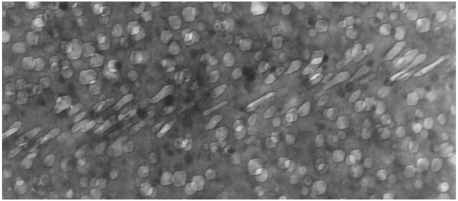
Coalescence criteria for porous materials with small-scale voids



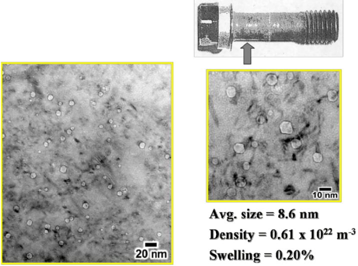
Jérémy HURE[1], Valentin GALLICAN[1], Kim Lau NIELSEN[2]

[1]Department of Materials for Nuclear Applications
French Alternative Energies and Atomic Energy Commission

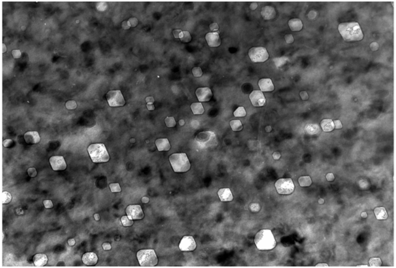
[2]Department of Mechanical Engineering - Section of Solid Mechanics
Technical University of Denmark (DTU)

16th European Mechanics of Materials Conference
Nantes, March 26th-28th, 2018

From the Nuclear Industry: **Irradiated materials**



PWR, (Edwards *et al.*, 2003)



Fast reactor, (Garner *et al.*, 2002)

Austenitic stainless steels irradiated by **high-energy particles**:

- Creation of **crystalline defects** in the microstructure
- Under specific conditions: **Nanovoids** (5nm $\lesssim R \lesssim$ 100nm)

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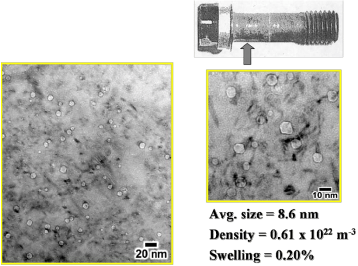

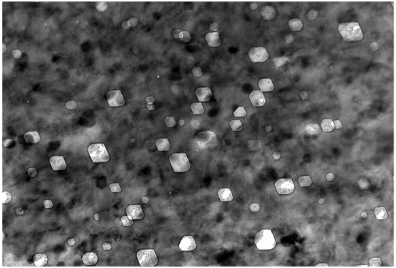

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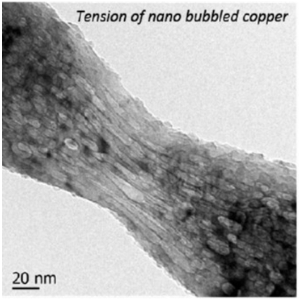
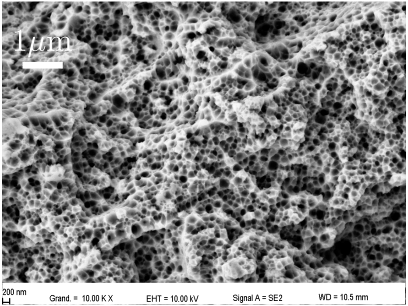
The material becomes nanoporous: Behavior under stress ?

From the Nuclear Industry: **Irradiated materials**



(Ding *et al.*, 2016)



(CEA - DMN/SEMI/LM2E Microscopy team)

Nanovoids are observed to contribute to the fracture of the material through **classical mechanisms of ductile fracture:**

- Void growth to coalescence
- *Small* dimples on fracture surfaces

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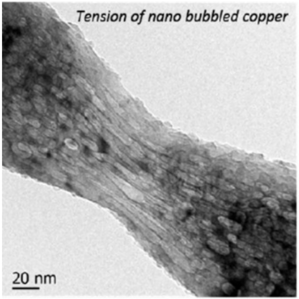

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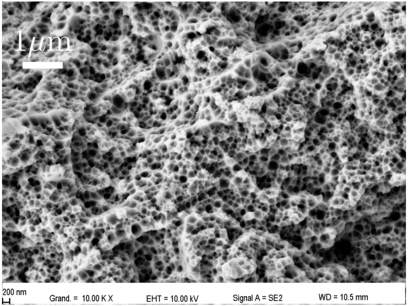

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Towards homogenized models of nanoporous materials

Some **porous unit-cell** simulations accounting for **void size effects**

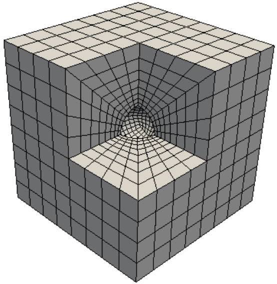
With interface stresses
(Dormieux & Kondo, 2010)

Void/Matrix interface ⇒ 2D plasticity

$$\frac{3}{2}\boldsymbol{\sigma}_D^{2D} : \boldsymbol{\sigma}_D^{2D} \leq \gamma^2$$

with 2D yield stress γ.

Lengthscale: $l = \dfrac{\gamma}{\sigma_0} \Rightarrow \Gamma = \dfrac{\gamma}{\sigma_0 R}$



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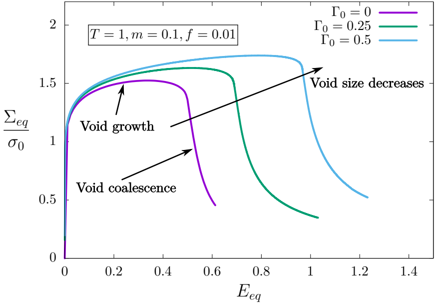
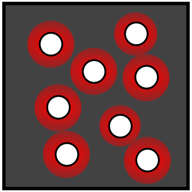
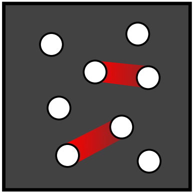


(Scherer *et al.*)



Growth regime
Diffuse plastic flow



Coalescence regime
Localized plastic flow

Some **porous unit-cell** simulations accounting for **void size effects**

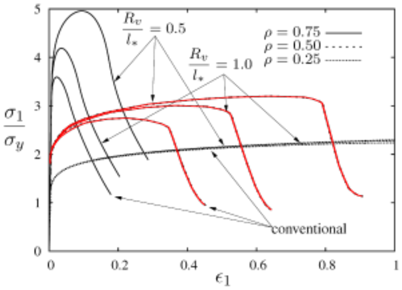
With strain-gradient plasticity (*e.g.*, Fleck & Hutchinson, 2001)

Hardening due to strain-gradient

$$\dot{E}_p^2 = \dot{\varepsilon}_p^2 + l^2 \dot{\varepsilon}_{p,i}\dot{\varepsilon}_{p,i}$$

Lengthscale l related to the presence of GND's.

$$\Upsilon = \frac{l}{R}$$



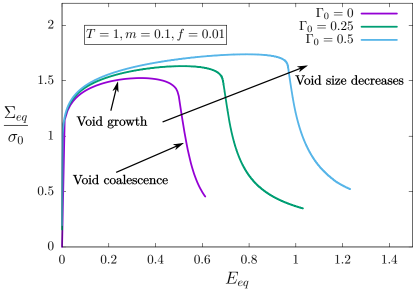
(Niordson, 2008)

For both models: qualitatively similar observations ...

- Hardening
- Delayed softening

... as **void size decreases** down to the characteristic lengthscale.

Some **porous unit-cell** simulations accounting for **void size effects**



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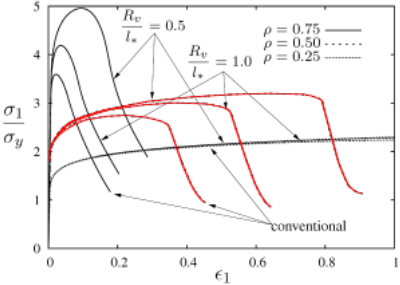

(Niordson, 2008)

Analytical homogeneized yield criteria for porous materials with **size effects**, under the assumption of isotropy:

- **Growth regime**: (Wen *et al.*, 2005), (Monchiet & Bonnet, 2013), (Dormieux & Kondo, 2010), (Monchiet & Kondo, 2013), ...

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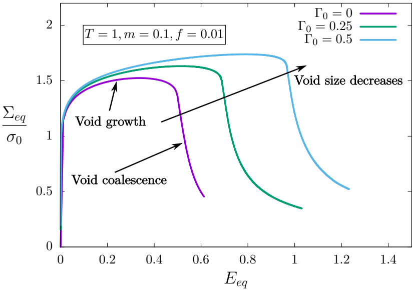

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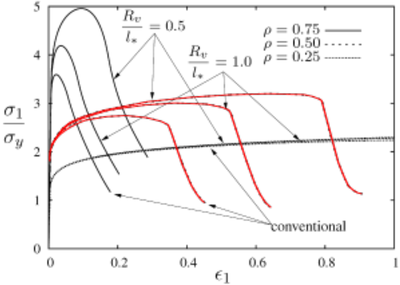

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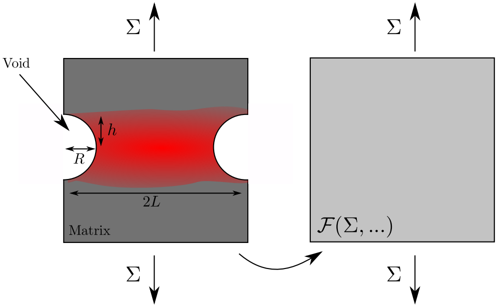
Coalescence yield criteria showing size effects are needed

Yield criterion **in the coalescence regime** for nanoporous material

- Relevant for large porosity: localization of plastic flow between voids



Key parameters:

Void aspect ratio:
$$W = \frac{h}{R}$$

Ligament length:
$$\chi = \frac{R}{L}$$

Thomason analysis (1985) to be re-done accounting for:

- Interface stresses
- Strain-gradient plasticity

Main assumption: Periodic arrangement of voids

Yield criterion for nanoporous material $\boxed{\mathcal{F}(\mathbf{\Sigma}, ...)}$

Homogenisation and limit analysis (Rigid-non hardening solid)

- RVE homogenisation with appropriate boundary conditions

$$\mathbf{\Sigma} = \frac{1}{vol\Omega} \int_{\Omega} \boldsymbol{\sigma} \, d\Omega \qquad \mathbf{D} = \frac{1}{vol\Omega} \int_{\Omega} \mathbf{d} \, d\Omega$$

- Limit analysis (Dormieux & Kondo, 2010)

$$\mathbf{\Sigma} : \mathbf{D} \leq \Pi(\mathbf{D}) = \inf_{\underline{v} \in \kappa(\mathbf{D})} \frac{1}{vol(\Omega)} \left[\int_{\Omega_m} \sigma_0 d_{eq}^{VM} \, dV + \int_{S_{int}} \gamma d_{S,eq}^{VM} \, dS \right]$$

where $\kappa(\mathbf{D})$ is a subset of velocity field compatible with $\mathbf{D}$ and verifying the property of incompressibility

- Effective yield criterion for porous RVE

$$\mathbf{\Sigma} = \frac{\partial \Pi(\mathbf{D})}{\partial \mathbf{D}}$$

This theoretical approach stands on the ***choice*** of a ***trial velocity field*** $\underline{v}$

Yield criterion **in the coalescence regime** for nanoporous material

$$\boxed{\mathcal{F}(\boldsymbol{\Sigma}, \sigma_0, \gamma, ...)} \text{ or } \boxed{\Sigma_{33} = \mathcal{G}(\sigma_0, \gamma, ...)}$$

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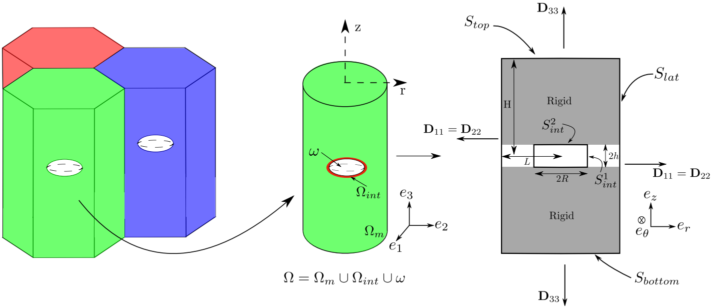
Geometry and boundary conditions

- Cylindrical void in cylindrical unit-cell
- Axisymmetric loading conditions



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Constitutive equations: Rigid / Perfect plasticity

- Matrix: Isotropic von Mises criterion (3D yield stress σ_0)

$$\frac{3}{2}\boldsymbol{\sigma}_D : \boldsymbol{\sigma}_D \leq \sigma_0^2$$

- Void/Matrix interface: Isotropic von Mises criterion (2D yield stress γ)

$$\frac{3}{2}\boldsymbol{\sigma}_D^{2D} : \boldsymbol{\sigma}_D^{2D} \leq \gamma^2$$

Homogenisation and limit analysis

$$\Pi(\mathbf{D}) = \inf_{\underline{v} \in \kappa(\mathbf{D})} \frac{1}{vol(\Omega)} \left[\int_{\Omega_m} \sigma_0 d_{eq}^{VM} \, dV + \int_{S_{int}} \gamma d_{S,eq}^{VM} \, dS \right]$$

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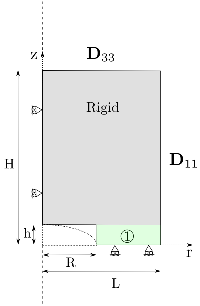
Trial velocity field kinematically admissible, incompressible

- Proposed by (Keralavarma & Chockalingham, 2016):

$$\begin{cases} v_r^{KC}(r,z) = \dfrac{3HD_{33}}{4h}\left(1 - \dfrac{z^2}{h^2}\right)\left(\dfrac{L^2}{r} - r\right) \\ v_z^{KC}(r,z) = \dfrac{3HD_{33}}{2h}\left(z - \dfrac{z^3}{3h^2}\right) \end{cases}$$



- Other trial velocity fields are possible (see (Morin *et al.*, 2015))

Yield criterion **in the coalescence regime** for nanoporous material

$$\boxed{\mathcal{F}(\mathbf{\Sigma}, \sigma_0, \gamma, ...)} \text{ or } \boxed{\Sigma_{33} = \mathcal{G}(\sigma_0, \gamma, ...)}$$

Estimation of the coalescence stress (isotropic, axisymmetric loading):

$$\left(\frac{\Sigma_{33}}{\sigma_0}\right)_c = \sqrt{\frac{6}{5}}\left[b \ln\frac{1}{\chi^2} + \sqrt{b^2+1} - \sqrt{b^2+\chi^4} + b\ln\left(\frac{b+\sqrt{b^2+\chi^4}}{b+\sqrt{b^2+1}}\right)\right] + \frac{2\Gamma}{\sqrt{3}}\sqrt{1+3\chi^4}$$

$$\text{with } b^2 = \frac{1}{3} + \alpha\frac{1}{3}\frac{5}{8W^2\chi^2},\ \alpha = [1+\chi^2-5\chi^4+3\chi^6]/12.$$

Can be extended to account for **anisotropy and shear**:

$\Rightarrow$ see (Gallican & Hure, 2017)

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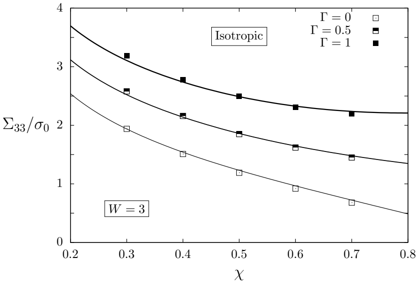
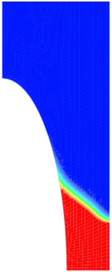
How good is this analytical coalescence criterion ?:
⇒ Comparison to **Numerical limit-analysis**

Yield criterion **in the coalescence regime** for nanoporous material

$$\boxed{\mathcal{F}(\boldsymbol{\Sigma}, \sigma_0, \gamma, ...)} \text{ or } \boxed{\Sigma_{33} = \mathcal{G}(\sigma_0, \gamma, ...)}$$

- **Numerical limit-analysis simulations**: Standard finite element simulations, coalescence boundary conditions, no geometry update, perfectly plastic von Mises matrix and interface





$$\Sigma = \frac{1}{vol\Omega} \int_{\Omega} \sigma \, d\Omega$$

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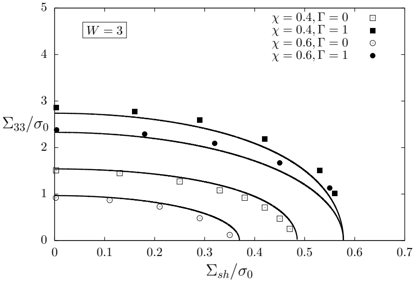

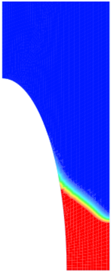

$$\Sigma = \frac{1}{vol\Omega} \int_{\Omega} \sigma \, d\Omega$$

☑ for elongated spheroidal voids $W \gg 1$

☑ for spherical voids $W \sim 1$ with additional fitting parameter

Yield criterion for porous strain-gradient material $\boxed{\mathcal{F}(\mathbf{\Sigma}, ...) = 0}$

Similar framework as for the case of interface stresse

- **Fleck & Willis** version of strain gradient plasticity

$$\dot{E}_p^2 = \dot{\varepsilon}_p^2 + L_D^2 \dot{\varepsilon}_{ij,k}^2 \dot{\varepsilon}_{ij,k}^2$$

- **Extension** of Hill-Mandel lemma (Azizi *et al.*, 2014):

$$\mathbf{\Sigma} : \mathbf{D} = \frac{1}{vol\Omega} \int_{\partial\Omega} [T_i v_i + t_{ij} d_{ij}] dS$$

  for periodic boundary conditions

- **Extension** of Limit analysis theorem (Fleck & Willis, 2009)

$$\mathbf{\Sigma} : \mathbf{D} = \inf_{\underline{v} \in \kappa(\mathbf{D})} \frac{1}{vol(\Omega)} \int_{\Omega} \sigma_0 \sqrt{\frac{2}{3} d_{ij} d_{ij} + L_D^2 d_{ij,k} d_{ij,k}}\, dV$$

where $\kappa(\mathbf{D})$ is a subset of velocity field compatible with $\mathbf{D}$ and verifying the property of incompressibility

Yield criterion **in the coalescence regime** for porous strain-gradient material

$$\boxed{\mathcal{F}(\boldsymbol{\Sigma}, \sigma_0, \gamma, ...)} \quad \text{or} \quad \boxed{\Sigma_{33} = \mathcal{G}(\sigma_0, \gamma, ...)}$$

Trial velocity field (Morin *et al.*, 2015)

$$\begin{cases} v_r^M(r,z) = \dfrac{HD_{33}}{h^2}(h-z)\left(\dfrac{L^2}{r} - r\right) \\ v_z^M(r,z) = \dfrac{HD_{33}}{h^2}(2hz - z^2) \end{cases}$$

Estimation of the coalescence stress (isotropic, axisymmetric loading):

$$\left(\frac{\Sigma_{33}}{\sigma_0}\right)_c = \frac{2}{W^2\chi^2}\int_0^{W\chi} dz \int_\chi^1 \sqrt{\alpha(r,z) + L_D^2 \beta(r,z)}\, r dr$$

with $$\alpha(r,z) = \frac{4}{3}(W\chi - z)^2\left(\frac{1}{r^4} + 3\right) + \frac{1}{3}\left(\frac{1}{r} - r\right)^2$$

and $$\beta(r,z) = \frac{16}{r^6}(W\chi - z)^2 + \frac{3}{r^4} + 7$$

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How good is this analytical coalescence criterion ?:

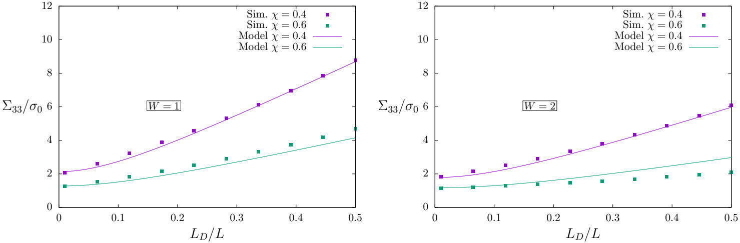
$\Rightarrow$ Comparison to **Numerical limit-analysis**

Yield criterion **in the coalescence regime** for nanoporous material

$$\boxed{\mathcal{F}(\mathbf{\Sigma}, \sigma_0, \gamma, \ldots)} \text{ or } \boxed{\Sigma_{33} = \mathcal{G}(\sigma_0, \gamma, \ldots)}$$

Numerical limit-analysis simulations:

- Cubic-unit cell with pediodic boundary conditions
- Coalescence boundary conditions
- Fleck-Willis strain-gradient material without hardening
- Coalescence boundary conditions



The model **captures well** the increase of coalescence stress as L_D increases

- One parameter needed to account for unit-cell shapes (cylindrical *vs.* cubic)

Accounting for interface stresses:

$$\left(\frac{\Sigma_{33}}{\sigma_0}\right)_c = \sqrt{\frac{6}{5}}\left[b\ln\frac{1}{\chi^2} + \sqrt{b^2+1} - \sqrt{b^2+\chi^4} + b\ln\left(\frac{b+\sqrt{b^2+\chi^4}}{b+\sqrt{b^2+1}}\right)\right]$$
$$+\frac{2\Gamma}{\sqrt{3}}\sqrt{1+3\chi^4}$$

Accounting for strain-gradient plasticity (Fleck-Willis):

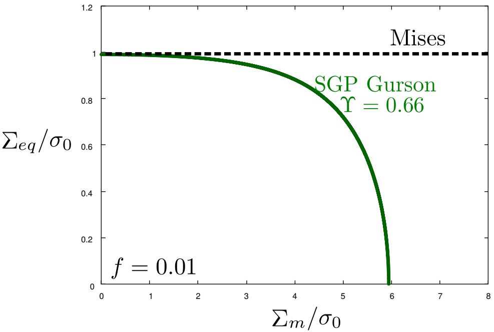
$$\left(\frac{\Sigma_{33}}{\sigma_0}\right)_c = \frac{2}{W^2\chi^2}\int_0^{W\chi} dz \int_\chi^1 \sqrt{\alpha(r,z) + L_D^2\beta(r,z)}\, r\,dr$$

From coalescence criterion to yield criterion in the coalescence regime (axisymmetric loading conditions)

$$\mathcal{F}(\boldsymbol{\Sigma}) = \frac{\Sigma_{eq}}{\sigma_0} + \frac{3}{2}\frac{\Sigma_m}{\sigma_0} - \frac{3}{2}\left(\frac{\Sigma_{33}}{\sigma_0}\right)_c \leq 0$$

A hybrid yield criterion for porous material exhibiting size effects:

- Growth criterion $\mathcal{F}_g(\mathbf{\Sigma}, \boldsymbol{\alpha}, \Gamma) \leq 0$



A hybrid yield criterion for porous material exhibiting size effects:

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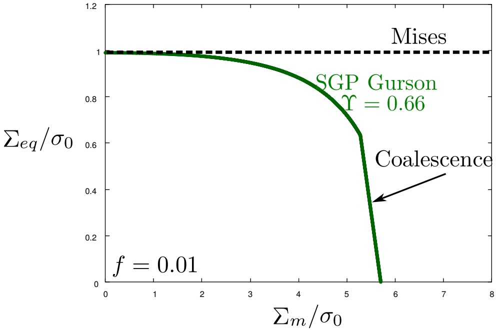
- Coalescence criterion $\mathcal{F}_c(\mathbf{\Sigma}, \boldsymbol{\alpha}, \Gamma) \leq 0$

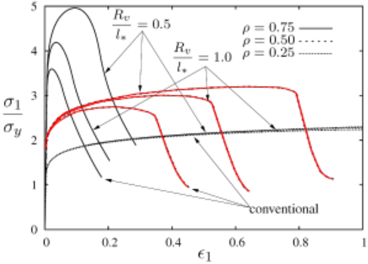


Complete homogenized model:

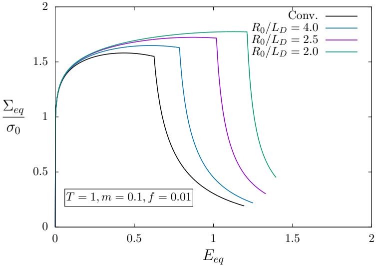
- Adding evolution laws
- Numerical implementation of constitutive equations

Numerical implementation of the constitutive equations:

- Strain-gradient plasticity: qualitative agreement to be further validated



(Niordson, 2008)



Hardening and delayed softening observed as R/L_D decreases

- Interface stresses: **Talk of J.M. Scherer)**