A Variational Framework for Phase-Field Fracture Modeling with Applications to Fragmentation, Desiccation, Ductile Failure, and Spallation

Dissertation Defense

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Overview

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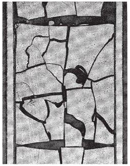

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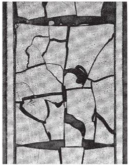


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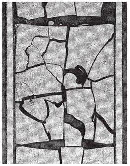

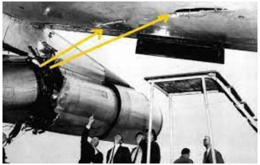

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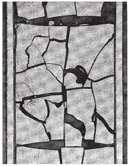

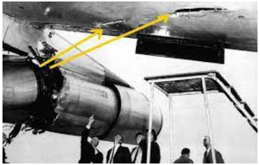


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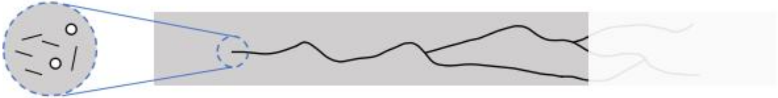

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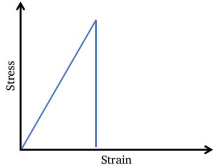

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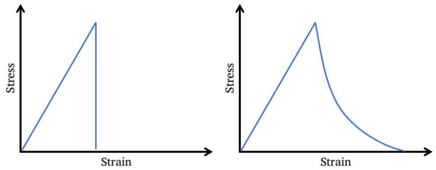

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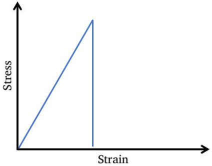

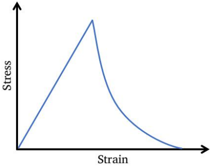

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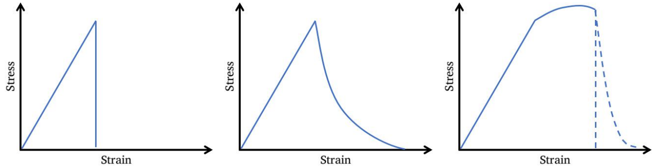

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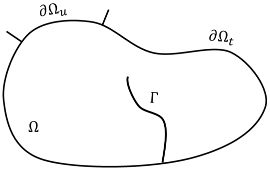
To date, fracture is still one of the most challenging phenomena to model and predict.

The permanent crack set Γ and its associated fracture energy

$$\Psi^f = \int_\Gamma \mathcal{G}_c \; \mathrm{d}A$$



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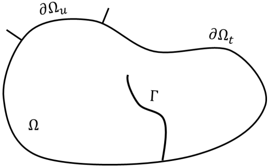
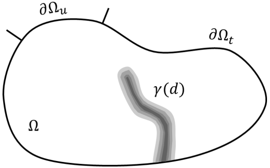


is approximated with

the crack surface density function $\gamma = \widehat{\gamma}_l(d)$:

$$\Psi^f \approx \int_\Omega \mathcal{G}_c \gamma \, \mathrm{d}V, \quad \gamma = \frac{1}{c_0 l}\left(\alpha + l^2 \nabla d \cdot \nabla d\right).$$



- $d \in [0, 1]$ is the phase field;
- $\alpha = \widehat{\alpha}(d)$ is the crack geometric function, $\widehat{\alpha}(0) = 0$, $\widehat{\alpha}(1) = 1$;
- $g = \widehat{g}(d)$ is the degradation function, $\widehat{g}(0) = 1$, $\widehat{g}(1) = 0$;
- c_0 is chosen such that

$$\lim_{l \to 0+} \int_\Omega \mathcal{G}_c \gamma \, \mathrm{d}V = \int_\Gamma \mathcal{G}_c \, \mathrm{d}A.$$

See [1] for more details.

- Working with the Helmholtz free energy density ψ, variables we are concerned with are

$$\boldsymbol{\phi}, \quad \boldsymbol{F}^p, \quad \bar{\varepsilon}^p, \quad d, \quad T.$$

- Conservations and thermodynamic laws:

$$\begin{aligned}
&\dot{\rho}_0 = 0,\\
&\rho_0 \mathbf{a} = \boldsymbol{\nabla}\cdot \boldsymbol{P} + \rho_0 \mathbf{b},\\
&\boldsymbol{P}\boldsymbol{F} = \boldsymbol{F}\boldsymbol{P}^T,\\
&f - \boldsymbol{\nabla}\cdot \boldsymbol{\xi} = 0,\\
&\dot{u} + \dot{k} = \mathcal{P}^{\text{ext}} + \rho_0 q - \boldsymbol{\nabla}\cdot \mathbf{h},\\
&\dot{s}^{\text{int}} = \dot{s} - \frac{\rho_0 q}{T} + \boldsymbol{\nabla}\cdot \frac{\mathbf{h}}{T} \geqslant 0.
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- Generalized forces are

$$\boldsymbol{P} = \boldsymbol{P}^{\text{eq}} + \boldsymbol{P}^{\text{vis}}, \quad \boldsymbol{T} = \boldsymbol{T}^{\text{eq}} + \boldsymbol{T}^{\text{vis}}, \quad Y = Y^{\text{eq}} + Y^{\text{vis}},$$
$$f = f^{\text{eq}} + f^{\text{vis}}, \quad \boldsymbol{\xi} = \boldsymbol{\xi}^{\text{eq}} + \boldsymbol{\xi}^{\text{vis}},$$

- Following the Coleman-Noll procedure:

$$\boldsymbol{P}^{\text{eq}} = \psi_{,\boldsymbol{F}}, \quad \boldsymbol{T}^{\text{eq}} = \psi_{,\boldsymbol{F}^p}, \quad Y^{\text{eq}} = \psi_{,\bar{\varepsilon}^p},$$
$$f^{\text{eq}} = \psi_{,d}, \quad \boldsymbol{\xi}^{\text{eq}} = \psi_{,\boldsymbol{\nabla} d}, \quad -s = \psi_{,T}.$$

- Viscous forces follow from the dual kinetic potential Δ^*:

$$\boldsymbol{P}^{\text{vis}} = \Delta^*_{,\dot{\boldsymbol{F}}}, \quad \boldsymbol{T}^{\text{vis}} = \Delta^*_{,\dot{\boldsymbol{F}}^p}, \quad Y^{\text{vis}} = \Delta^*_{,\dot{\bar{\varepsilon}}^p},$$
$$f^{\text{vis}} = \Delta^*_{,\dot{d}}, \quad \boldsymbol{\xi}^{\text{vis}} = \Delta^*_{,\boldsymbol{\nabla}\dot{d}}.$$

- To satisfy the second law:

$$\delta = \boldsymbol{P}^{\text{vis}} : \dot{\boldsymbol{F}} + \boldsymbol{T}^{\text{vis}} : \dot{\boldsymbol{F}}^p + Y^{\text{vis}}\dot{\bar{\varepsilon}}^p + f^{\text{vis}}\dot{d} + \boldsymbol{\xi}^{\text{vis}} \cdot \boldsymbol{\nabla}\dot{d} \geqslant 0.$$

With $\mathcal{V} = \{\dot{\boldsymbol{\phi}}, \dot{\boldsymbol{F}}^p, \dot{\bar{\varepsilon}}^p, \dot{d}\}$:

$$(\mathcal{V}, \dot{s}, T) = \arg\left(\inf_{\mathcal{V}, \dot{s}} \sup_{T} L\right)$$

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Benefits:

- From a theoretical standpoint:
  - The direct method of calculus of variations informs conditions for the existence and uniqueness of solutions.
  - Localization effects can be studied within the framework of free-discontinuity problems.
- From a computational standpoint:
  - Discretization leads to a symmetric operator.
  - Discretization leads to robust and efficient variational constitutive update.
  - The total potential can assist line search.
  - The total potential can be directly used as an error indicator for adaptive mesh refinement.
  - Many powerful optimization packages exist, e.g. PETSc/TAO, Trilinos, Matlab, etc..

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- Construction of such a potential is no easy task.
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State-of-the-art: variational brittle fracture that concerns with

$$\boldsymbol{\phi}, \quad d,$$

while we are looking at

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The total potential L is constructed as

$$L = \int_{\Omega_0} \varphi \, \mathrm{d}V - \mathcal{P}^{\text{ext}},$$

$$\varphi = \dot{k} + \dot{u} + \Delta^* - T\dot{s} - \chi,$$

The external power expenditure $\mathcal{P}^{\text{ext}}(\dot{\boldsymbol{\phi}}, T)$ is defined as

$$\mathcal{P}^{\text{ext}} = \underbrace{\int_{\Omega_0} \rho_0 \mathbf{b} \cdot \dot{\boldsymbol{\phi}} \, \mathrm{d}V}_{\text{body force}} + \underbrace{\int_{\partial_t \Omega_0} \mathbf{t} \cdot \dot{\boldsymbol{\phi}} \, \mathrm{d}A}_{\text{surface traction}} + \underbrace{\int_{\partial_h \Omega_0} \bar{h}_n \ln\left(\frac{T}{T_0}\right) \mathrm{d}A}_{\text{external heat flux}}$$
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$$\mathcal{P}^{\text{ext}} = \underbrace{\int_{\Omega_0} \rho_0 \mathbf{b} \cdot \dot{\boldsymbol{\phi}} \, \mathrm{d}V}_{\text{body force}} + \underbrace{\int_{\partial_t \Omega_0} \mathbf{t} \cdot \dot{\boldsymbol{\phi}} \, \mathrm{d}A}_{\text{surface traction}} + \underbrace{\int_{\partial_h \Omega_0} \bar{h}_n \ln\left(\frac{T}{T_0}\right) \, \mathrm{d}A}_{\text{external heat flux}}$$
$$+ \underbrace{\int_{\partial_r \Omega_0} h \left[T - T_0 \ln\left(\frac{T}{T_0}\right)\right] \, \mathrm{d}A}_{\text{external heat convection}} - \underbrace{\int_{\Omega_0} \rho_0 q \ln\left(\frac{T}{T_0}\right) \, \mathrm{d}V}_{\text{heat source}},$$

- Mass balance and angular momentum balance are satisfied by construction.
- Linear momentum balance:

$$\rho_0 \mathbf{a} = \boldsymbol{\nabla} \cdot \boldsymbol{P} + \mathbf{b}.$$

- Micro-macro force balance:

$$\boldsymbol{\nabla} \cdot \boldsymbol{\xi} - f = 0.$$

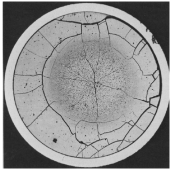
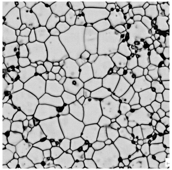
- Plastic flow:

$$\left(\dot{\boldsymbol{F}}^p, \dot{\bar{\varepsilon}}^p\right) = \arg \inf_{\dot{\boldsymbol{F}}^p, \dot{\bar{\varepsilon}}^p} \left[\boldsymbol{T}^{\text{eq}} : \dot{\boldsymbol{F}}^p + Y^{\text{eq}} \dot{\bar{\varepsilon}}^p + \Delta^*\right]$$
$$\text{subject to} \quad \boldsymbol{L}(\boldsymbol{Z}) \dot{\boldsymbol{Z}} = \mathbf{0}.$$

- Heat transfer:

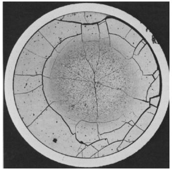
$$T\dot{s} = \rho_0 q - \boldsymbol{\nabla} \cdot \mathbf{h} + \delta.$$

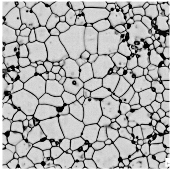
- (Strict) dissipation inequality requires Δ^* to be convex in each rate.

Background:

- Fission of UO_2 produces a variety of fission products.
- Properties of UO_2 are strongly influenced by fracture.
- Gas bubbles, grains, and grain boundaries alter fracture properties.
- Existing 2D models over-simplifies the microstructure and results in inaccurate strength-porosity relations.





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Model:

- Helmholtz free energy density:

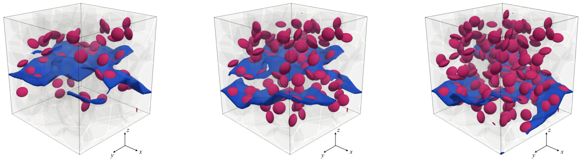
$$\psi = \psi^e + \psi^f .$$

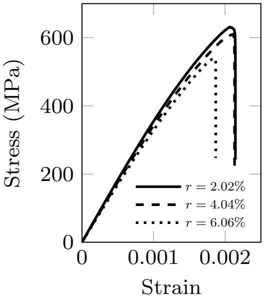
- Strain energy density:

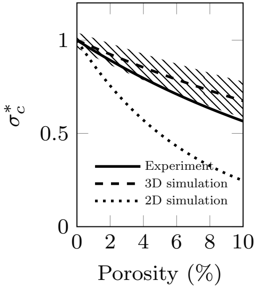
$$\begin{aligned}
\psi^e &= g\psi^e_{\langle A \rangle} + \psi^e_{\langle I \rangle}, \\
\psi^e_{\langle A \rangle} &= \frac{1}{2}\lambda \left\langle \mathrm{tr}(\boldsymbol{\varepsilon}) \right\rangle_+^2 + G\boldsymbol{\varepsilon}^+ : \boldsymbol{\varepsilon}^+, \\
\psi^e_{\langle I \rangle} &= \frac{1}{2}\lambda \left\langle \mathrm{tr}(\boldsymbol{\varepsilon}) \right\rangle_-^2 + G\boldsymbol{\varepsilon}^- : \boldsymbol{\varepsilon}^-,
\end{aligned}$$

- Fracture energy density:

$$\begin{aligned}
\psi^f &= \frac{\mathcal{G}_c}{c_0 l} \left(\alpha + l^2 \boldsymbol{\nabla} d \cdot \boldsymbol{\nabla} d \right), \\
\alpha &= d^2, \quad g = (1-d)^2 .
\end{aligned}$$

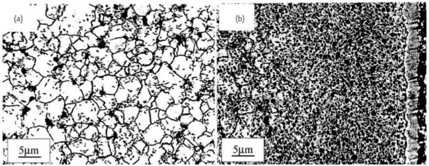






- A set of random close-packing voronoi structures are realized by maximal Poisson-disk sampling.
- The microstructure is generated using a phase-field grain growth model [2].
- Grain boundaries have an arbitrarily high fracture toughness to facilitate intergranular fracture.
- Numerical studies are performed to investigate the effects of bubble geometry, loading conditions, and porosity on the critical fracture strength.
- Results of 15 realizations of 3 porosity levels are fitted using the relation suggested by experiments [3]:

$$\frac{\sigma_c}{\sigma_0} = \exp(-ar).$$

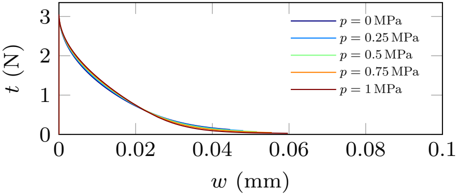


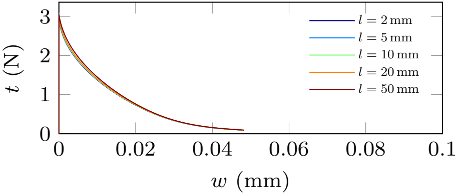
Background:

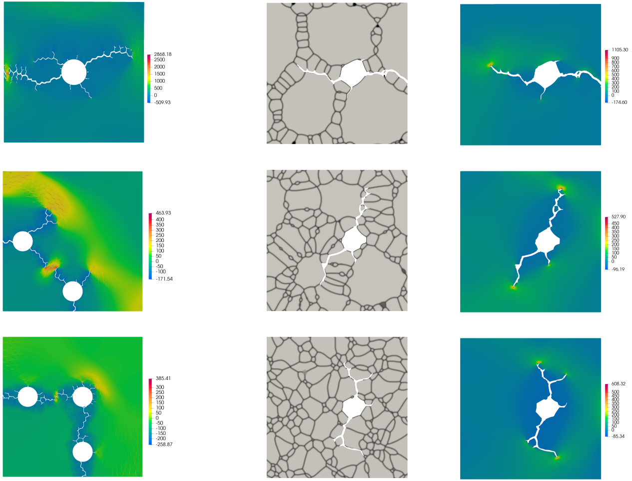
- Utilities are seeking to increase the allowable burnup limit for UO_2 fuel.
- The risk of fragmentation during a loss-of-coolant accident (LOCA) is a major limitation.
- Over-pressurization of fission gas bubbles results in fine fragmentation of high burnup structures.
- A model for predicting the onset of fragmentation is essential.

External pressure power:

$$\mathcal{P}^{\text{ext}} = -\int_{\Omega_0} \bar{p}\boldsymbol{\nabla} d \cdot \dot{\boldsymbol{\phi}} I_{,d} \, \mathrm{d}V.$$







- A 2D REV is considered. Plane strain conditions are assumed to hold.
- LOCA pressure transients:
  - The temperature as a function of time at the edge of a representative pellet for each rod is obtained from simulations.
  - The temperature transient is used as an input to a Kim-Kim-Suzuki (KKS) phase-field model [4] to determine the pressure transient.
  - The pressure transient is treated as a known in the fracture model.
- Effects of bubble size, bubble pressure, surrounding pressure, and multi-bubble interaction are investigated.
- Defect evolution and recrystallization can be incorporated into the fracture model.

Background:

- Film-substrate systems widely exist in nature and in engineering applications.
- Fracture of thin films has been studied using model-based simulations based on a wide range of methodologies.
- Many soil materials are "cohesive" in nature. It calls for a phase-field model for cohesive fracture.
- Many film-substrate systems are symmetric or axisymmetric. It is important to incorporate stochastic models for material properties.

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Model:

- Enforcing traction-free boundary conditions:

$$
\begin{aligned}
&\psi^e = g\psi^e_{\langle A\rangle} + \psi^e_{\langle I\rangle}, \\
&\psi^e_{\langle A\rangle} = \frac{1}{2}\boldsymbol{\sigma}_{\langle A\rangle} : \boldsymbol{\varepsilon}, \quad \psi^e_{\langle I\rangle} = \frac{1}{2}\boldsymbol{\sigma}_{\langle I\rangle} : \boldsymbol{\varepsilon}, \\
&\boldsymbol{\sigma}_{\langle A\rangle} = \boldsymbol{\sigma}_n^+ + \boldsymbol{\sigma}_t, \quad \boldsymbol{\sigma}_{\langle I\rangle} = \boldsymbol{\sigma}_n^-, \\
&\boldsymbol{\sigma}_n^\pm = \langle -t_N\rangle_\pm \, \widetilde{\mathbf{n}} \otimes \widetilde{\mathbf{n}}, \quad \boldsymbol{\sigma}_t = \boldsymbol{\sigma} - \boldsymbol{\sigma}_n^+ - \boldsymbol{\sigma}_n^-.
\end{aligned}
$$

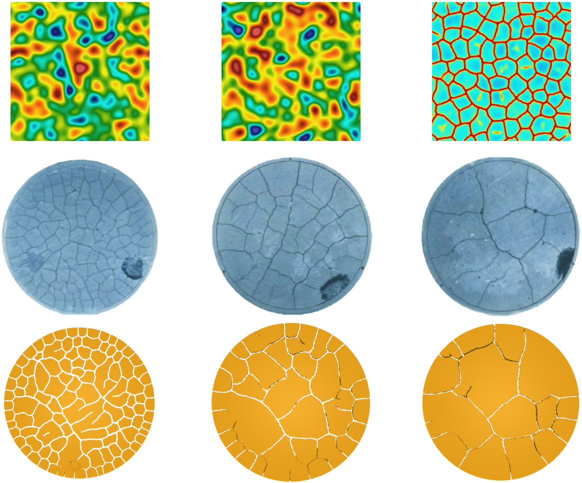
- Cohesive fracture:

$$
\alpha = \xi d - (1-\xi)d^2, \quad g = \frac{1}{1+\phi},
$$

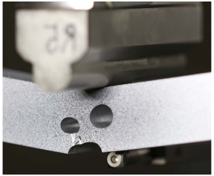
$$
\phi = \frac{a_1 d + a_1 a_2 d^2 + a_1 a_2 a_3 d^3}{(1-d)^p}.
$$

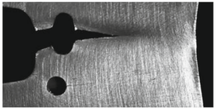
- A nonlinear softening law:

$$
\xi = 1, \quad p = 2, \quad a_1 = \frac{\mathcal{G}_c}{c_0 l \psi_c}, \quad a_2 = 1, \quad a_3 = 0.
$$

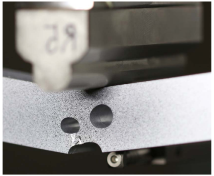


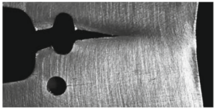
- Only "channeling" cracks in the thin film are considered.
- Thermal effects are neglected. Dehydration is modeled as pre-stress (or equivalent eigenstrains).
- The fracture model is verified with analytical solutions in a periodic quasi-1D context.
- Pervasive fracture is studied with a 2D simplification.
- Material property inhomogeneity is represented by two pointwise correlated random fields $\{\mathcal{G}_c(\boldsymbol{X}), \boldsymbol{X} \in \Omega\}$ and $\{\psi_c(\boldsymbol{X}), \boldsymbol{X} \in \Omega\}$.
- The versatility offered by the probabilistic framework is highlighted by solving a 3D problem based on physical experiments.





There exist many approaches to modeling plasticity in the context of phase-field fracture [5, 6, 7, 8, 9, 10, 11, 12].





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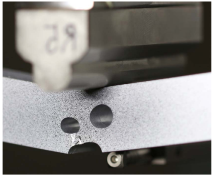
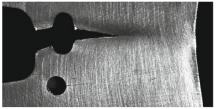
How to best design the coupling between plasticity and fracture remains an open question. Some challenges/issues:

- Fracture tends to propagate along the plastic zone.





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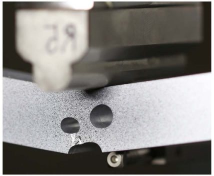

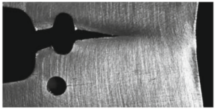

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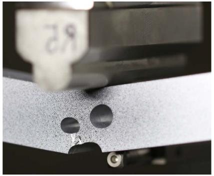

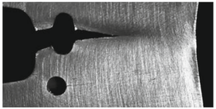

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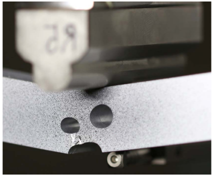

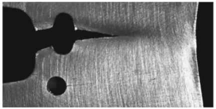

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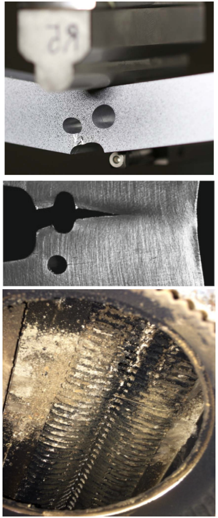

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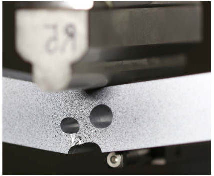

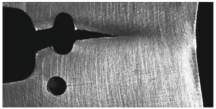

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- How much plastic dissipation contributes to fracture evolution?
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All of the issues above can be addressed by the proposed framework (with proper constitutive choices).

$$L = \int_{\Omega_0} \left[\dot{\psi}^e + \psi^{e\,*} + (1-\mathcal{Q})\dot{\psi}^p + \mathcal{Q}\psi^{p\,*} + \dot{\psi}^f + \psi^{f\,*} - T\dot{s} - \chi \right] \, \mathrm{d}V - \mathcal{P}^{\mathrm{ext}},$$

$$\text{subject to } \boldsymbol{L}(\boldsymbol{Z})\dot{\boldsymbol{Z}} = \boldsymbol{0}.$$

Option 1 (Compressible Neo-Hookean):

$$\begin{aligned}
\psi^e &= g^e \psi^e_{\langle A \rangle} + \psi^e_{\langle I \rangle}, \\
\psi^e_{\langle A \rangle} &= \mathbb{H}_1(J) \left\{ \frac{1}{2} K \left[\frac{1}{2}(J^2 - 1) - \ln(J) \right] \right\} \\
&\quad + \frac{1}{2} G \left(\overline{\boldsymbol{C}} : \boldsymbol{C}^{p\,-1} - 3 \right), \\
\psi^e_{\langle I \rangle} &= (1 - \mathbb{H}_1(J)) \left\{ \frac{1}{2} K \left[\frac{1}{2}(J^2 - 1) - \ln(J) \right] \right\}.
\end{aligned}$$

Option 2 (Hencky):

$$\begin{aligned}
\psi^e &= g^e \psi^e_{\langle A \rangle} + \psi^e_{\langle I \rangle}, \\
\psi^e_{\langle A \rangle} &= \frac{1}{2} K \left\langle \mathrm{tr}(\boldsymbol{\varepsilon}^e) \right\rangle_+^2 + G \, \mathrm{dev}\, \boldsymbol{\varepsilon}^e : \mathrm{dev}\, \boldsymbol{\varepsilon}^e, \\
\psi^e_{\langle I \rangle} &= \frac{1}{2} K \left\langle \mathrm{tr}(\boldsymbol{\varepsilon}^e) \right\rangle_-^2, \\
\boldsymbol{\varepsilon}^e &= \frac{1}{2} \ln\left(\boldsymbol{C}^e \right).
\end{aligned}$$

$$L = \int_{\Omega_0} \left[\dot{\psi}^e + \psi^{e\,*} + (1-\mathcal{Q})\dot{\psi}^p + \mathcal{Q}\psi^{p\,*} + \dot{\psi}^f + \psi^{f\,*} - T\dot{s} - \chi\right] \,\mathrm{d}V - \mathcal{P}^{\mathrm{ext}},$$

$$\text{subject to } \boldsymbol{L}(\boldsymbol{Z})\dot{\boldsymbol{Z}} = \boldsymbol{0}.$$

Option 1 (Linear hardening):

$$\psi^e = g^e \psi^e_{\langle A\rangle} + \psi^e_{\langle I\rangle},$$

$$\psi^e_{\langle A\rangle} = \mathbb{H}_1(J)\left\{\frac{1}{2}K\left[\frac{1}{2}(J^2-1) - \ln(J)\right]\right\} + \frac{1}{2}G\left(\overline{\boldsymbol{C}} : \boldsymbol{C}^{p\,-1} - 3\right),$$

$$\psi^e_{\langle I\rangle} = (1-\mathbb{H}_1(J))\left\{\frac{1}{2}K\left[\frac{1}{2}(J^2-1) - \ln(J)\right]\right\}.$$

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