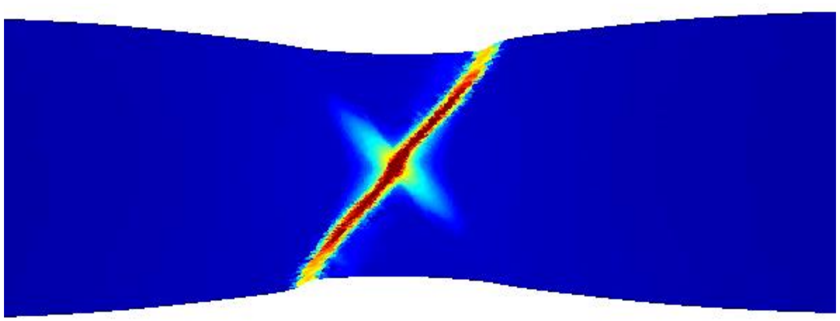
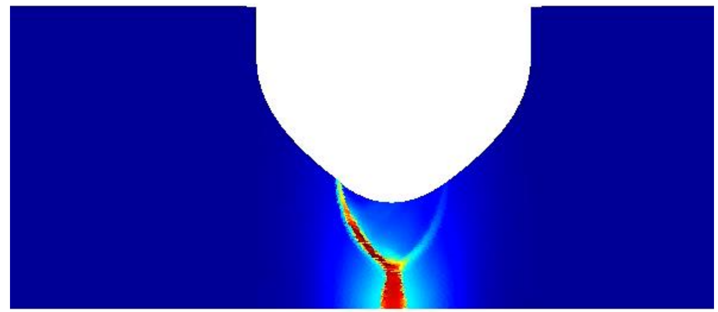
A multi-mechanism non-local porosity model for highly-ductile materials; application to high entropy alloys

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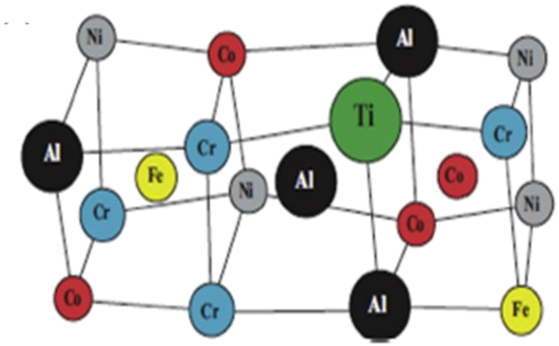
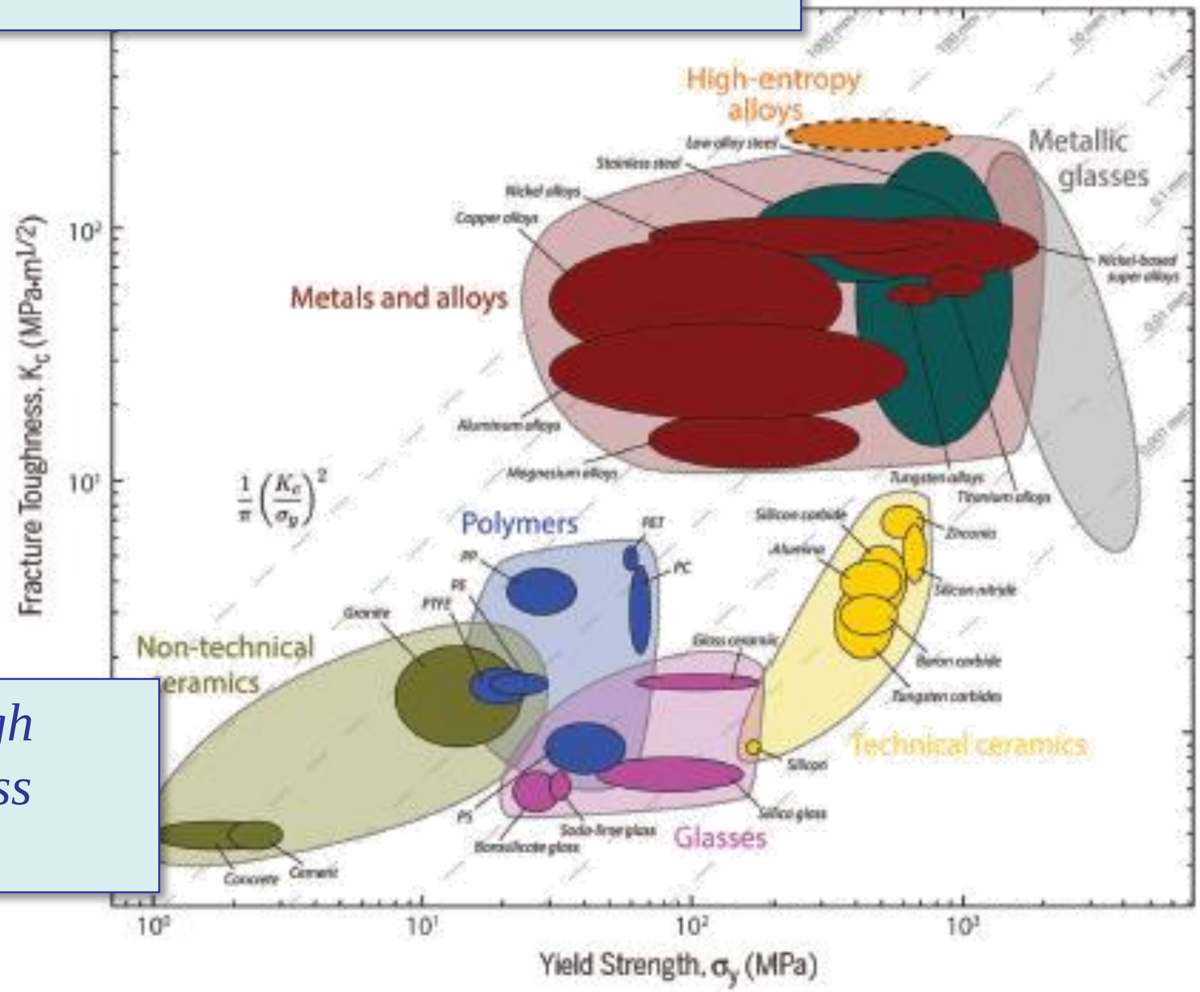
- High Entropy Alloy



Zhang et al. 2014

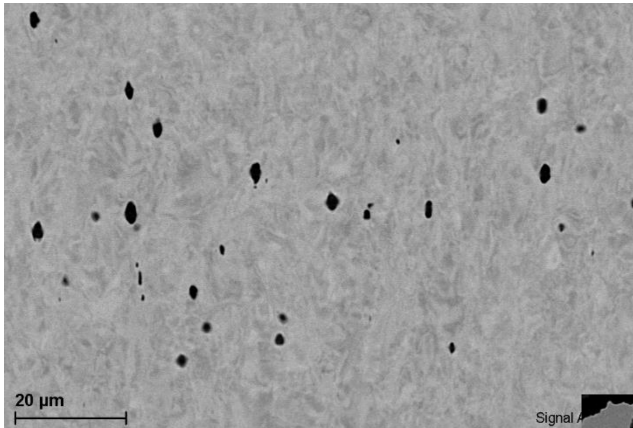
Distorted lattice of several elements in equivalent proportions



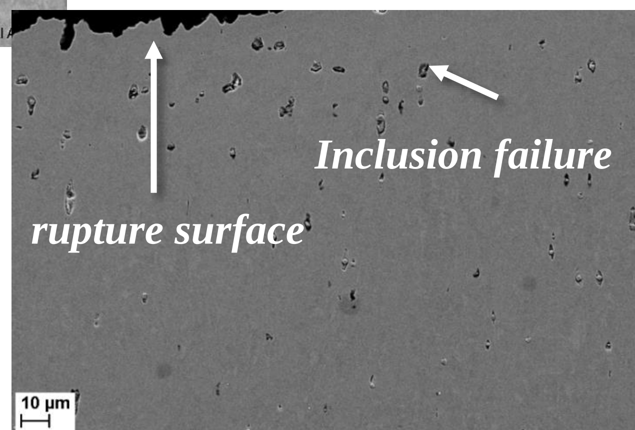
Unexpectedly high fracture toughness

Introduction

- HEAs follow a ductile failure mechanism



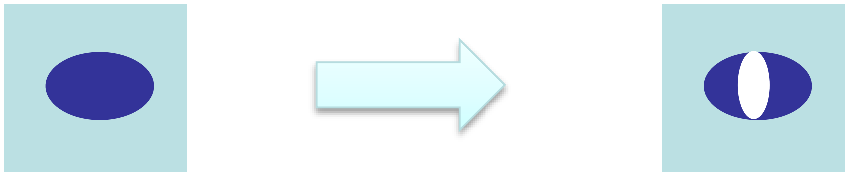
Porosity free
Initial inclusions



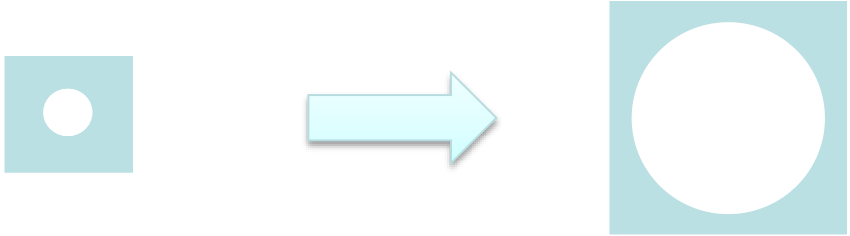
Nucleation from inclusion failure

Tests performed at UCL by Antoine Hilhorst

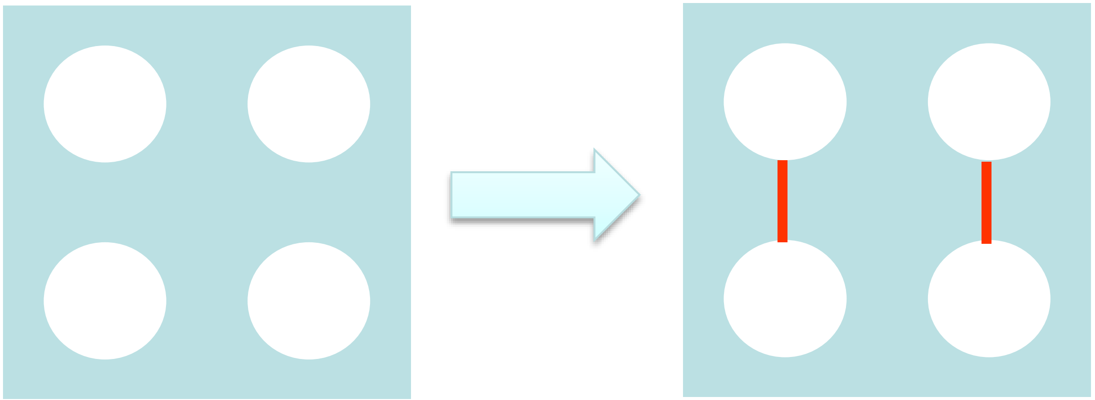
- Ductile failure: failure mechanism
  - Void nucleation (dislocation motion, particle/matrix decohesion, particle cracking, …)



  - Void growth of existing voids (because of plastic incompressibility)

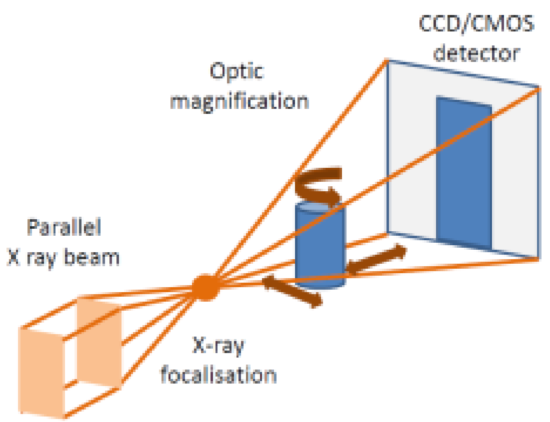


  - Void coalescence (crack growth by shrinking of ligaments between voids)

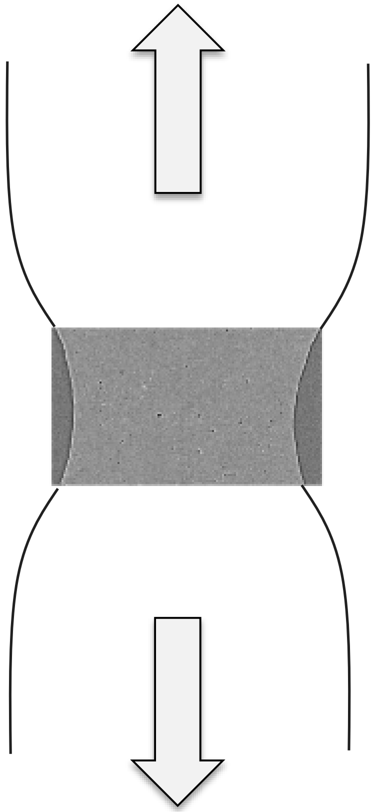


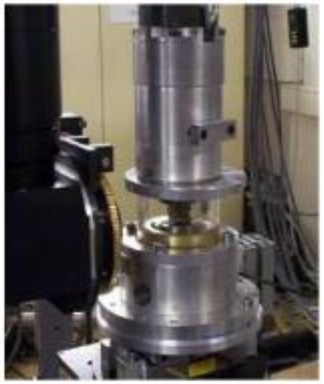
- Ductile failure: complex coalescence scenarios
  - What does happen inside a « ductile » material under large strain ?

X-ray tomography of in-situ tensile tests
= scanner for materials



Tests performed at the ESRF synchrotron in Grenoble by F. *Hannard (Ph. D. UCL) collaboration with Dr. E. maire INSA Lyon*

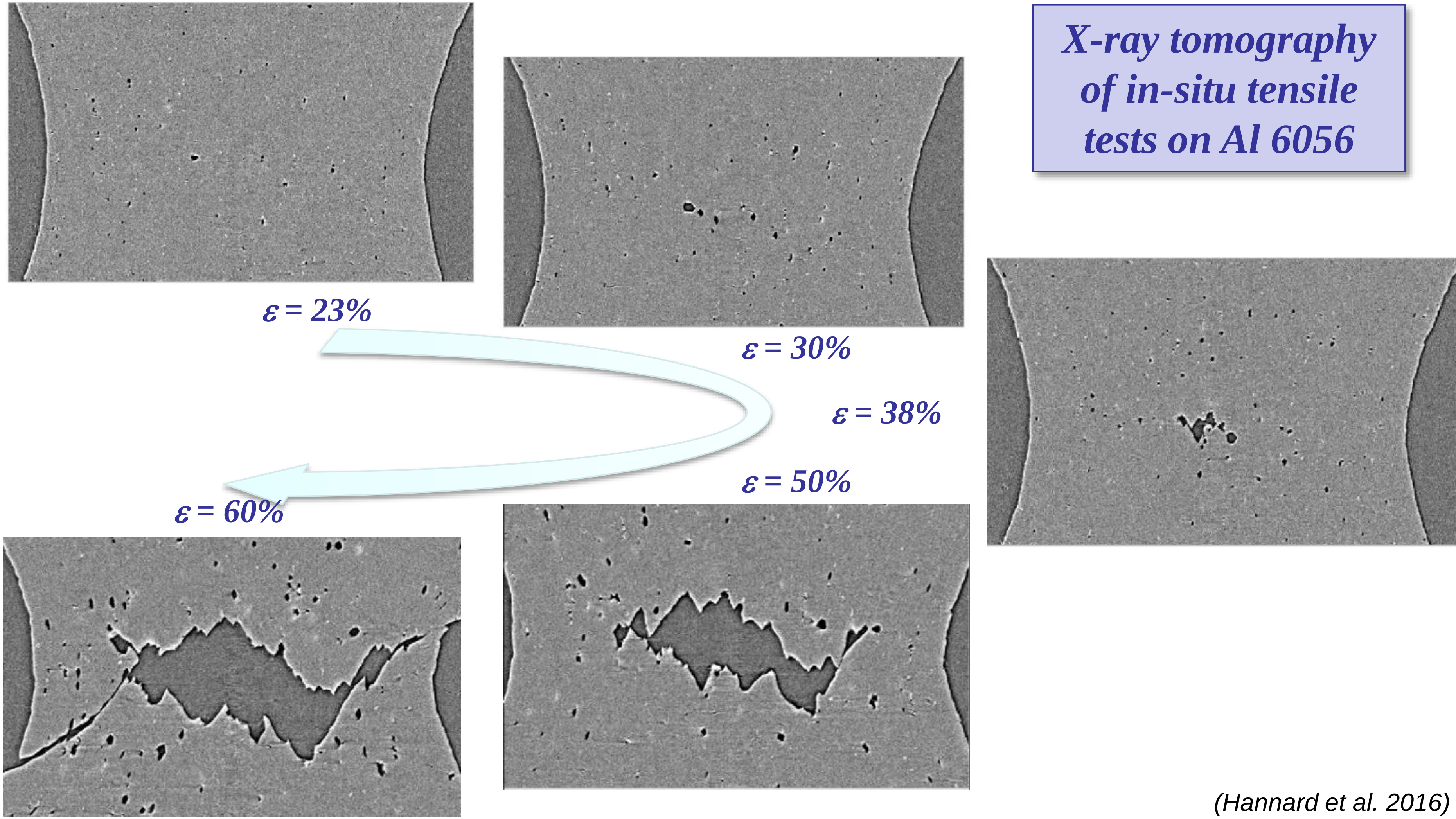




(Hannard et al. 2016)

- Ductile failure: complex coalescence scenarios
  - What does happen inside a « ductile » material under large strain ?

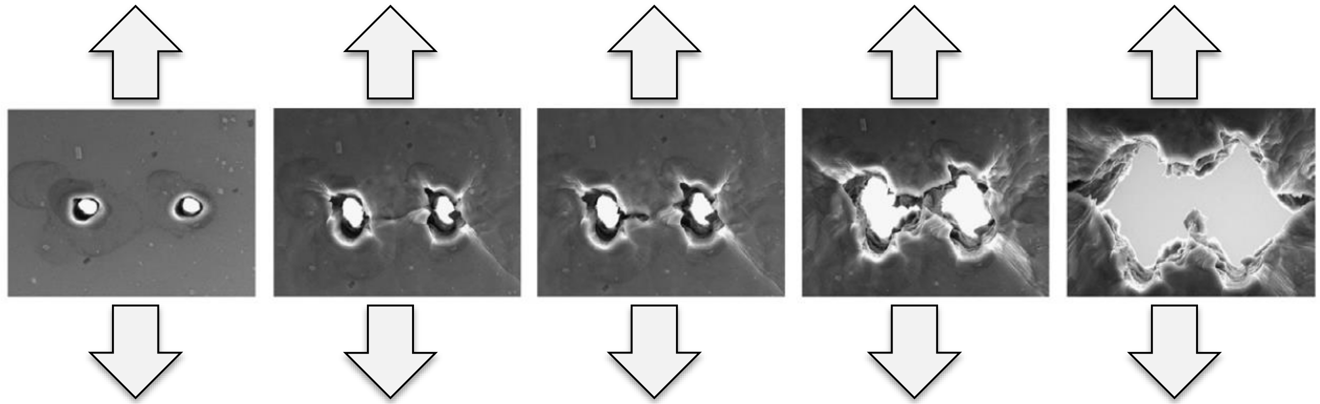
X-ray tomography of in-situ tensile tests on Al 6056



(Hannard et al. 2016)

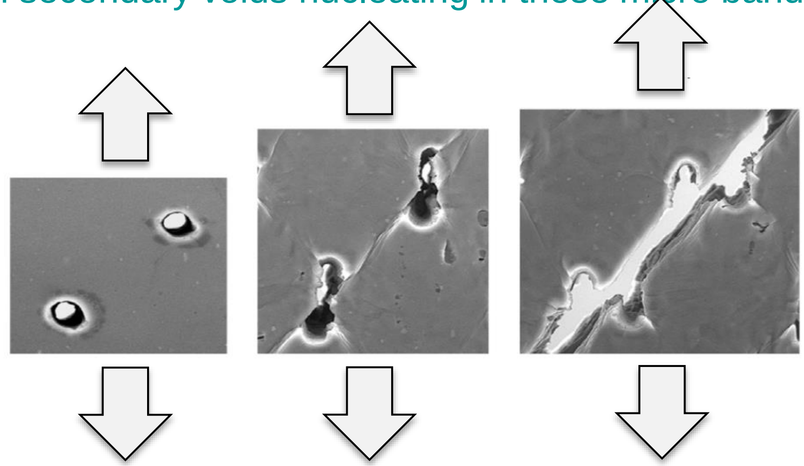
- Ductile failure: complex coalescence scenarios
  - Localization band perpendicular to the main loading direction
    - Shrinking of ligaments between voids

Internal necking coalescence



  - Micro shear bands inclined to the main loading direction
    - Joining primary voids
    - Possibly with secondary voids nucleating in these micro bands

Shear driven coalescence



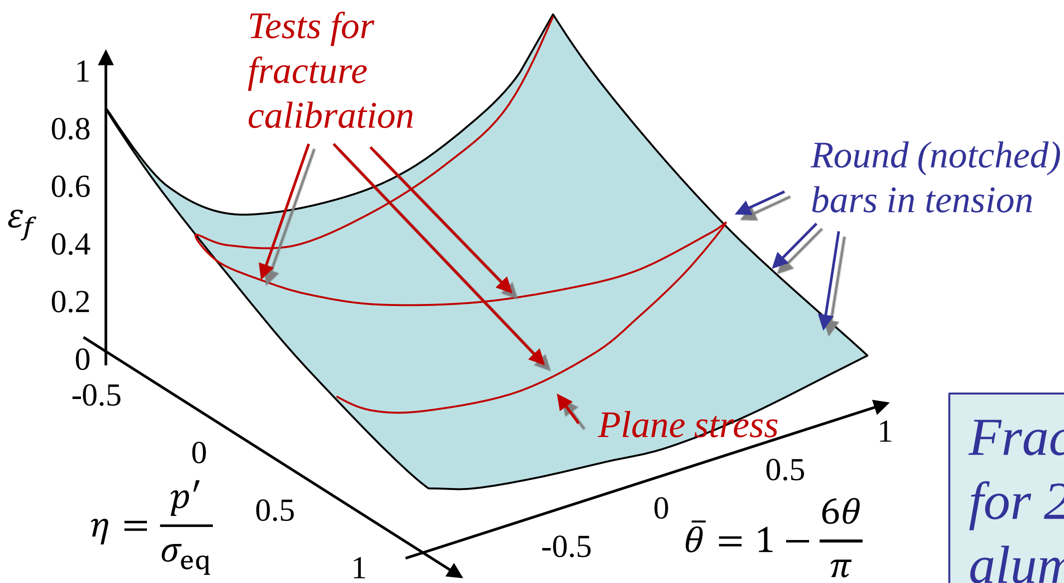
(Weck & Wilkinson 2008)

- Ductile failure: stress-state dependent fracture strain
  - Stress triaxiality dependent

$$\eta = \frac{p'}{\sigma_{\mathrm{eq}}} \in [-\infty \ \infty] \qquad p' = \frac{\mathrm{tr}\,(\boldsymbol{\sigma})}{3} \qquad \sigma_{\mathrm{eq}} = \sqrt{\frac{3}{2}\mathrm{dev}\,(\boldsymbol{\sigma}) : \mathrm{dev}\,(\boldsymbol{\sigma})}$$

  - Lode dependent

$$\theta = \frac{1}{3}\arccos\left(\frac{27J_3}{2\sigma_{\mathrm{eq}}^3}\right) \qquad J_3 = \det\left(\mathrm{dev}\,(\boldsymbol{\sigma})\right)$$



Fracture locus for 2024-T351 aluminum alloy

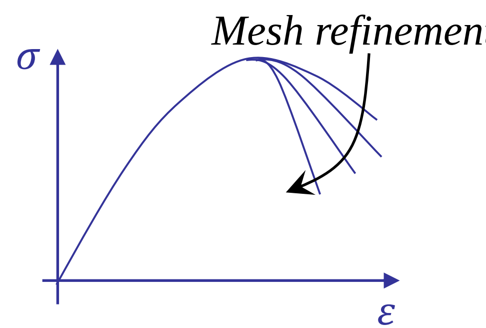
(Bai & Wierzbicki 2010)

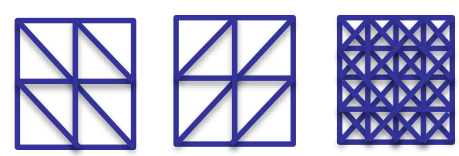
- Objective & Methodology
  - Develop a multi-surface model incorporating
    - Void growth phase
    - Internal necking coalescence phase
      - Driven by maximum principal stress
    - Shear driven coalescence phase
      - Driven by maximum shear stress
  - In a nonlocal formalism
    - Why?
      - Local forms suffer from mesh-dependency
    - Implicit formulation (Peerlings et al. 1998)
      - Introduction of a characteristic length l_c
      - New non-local degrees of freedom $\bar{Z}_k$
      - New Helmholtz-type equation to be solved

$$\bar{Z}_k - Z_k - l_{ck}^2 \Delta_0 \bar{Z}_k = 0\,, \text{ with } k = 1, \dots, N$$

      - Damage indicators depend on the nonlocal variable
    - Multiple nonlocal variables can be considered
      - Damage indicators depend on N different sources

The maximum principal stress & maximum shear stress are Lode-dependent!





The numerical results change without convergence

- Porous plasticity corotational approach
  - Yield condition

$$\Phi_{\mathrm{nl}} = \Phi_{\mathrm{nl}}\left(\boldsymbol{\sigma}; \sigma_{\mathrm{Y}}, \mathbf{Y}\right) = 0$$

  - Plastic flow

$$\mathbf{D}^{\mathrm{p}} = \dot{\mathbf{F}}^{\mathrm{p}} \cdot \mathbf{F}^{\mathrm{p}-1} = \dot{\mu} \frac{\partial \Phi_{\mathrm{nl}}}{\partial \boldsymbol{\sigma}}$$

  - Evolution laws
    - Equivalent matrix plastic strain rate:

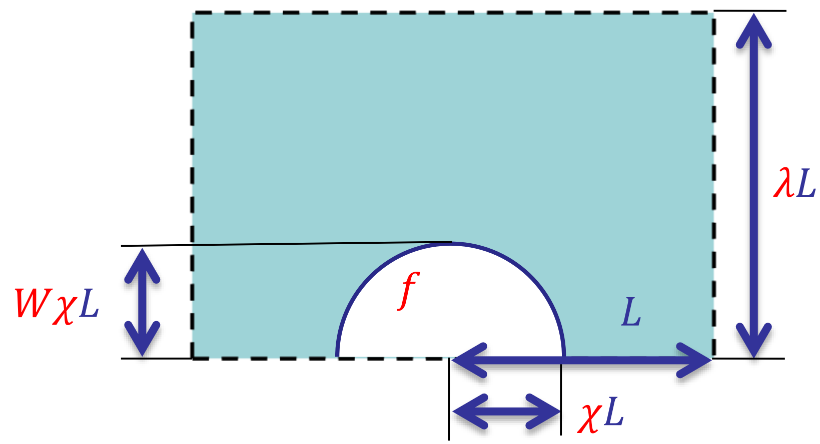
$$\dot{\varepsilon}_{\mathrm{m}} = \frac{\boldsymbol{\sigma} : \mathbf{D}^{\mathrm{p}}}{(1-f)\,\sigma_{\mathrm{Y}}}$$

    - Isotropic hardening law:

$$\sigma_{\mathrm{Y}} = \sigma_{\mathrm{Y}}^{0} + R\left(\varepsilon_{\mathrm{m}}\right)$$

    - Evolution laws for void characteristics

$$\mathbf{Y} = \begin{bmatrix} f & \chi & W & \lambda \end{bmatrix}^{T}$$



Void characteristics Y:

Porosity : f
Void ligament ratio: χ
Void aspect ratio: W
Void spacing ratio: λ

Yield surface Φ_{nl} and evolution laws for Y depend on the void expansion solution:
- *Void growth;*
- *Internal necking coalescence; or*
- *Shear driven coalescence*

- Void growth phase – GTN model
  - Yield condition

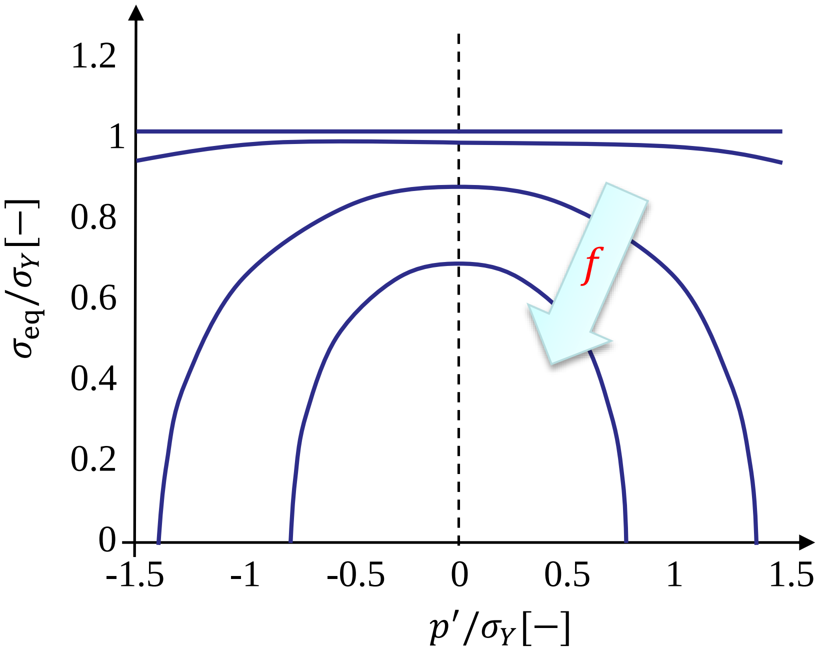
$$\begin{cases} \Phi_{\text{nl}} = \Phi_{\text{G}} = \dfrac{\hat{\sigma}_{\text{G}}}{\sigma_{\text{Y}}} - 1 = 0 \\ \hat{\sigma}_{\text{G}}\left(\sigma_{\text{eq}}, p', \sigma_{\text{Y}}, f\right) = \dfrac{\sqrt{\sigma_{\text{eq}}^2 + 2\sigma_{\text{Y}}^2 f q_1 \left[\cosh\left(\frac{3}{2} q_2 \frac{p'}{\sigma_{\text{Y}}}\right) - 1\right]}}{1 - q_1 f} \end{cases}$$

$$p' = \frac{\text{tr}\left(\boldsymbol{\sigma}\right)}{3}$$

$$\sigma_{\text{eq}} = \sqrt{\frac{3}{2}\text{dev}\left(\boldsymbol{\sigma}\right) : \text{dev}\left(\boldsymbol{\sigma}\right)}$$

  - Parameters:
    - q_1 and q_2
  - Hardening law
    - $\sigma_{\text{Y}}(\varepsilon_m)$
    - Matrix plastic deformation ε_m
  - Nonlocal evolution laws for void characteristics

$$\mathbf{Y}_{\text{nl}} = \mathbf{Y}_{\text{G}}(\varepsilon_{\text{m}}, \varepsilon_{\text{v}}, \varepsilon_{\text{d}}, \bar{\varepsilon}_{\text{m}}, \bar{\varepsilon}_{\text{v}}, \bar{\varepsilon}_{\text{d}}, \boldsymbol{\sigma})$$



Multi-surface nonlocal porous model

- Void growth phase - $\mathbf{Y}_{\mathrm{nl}} = \mathbf{Y}_{\mathrm{G}}(\varepsilon_{\mathrm{m}}, \varepsilon_{\mathrm{v}}, \varepsilon_{\mathrm{d}}, \bar{\varepsilon}_{\mathrm{m}}, \bar{\varepsilon}_{\mathrm{v}}, \bar{\varepsilon}_{\mathrm{d}}, \boldsymbol{\sigma})$
  - Nonlocal porosity evolution

$$\dot{f} = \dot{f}_{\mathrm{gr}} + \dot{f}_{\mathrm{nu}} + \dot{f}_{\mathrm{sh}}$$

- Growth part

$$\dot{f}_{\mathrm{gr}} = (1-f)\,\mathrm{tr}\,(\mathbf{D}^{\mathrm{p}}) \Rightarrow \dot{f}_{\mathrm{gr}} = (1-f)\,\dot{\bar{\varepsilon}}_{\mathrm{v}}$$

- Nucleation part

$$\dot{f}_{\mathrm{nu}} = A_n\,(\varepsilon_{\mathrm{m}})\,\dot{\varepsilon}_{\mathrm{m}} \Rightarrow \dot{f}_{\mathrm{nu}} = A_n\,(\bar{\varepsilon}_{\mathrm{m}})\,\dot{\bar{\varepsilon}}_{\mathrm{m}}$$

- Shear part

$$\dot{f}_{\mathrm{sh}} = k_w \phi_\eta \phi_\omega f \frac{\mathrm{dev}(\boldsymbol{\sigma}) : \mathbf{D}^{\mathrm{p}}}{\sigma_{\mathrm{eq}}} \Rightarrow \dot{f}_{\mathrm{sh}} = k_w \phi_\eta \phi_\omega f \dot{\bar{\varepsilon}}_d$$

(Nahshon and Hutchinson 2008)

- Parameter: η_s, k_w

$$\phi_\eta = \exp\left(-\frac{1}{2}\left(\frac{\eta}{\eta_s}\right)^2\right) \quad \& \quad \phi_\omega = 1 - \omega^2$$

$$\mathbf{D}^{\mathrm{p}} = \dot{\mathbf{F}}^{\mathrm{p}} \cdot \mathbf{F}^{\mathrm{p}-1} = \dot{\mu} \frac{\partial \Phi_{\mathrm{nl}}}{\partial \boldsymbol{\sigma}}$$

$$\varepsilon_{\mathrm{v}} = \mathrm{tr}\,(\mathbf{D}^{\mathrm{p}})$$

$$\frac{\mathrm{dev}\,(\boldsymbol{\sigma}) : \mathbf{D}^{\mathrm{p}}}{\sigma_{\mathrm{eq}}} = \dot{\varepsilon}_{\mathrm{d}}$$

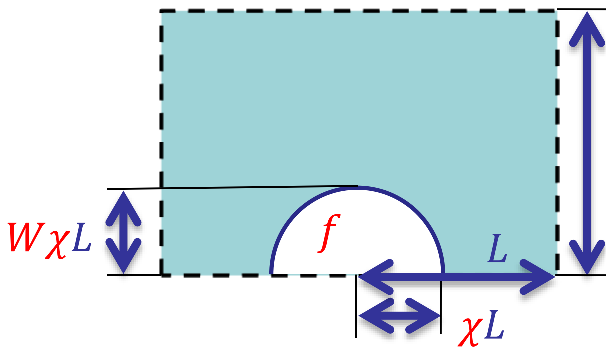
$$\omega = \frac{27 J_3}{2{\sigma_{\mathrm{eq}}}^3}.$$

  - Voids shape evolution

$$\begin{cases} \dot{\lambda} = \kappa \lambda \dot{\bar{\varepsilon}}_{\mathrm{d}} \\ \chi = \left(\frac{3 f \lambda}{2W}\right)^{\frac{1}{3}} \\ \dot{W} = 0 \end{cases}$$

Periodic distribution $\kappa = 1.5$,
Random distribution $\kappa = 0$,
Clustered distribution $0 < \kappa < 1.5$

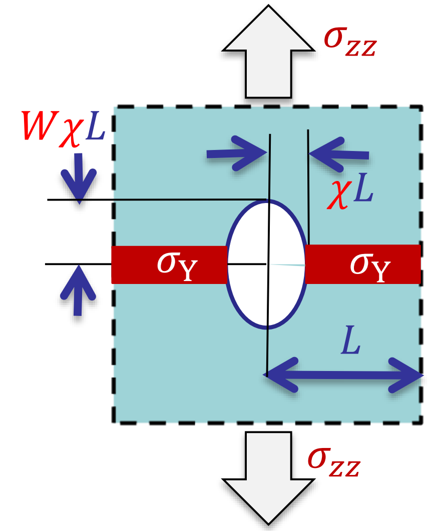
(Benzerga et al. 2016)



- Internal necking – Coalescence
  - Thomason coalescence onset
    - Localized plastic flow in ligament
    - Limit load factor for uniaxial tension

(Thomason 1985)

$$C_{\mathrm{Tf}}(\mathbf{Y}) = \frac{\sigma_{zz}}{\sigma_{\mathrm{Y}}} = (1-\chi^2)\left[h\left(\frac{1-\chi}{W\chi}\right)^2 + g\sqrt{\frac{1}{\chi}}\right]$$

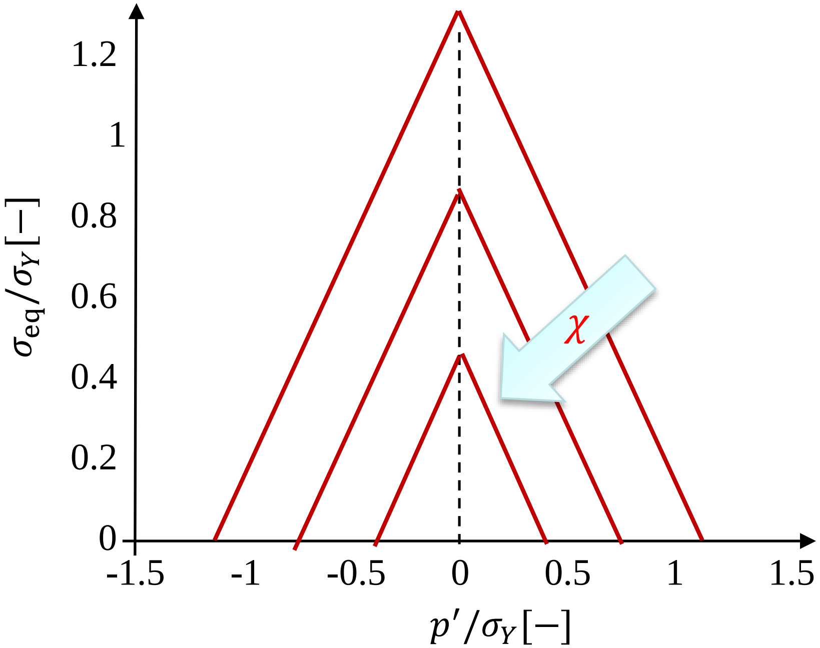


- Parameters:
  - $g = 0.1,\ h = 1.24$ are generally adopted
- New yield surface accounting for general loading
  - Driven by maximum principal stress (MPS)

$$\begin{cases} \Phi_{\mathrm{nl}} = \Phi_{\mathrm{T}} = \dfrac{\hat{\sigma}_{\mathrm{T}}}{\sigma_{\mathrm{Y}}} - 1 = 0 \\ \hat{\sigma}_{\mathrm{T}} = \dfrac{1}{C_{\mathrm{Tf}}}\left(\dfrac{2}{3}\sigma_{\mathrm{eq}}\cos\theta + |p'|\right) \end{cases}$$

MPS

$$\theta(\sigma_{\mathrm{eq}}, J_3) = \frac{1}{3}\arccos\frac{27J_3}{2\sigma_{\mathrm{eq}}{}^3}. \qquad p' = \frac{\mathrm{tr}(\boldsymbol{\sigma})}{3}$$



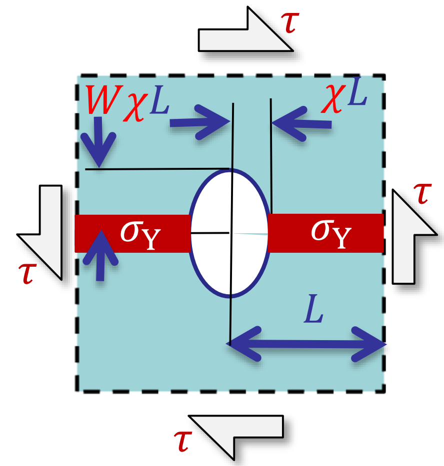
- Evolution laws for void characteristics

$$\mathbf{Y}_{\mathrm{nl}} = \mathbf{Y}_{\mathrm{T}}(\varepsilon_{\mathrm{m}}, \varepsilon_{\mathrm{v}}, \varepsilon_{\mathrm{d}}, \bar{\varepsilon}_{\mathrm{m}}, \bar{\varepsilon}_{\mathrm{v}}, \bar{\varepsilon}_{\mathrm{d}}, \boldsymbol{\sigma})$$

Multi-surface nonlocal porous model

- Shear driven – Coalescence
  - Thomason-like coalescence onset
    - Limit load factor

$$C_{\mathrm{Sf}}\left(\mathbf{Y}\right) = \frac{\sqrt{3}\tau}{\sigma_{\mathrm{Y}}} = \xi\left(1-\chi^2\right)$$



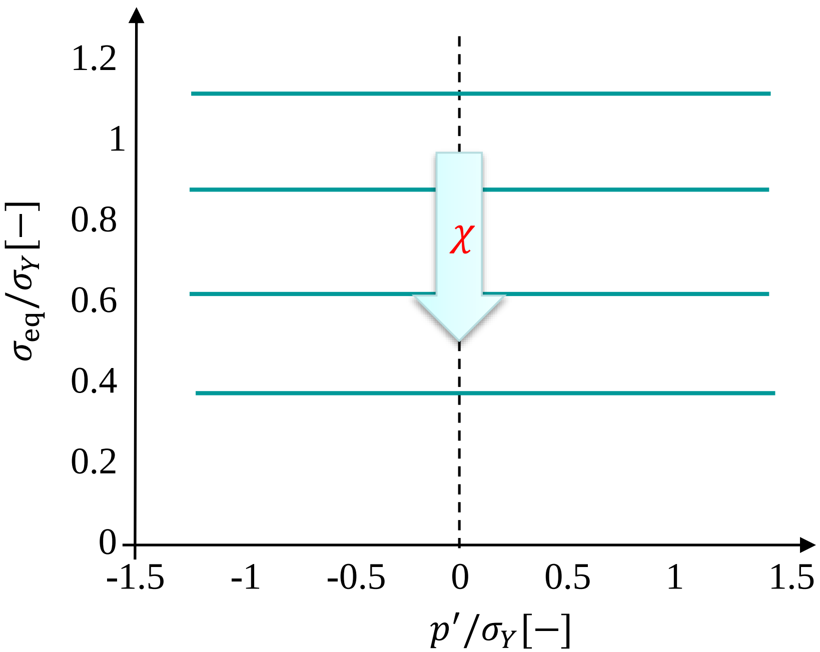
- Parameter ξ
  - $\xi = 1$ for σ_Y uniform inside localization band
  - $\xi > 1$ is used for real distribution

  - New yield surface
    - Driven by maximum shear stress (MSS)

$$\begin{cases} \Phi_{\mathrm{nl}} = \Phi_{\mathrm{S}} = \dfrac{\hat{\sigma}_{\mathrm{S}}}{\sigma_{\mathrm{Y}}} - 1 = 0 \\ \hat{\sigma}_{\mathrm{S}} = \dfrac{\sqrt{3}\tau}{C_{\mathrm{Sf}}} = \dfrac{\sigma_{\mathrm{eq}}}{C_{\mathrm{Sf}}}\left(\dfrac{\sin\theta}{2} + \dfrac{\sqrt{3}\cos\theta}{2}\right) \end{cases}$$

MSS

$$\theta\left(\sigma_{\mathrm{eq}}, J_3\right) = \frac{1}{3}\arccos\frac{27J_3}{2{\sigma_{\mathrm{eq}}}^3}$$



  - Evolution laws for void characteristics

$$\mathbf{Y}_{\mathrm{nl}} = \mathbf{Y}_{\mathrm{S}}(\varepsilon_{\mathrm{m}}, \varepsilon_{\mathrm{v}}, \varepsilon_{\mathrm{d}}, \bar{\varepsilon}_{\mathrm{m}}, \bar{\varepsilon}_{\mathrm{v}}, \bar{\varepsilon}_{\mathrm{d}}, \boldsymbol{\sigma})$$

Multi-surface nonlocal porous model

- Competition between different modes
  - Yield surface

$$\Phi_{\mathrm{e}} = \frac{\hat{\sigma}}{\sigma_{\mathrm{Y}}} - 1 = 0$$

    - Effective stress

$$\hat{\sigma} = \max\left(\hat{\sigma}_{\mathrm{G}}, \hat{\sigma}_{\mathrm{T}}, \hat{\sigma}_{\mathrm{S}}\right)$$

    - Approximated form

$$\hat{\sigma} = \left(\hat{\sigma}_{\mathrm{G}}^{m} + \hat{\sigma}_{\mathrm{T}}^{m} + \hat{\sigma}_{\mathrm{S}}^{m}\right)^{\frac{1}{m}}$$

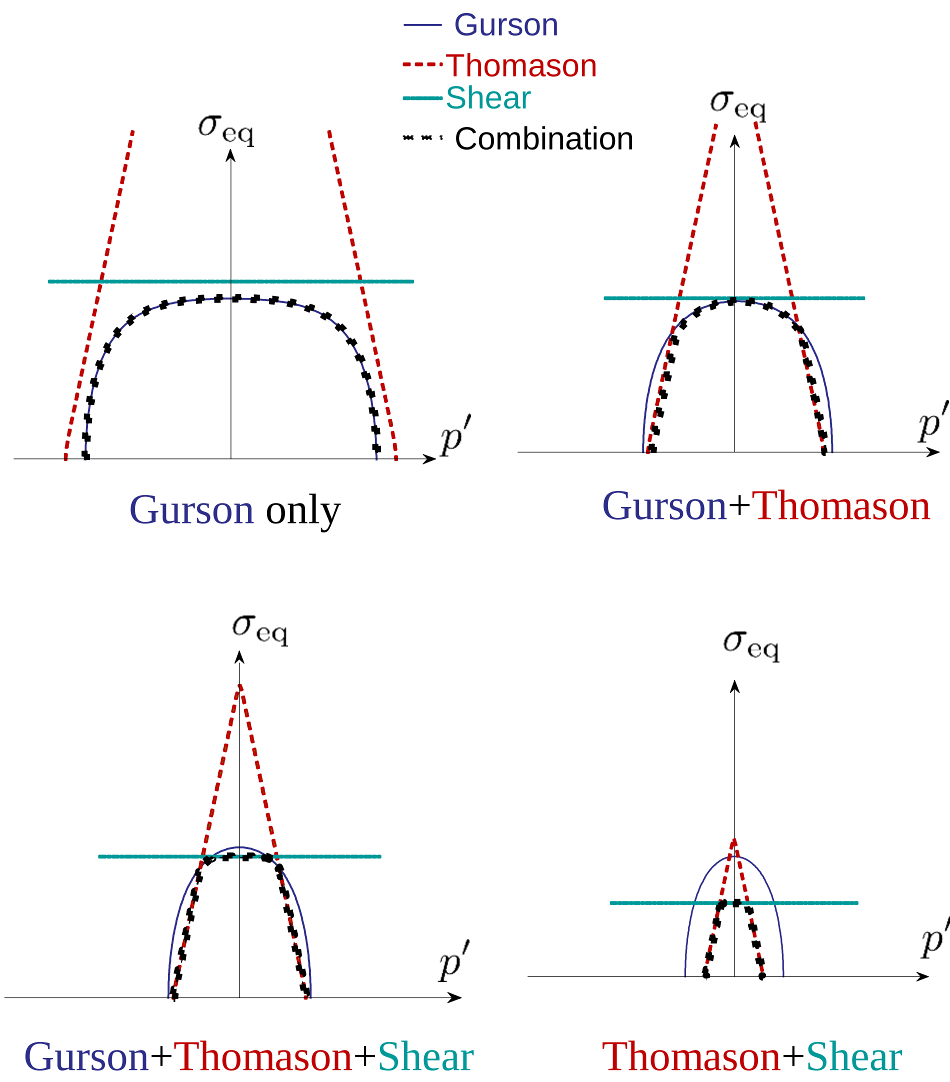
    - Smoothing using $m \gg 1$

  - Onset of void necking coalescence

$$\dot{\varepsilon}_{\mathrm{m}} > 0\,, \text{ and } \hat{\sigma}_T > \max\left(\hat{\sigma}_G, \hat{\sigma}_S\right)$$

  - Onset of void shear coalescence

$$\dot{\varepsilon}_{\mathrm{m}} > 0\,, \text{ and } \hat{\sigma}_S > \max\left(\hat{\sigma}_G, \hat{\sigma}_T\right)\,.$$



Multi-surface nonlocal porous model

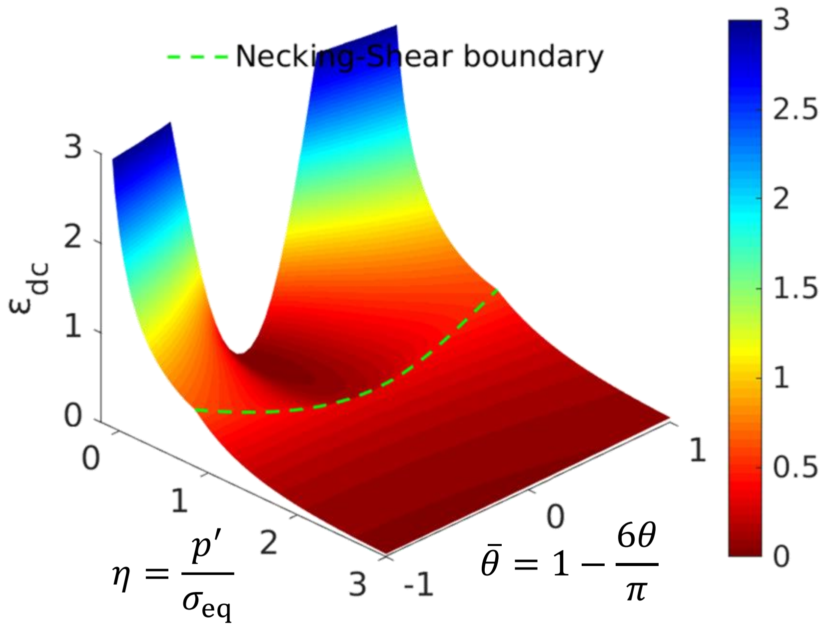
- Solution under proportional loadings
  - Constant
    - Stress triaxiality (η); and
    - Normalized Lode angle ($\bar{\theta}$)
  - ε_{dc}- ductility = plastic deformation at coalescence onset

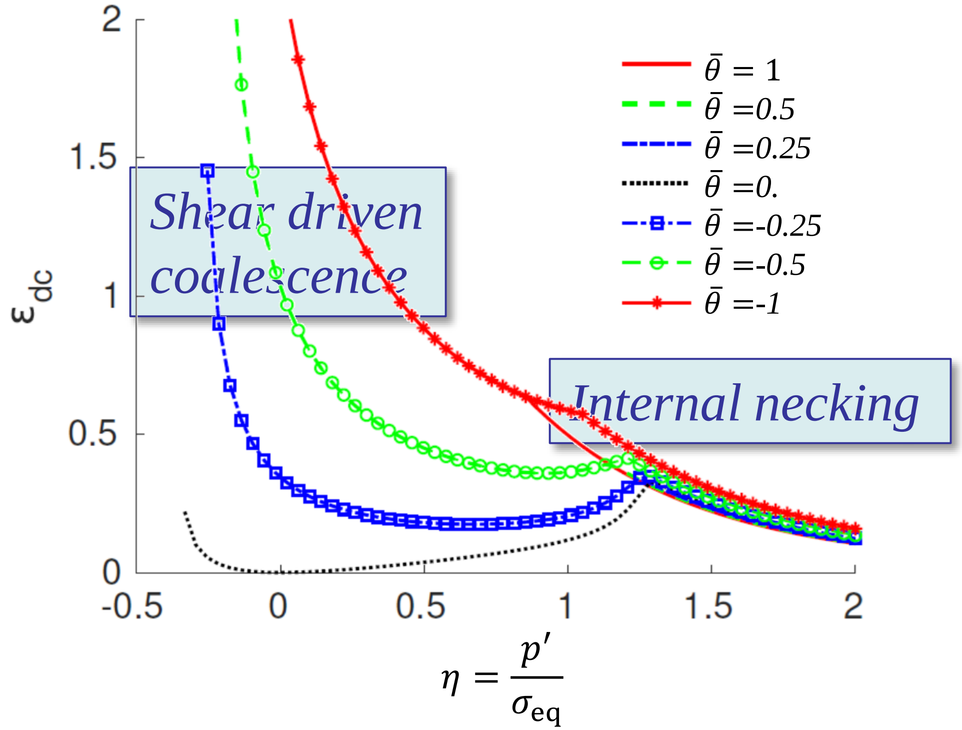
$$\eta = \frac{p'}{\sigma_{eq}} \qquad p' = \frac{\mathrm{tr}(\boldsymbol{\sigma})}{3}$$

$$\sigma_{eq} = \sqrt{\frac{3}{2}\mathrm{dev}(\boldsymbol{\sigma}) : \mathrm{dev}(\boldsymbol{\sigma})}$$

$$\bar{\theta} = 1 - \frac{6\theta}{\pi}$$

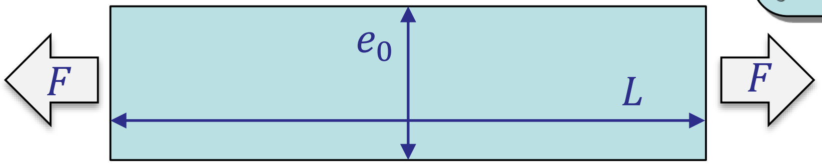
$$\theta(\sigma_{eq}, J_3) = \frac{1}{3}\arccos\frac{27 J_3}{2{\sigma_{eq}}^3}$$

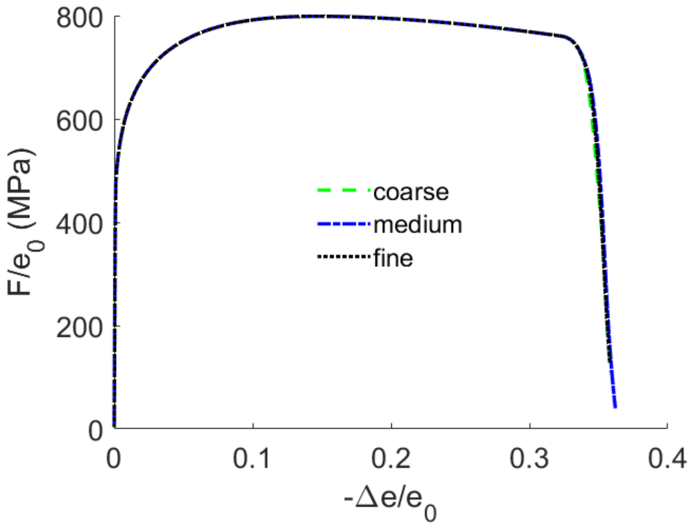




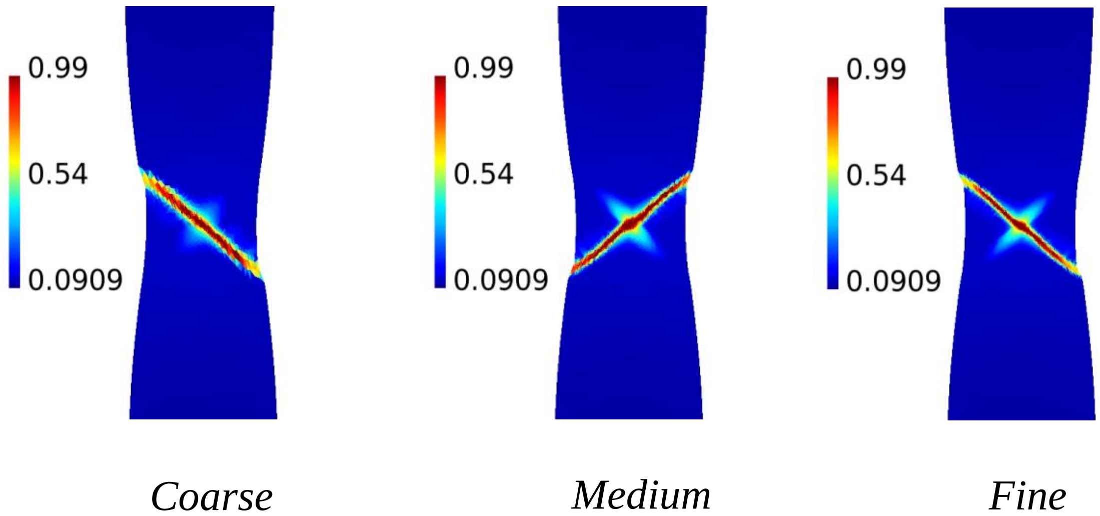
- Plane strain smooth specimen under tensile loading
  - Verification of the nonlocal model: mesh convergence

$L = 12.5$ mm
$e_0 = 3$ mm
$\xi = 1.015 \ (\varepsilon_{ds} = 0.95)$





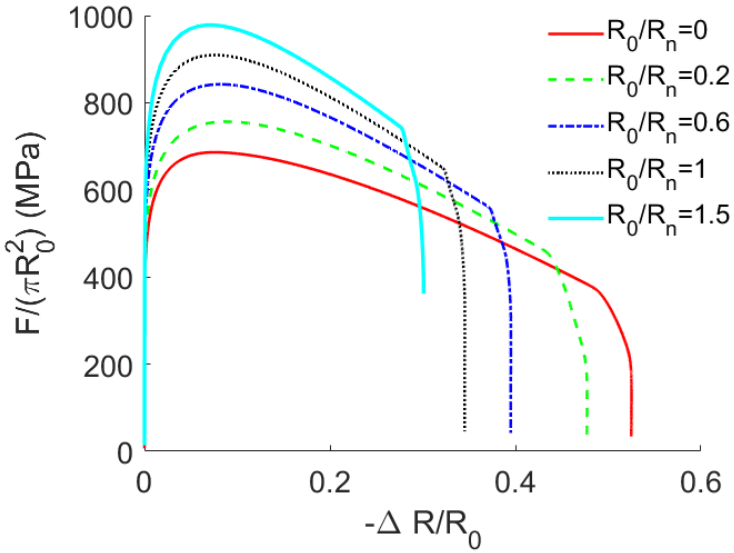
Distribution of void ligament ratio χ



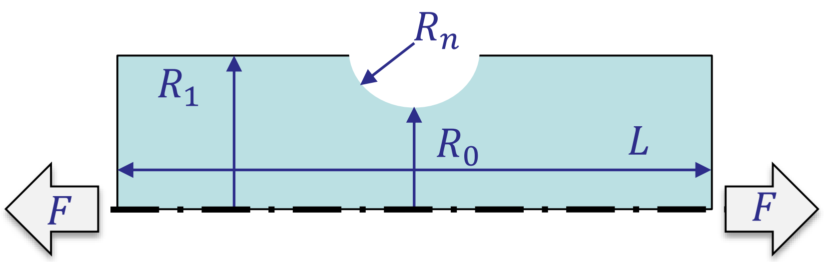
Capture slant fracture

Numerical examples

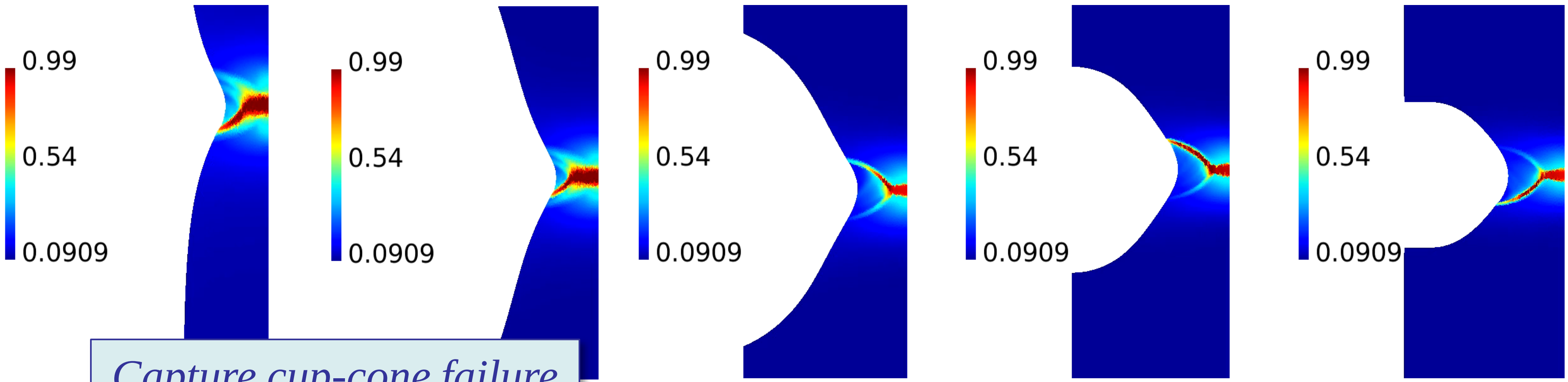
- Axisymmetric (notched) specimens under tensile loading
  - Different notch radii: $R_0/R_n = 0, 0.2, 0.6, 1, 1.5$



$R_0 = 3$ mm
$R_1 = 6$ mm
$L = 25$ mm
$\xi = 1.015 \;\; (\varepsilon_{ds} = 0.95)$



Distribution of void ligament ratio χ

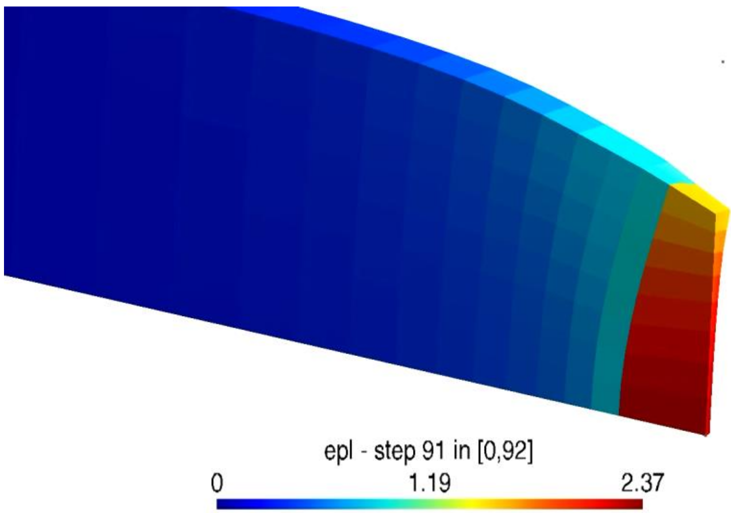


Capture cup-cone failure

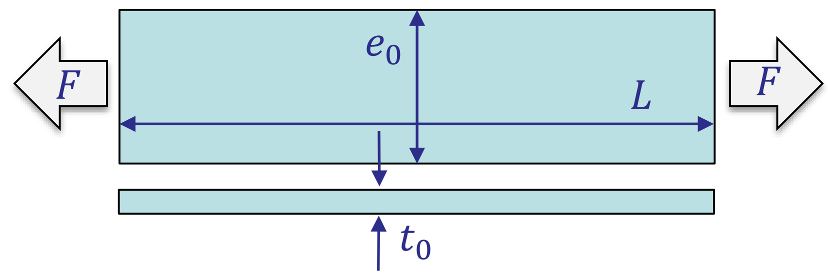
Application to HEA: Preliminary tests without MSS-driven coalescence

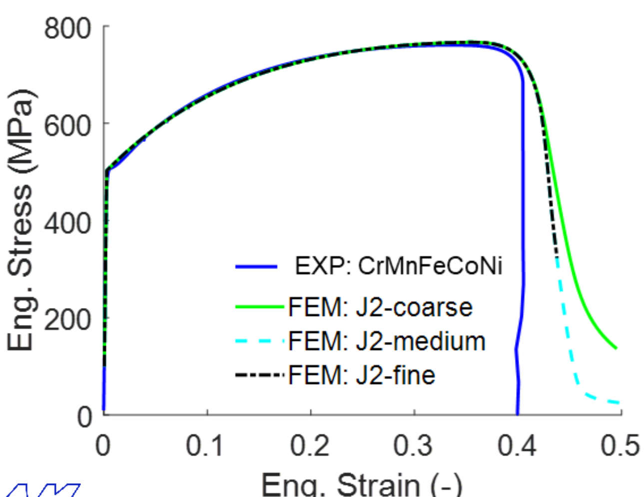
- Parameters identification of CrMnFeCoNi
  - Hardening law $\sigma_Y(\varepsilon_m)$ identification

Distribution of plastic strain ε_d

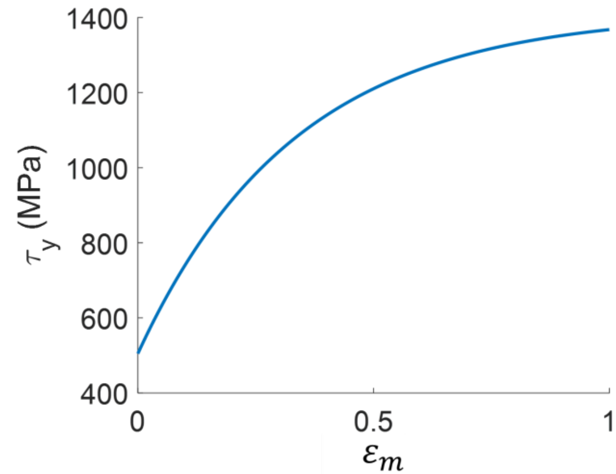


$e_0 = 6$ mm
$t_0 = 1.05$ mm
$L = 26$ mm





Elasto-plastic hardening identification

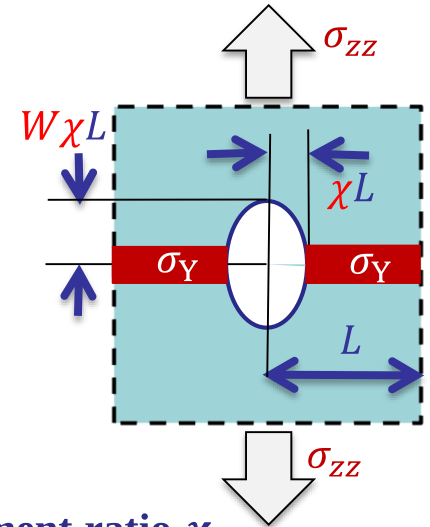


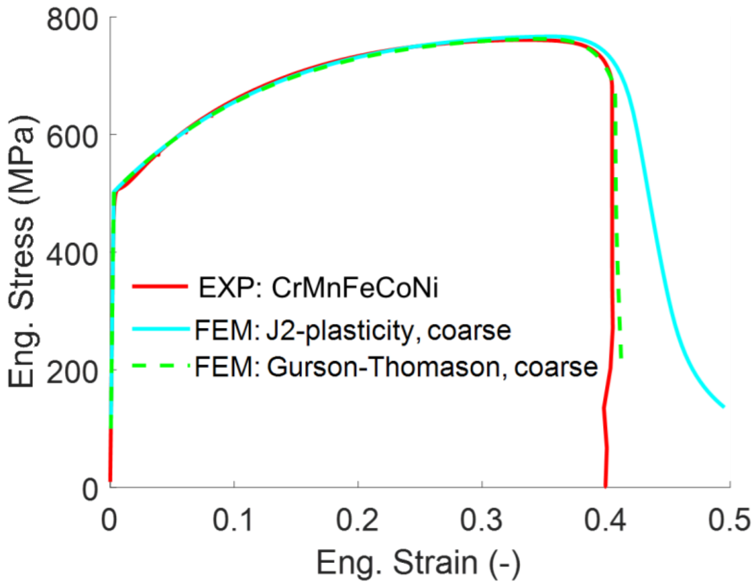
Application to HEA: Preliminary tests without MSS-driven coalescence

- Parameters identification of CrMnFeCoNi
  - Gurson-Thomason parameters identification

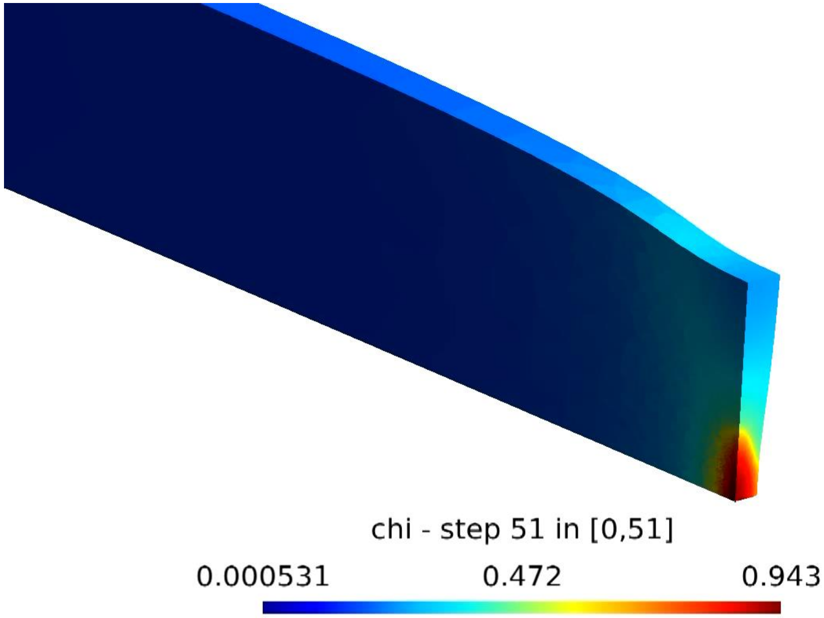
$$\begin{cases} \dot{\chi} &= \frac{3}{4}\frac{\lambda}{W}\left(\frac{3}{2\chi^2}-1\right)\dot{\bar{\varepsilon}}_{\mathrm{d}}\,, \\ \dot{W} &= \frac{9}{4}\frac{\lambda}{\chi}\left(1-\frac{1}{2\chi^2}\right)\dot{\bar{\varepsilon}}_{\mathrm{d}}\,, \\ \dot{\lambda} &= \kappa\lambda\dot{\bar{\varepsilon}}_{\mathrm{d}}\,, \end{cases}$$

$\lambda_0 = 1$
$\kappa = 1.5$





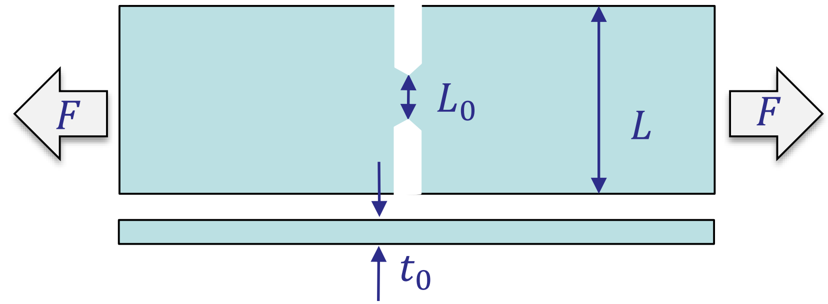
Distribution of void ligament ratio χ



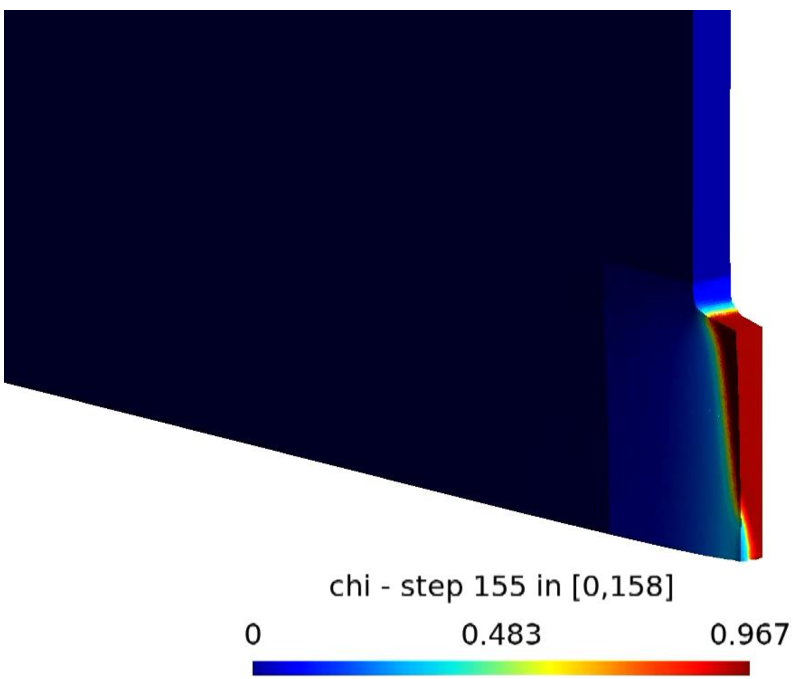
Application to HEA: Preliminary tests without MSS-driven coalescence

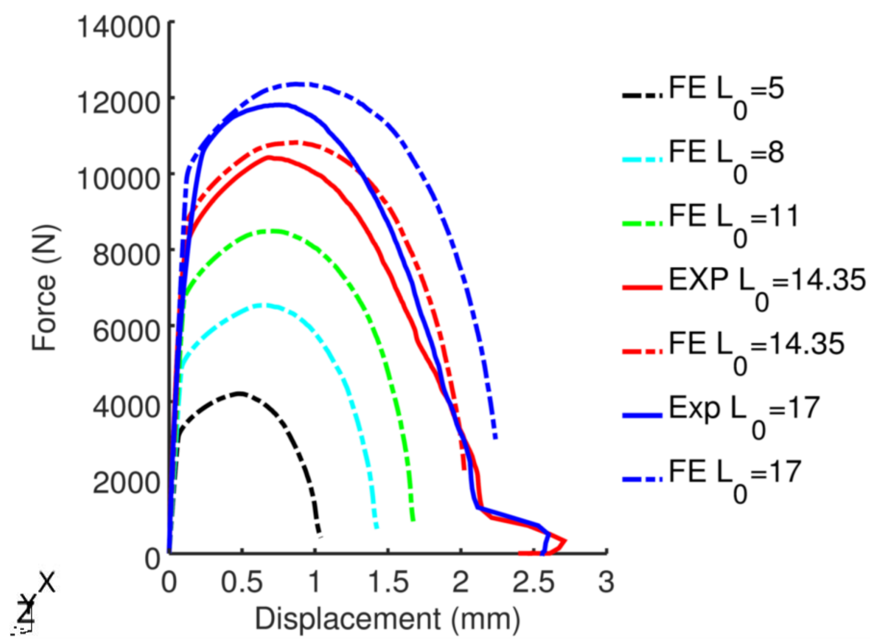
- Double notched specimen of CrMnFeCoNi
  - Preliminary results
  - To characterize non-local length
  - To extraction essential work of failure

$t_0 = 1.\ \text{mm}$
$L = 26\ \text{mm}$



Distribution of void ligament ratio χ





Conclusion

- Objective
  - Simulation of ductile failure incorporating void growth & coalescence deformation modes
- Methodology
  - Nonlocal porous plasticity
  - Multi-surface model incorporating
    - Void growth;
    - Internal necking coalescence; and
    - Shear driven coalescence
- Results
  - The proposed framework is able to model
    - The slant fracture mode in plane strain smooth specimens
    - The cup-cone fracture mode in axisymmetric smooth & notched specimens
- In progress
  - Validation/Calibration with HEAs

Thank you for your attention

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Predictor-corrector scheme

- Elastic predictor

$$\mathbf{F}^{\mathrm{ppr}} = \mathbf{F}_n^{\mathrm{p}} \qquad \mathbf{F}^{\mathrm{epr}} = \mathbf{F} \cdot \mathbf{F}^{\mathrm{ppr}-1}$$

- Plastic corrector (fully implicit radial return)

$$\begin{cases} \boldsymbol{\tau} = \boldsymbol{\tau}^{\mathrm{pr}} - \mathbb{C} : \Delta\mathbf{E}^p \,, \\ \boldsymbol{\sigma} = J^{-1}\boldsymbol{\tau} \,, \\ \sigma_{\mathrm{Y}} = \sigma_{\mathrm{Y}}\left(\varepsilon_{\mathrm{m}n} + \Delta\varepsilon_{\mathrm{m}}\right) \,, \\ \mathbf{Y} = \mathbf{Y}_n + \Delta\mathbf{Y}\left(\Delta\bar{\mathbf{Z}}, \boldsymbol{\sigma}\right) \,, \\ \Phi_{\mathrm{nl}}\left(\boldsymbol{\sigma}; \sigma_{\mathrm{Y}}, \mathbf{Y}\right) = 0 \,, \\ \Delta\mathbf{E}^p - \Delta\mu\mathbf{N}^{\mathrm{p}}\left(\boldsymbol{\sigma}; \sigma_{\mathrm{Y}}, \mathbf{Y}\right) = \mathbf{0} \,, \text{ and} \\ \boldsymbol{\sigma} : \Delta\mathbf{E}^p - (1-f)\,\sigma_{\mathrm{Y}}\Delta\varepsilon_{\mathrm{m}} = 0 \,. \end{cases}$$

Unknowns: $\boldsymbol{\tau}$, $\boldsymbol{\sigma}$, σ_{Y}, $\Delta\varepsilon_{\mathrm{m}}$, $\mathbf{Y}$, $\Delta\mathbf{E}^p$, and $\Delta\mu$