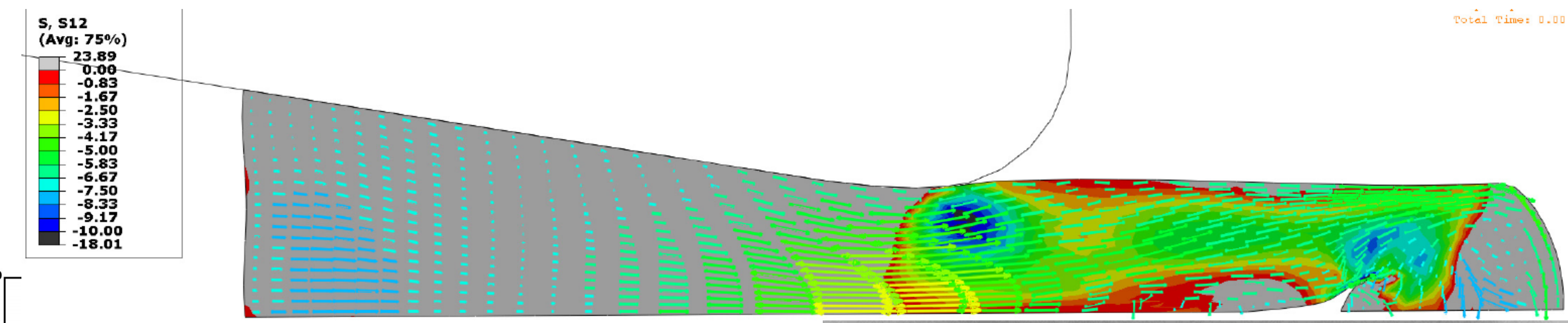
Dynamic-Tensile-Extrusion: Stress/Strain Fields

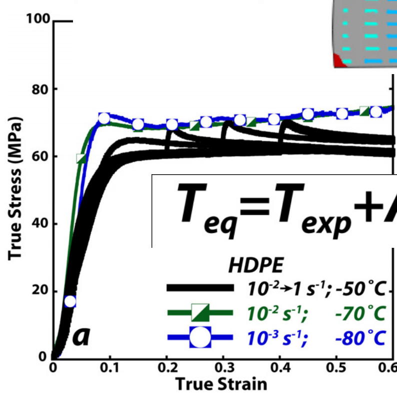
- *Taylor-validated* **constitutive scheme in ABAQUS/Explicit**
- **Simulations demonstrate extreme tensile behavior:**
  - *Strain>1, strain-rate>10,000, axial stress>0 (pressure<0)*



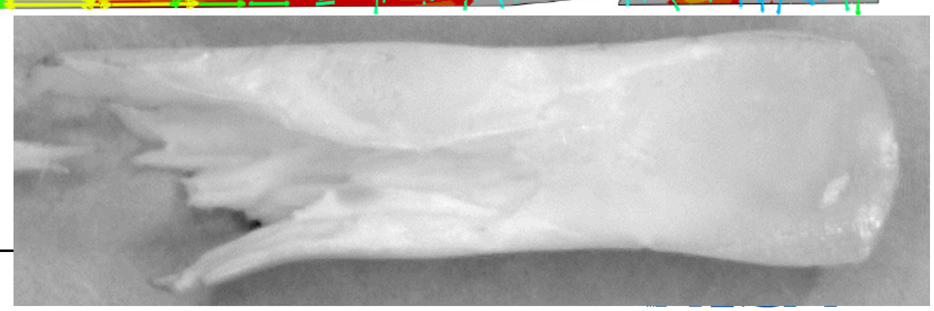
Taylor-validated scheme for damage mechanism inference:
Pressure-mediated shear damage







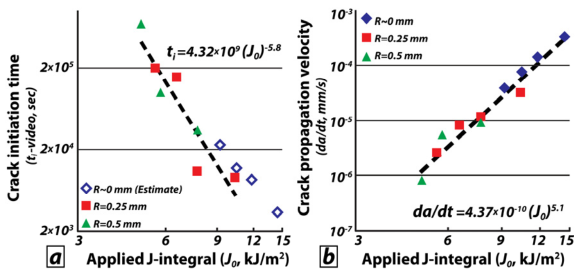
$$T_{eq}=T_{exp}+A[\log(\dot{\varepsilon}_{eq})-\log(\dot{\varepsilon}_{exp})]$$



Rate-shifted material definition is a first-order solution

- **Informs analytical model development (especially damage)**
  - ***Validation***
  - ***Short cut to interpretation of integrated dynamic tests***
- **Not a replacement for a true predictive model of material behavior**
- **Nevertheless, shows good agreement with dynamic integrated tests**

Analytical, experimental, and design efforts all benefit from seamless integration through simulation



Analytical Mechanics/Theory

Investigation
Sanity check

Constitutive Modeling

Verification
Consequences

Simulation
FEA and other mechanics codes

Model validation
Generality

Interpretation
Internal fields

Prediction/ Design

Experimental Observation/ Discovery