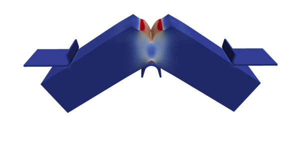
Extension of the StandardElastoViscoPlasticity brick to porous materials



DE LA RECHERCHE À L'INDUSTRIE

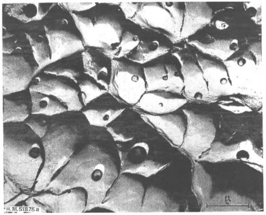
MFront User Meeting

25/11/2020

M. Shokeir, J. Hure, T. Helfer

Micromechanical modelling of ductile failure

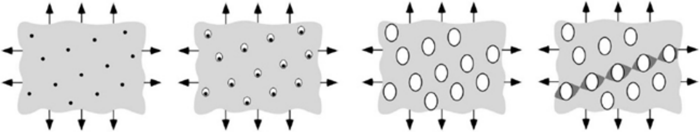
Observation of **fracture surfaces** of metal alloys



(Plateau et al., 1957)

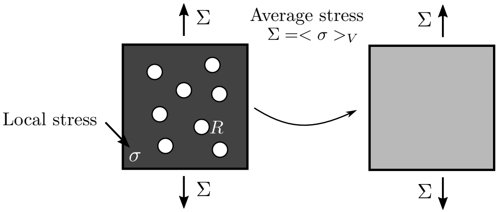
- Highly deformed material
- Presence of dimples
- Inclusions / Precipitates

Nucleation, growth and coalescence of internal voids fracture mechanism



(Anderson, 2005)

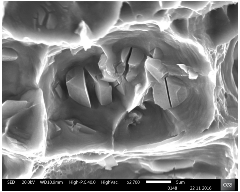
Simulation of ductile fracture requires **modelling of porous materials**



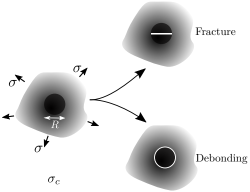
Homogenization leading to an **additional state variable** $f = \dfrac{V_{\text{void}}}{V_{\text{tot}}}$

- **Yield criterion / Flow rule** accounting for the porosity f
- **Evolution law** for the porosity f

Voids appear mostly through **inclusions fracture / debonding**



(Petit et al.)

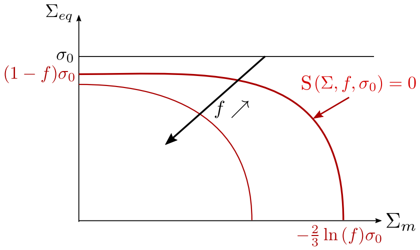


Typical evolution laws used to account for void nucleation $\dot{f} = A_n \dot{p}$

- (Chu & Needleman, 1980) $A_n = \dfrac{f_N}{s_N\sqrt{2\pi}} \exp\left(-\dfrac{1}{2}\left(\dfrac{p-\epsilon_N}{s_N}\right)^2\right)$
- Metallurgy-based $A_n = f_N \left\langle \dfrac{p}{\epsilon_N} - 1 \right\rangle^m$ if $\int A_n dp \leq f_{\mathrm{nuc}}^{max}$

Extension of von Mises yield criterion **to account for porosity**

- (Gurson, 1977) $\mathcal{S}(\underline{\Sigma}, f, \sigma_0) = \left(\frac{\Sigma_{eq}}{\sigma_0}\right)^2 + 2f\cosh\left(\frac{3}{2}\frac{\Sigma_m}{\sigma_0}\right) - 1 - f^2$



von Mises plasticity for $f = 0$

$$\mathcal{S}(\underline{\Sigma}, f, \sigma_0) = \left(\frac{\Sigma_{eq}}{\sigma_0}\right)^2 - 1$$

Mean stress dependence ($f \neq 0$)

$$\Sigma_m = \mathrm{tr}(\underline{\Sigma})/3$$

Plastic flow through normality rule $\qquad \underline{\dot{\epsilon}}_p = \dot{\lambda}\frac{\partial \mathcal{S}}{\partial \underline{\Sigma}}$

Porosity evolution through volume conservation $\qquad \dot{f} = (1-f)\mathrm{tr}\left(\underline{\dot{\epsilon}}_p\right)$

Homogenization of the strain hardening of porous materials

- Yield criterion $\mathcal{S}(\underline{\Sigma}, f)$ **as a definition** of the local yield stress $\sigma_\star$

$$\sigma_\star \quad \text{such that} \quad \mathcal{S}(\underline{\Sigma}, f, \sigma_\star) = 0$$

- **Energy balance** for the evolution of the **average plastic strain** p

$$\underline{\Sigma} : \underline{\dot{\varepsilon}}^{\mathrm{p}} = (1 - f) R(p) \dot{p}$$

- Generic **yield criterion** and associated **flow rule**

$$\mathcal{F}(\underline{\Sigma}, f) = \sigma_\star - R(p)$$

$$\underline{\dot{\varepsilon}}^{\mathrm{p}} = \dot{\lambda} \frac{\partial \mathcal{F}}{\partial \underline{\Sigma}} = \dot{\lambda} \frac{\partial \sigma_\star}{\partial \underline{\Sigma}} = (1 - f) \dot{p} \frac{\partial \sigma_\star}{\partial \underline{\Sigma}}$$

Generic constitutive equations for porous materials

- Additional state variables : **Porosity** f and **Average plastic strain** p
- **Definition** of an equivalent stress $\sigma_\star$, *i.e.* :
  - GTN : $\mathcal{S} = \left(\dfrac{\sigma_{eq}}{\sigma_\star}\right)^2 + 2q_1 f_\star \cosh\left(\dfrac{3}{2}q_2\dfrac{\sigma_m}{\sigma_\star}\right) - 1 - q_3 f_\star^2$
  - Rousselier-Tanguy-Besson : $\mathcal{S} = \dfrac{\sigma_{eq}}{(1-f)\sigma_\star} + \dfrac{2}{3} f D_R \exp\left(\dfrac{3}{2}q_R\dfrac{\sigma_m}{(1-f)\sigma_\star}\right) - 1$
- **Set of constitutive equations** to be solved

$$
\left\{
\begin{aligned}
\underline{\dot{\varepsilon}}^{\mathrm{el}} + \underline{\dot{\varepsilon}}^{\mathrm{p}} - \underline{\dot{\varepsilon}}^{\mathrm{to}} &= 0 \\
\sigma_\star - R(p) &= 0 \\
\dot{f} - (1-f)\,\mathrm{tr}\left(\underline{\dot{\varepsilon}}^{\mathrm{p}}\right) - \sum_j A_n^j \dot{p} &= 0
\end{aligned}
\right.
$$

Behaviour integration

- Implicit schemes turn an ordinary system of differential equations into a system of non linear equations.
- The unknowns are the increments of the integration variables :

$$\Delta\underline{\varepsilon}^{\mathrm{el}}, \Delta\, p, \Delta\, f$$

- The implicit system deduced from the constitutive equations is :

$$\begin{cases} f_{\underline{\varepsilon}^{\mathrm{el}}} = \Delta\,\underline{\varepsilon}^{\mathrm{el}} + \Delta\, p\, \underline{n}\big|_{t+\theta\,\Delta\,t} - \Delta\,\underline{\varepsilon}^{\mathrm{to}} & = 0 \\ f_p = \sigma_\star\big|_{t+\theta\,\Delta\,t} - R(p\big|_{t+\theta\,\Delta\,t}) & = 0 \\ f_f = \Delta f - (1 - f\big|_{t+\theta\,\Delta\,t})\,\Delta\, p\,\mathrm{tr}\left(\underline{n}\big|_{t+\theta\,\Delta\,t}\right) - \sum_j A_n^j\Big|_{t+\theta\,\Delta\,t}\Delta\, p & = 0 \end{cases}$$

where $\underline{n}\big|_{t+\theta\,\Delta\,t} = \dfrac{\partial\,\sigma_\star\big|_{t+\theta\,\Delta\,t}}{\partial\,\underline{\Sigma}\big|_{t+\theta\,\Delta\,t}}$, $p\big|_{t+\theta\,\Delta\,t} = p\big|_t + \theta\,\Delta\, p$, etc. and $\theta \in [0, 1]$

- This system is solved by a standard Newton-Raphson algorithm.

- Phenomenological nucleation laws with intrinsic bounds :

$$\dot{f}^{n} = A_n\,\dot{p} \quad \text{with} \quad A_n = f_N \left\langle \frac{\sigma_I}{\sigma_N} - 1 \right\rangle^{m} \quad \text{if} \quad \int A_n dp \leq f^{max}_{\mathrm{nuc}}$$

$A_n(\underline{\sigma})$ is continuous, $\dfrac{\mathrm{d}A_n}{\mathrm{d}\underline{\sigma}}$ is not

- Phenomenological coalescence laws :

$$f_{\star} = \begin{cases} \delta f & \text{if } f < f_c \\ f_c + \delta(f - f_c) & \text{otherwise} \end{cases} \quad \text{and} \quad \delta = \begin{cases} 1 & \text{if } f < f_c \\ \dfrac{\dfrac{1}{q_1} - f_c}{f_r - f_c} & \text{otherwise} \end{cases}$$

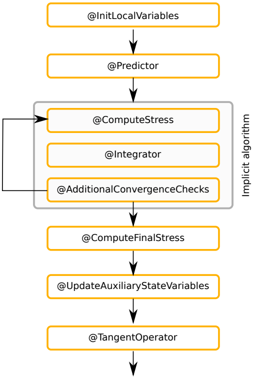
$f_{\star}$ is continuous, $\dfrac{\mathrm{d}f_{\star}}{\mathrm{d}f}$ is not

- Failure detection : $f \rightarrow f_r$
- Collapse of the yield surface

- **Main idea** : if the porosity is fixed, implicit equations $f_{\underline{\varepsilon}^{\mathrm{el}}}$ and f_p are much more easier to solve.
- Previous implementations used an **explicit** evolution of the porosity.
- The proposed scheme is based on an accelerated fixed point iterations around the porosity :

$$\Delta f^{(i_f+1)} = \left(1 - f|_t - \theta\,\Delta f^{(i_f)}\right)\Delta p^{(i_f)}\mathrm{tr}\left(\underline{n}|_{t+\theta\,\Delta\,t}{}^{(i_f)}\right) + \sum_j A_n^j\Big|_{t+\theta\,\Delta\,t}^{(i_f)}\Delta p^{(i_f)}$$

  where i_f is the iteration counter of the fixed point algorithm.
- The update formula can be easily adapted to take into account bounds in nucleations laws, failure detection, etc...
- Each time the porosity is updated, the implicit scheme is restarted using the solutions $\Delta\,\underline{\varepsilon}^{\mathrm{el}\,(i_f)}$, $\Delta\,p^{(i_f)}$ of the previous fixed point iteration.
- The Aitken acceleration scheme is used.



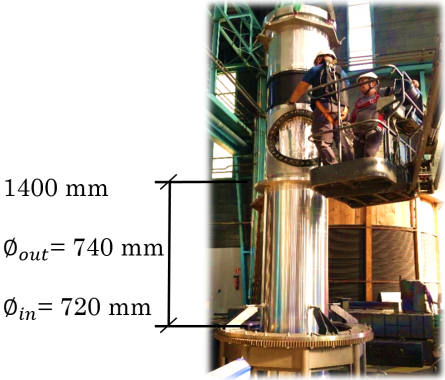
- Convergence of the fixed point algorithm and (accelerated) update of the porosity is performed in the `@AdditionalConvergenceChecks` code block once $\Delta\,\underline{\varepsilon}^{\mathrm{el}\,(i_f)}$, $\Delta\,p^{(i_f)}$ is found.
- The jacobian of the non standard implicit scheme leads to a secant tangent operator.
- The jacobian of the standard implicit scheme can be computed after the convergence of the explicit scheme to get the real consistent tangent operator.
- `http://tfel.sourceforge.net/implicit-dsl.html`

Integration in the `StandardElastoViscoPlastitity` brick

```
@Brick StandardElastoViscoPlasticity{
  stress_potential : "Hooke" {young_modulus : 70.e+03, poisson_ratio : 0.3},
  inelastic_flow : "Norton" {
    criterion : "GursonTvergaardNeedleman1982" {
      f_c : 0.04,    // coalescence porosity
      f_r : 0.056,   // fracture porosity
      q_1 : 2.,      // first Tvergaard parameter
      q_2 : 1.,      // second Tvergaard parameter
      q_3 : 4        // third Tvergaard parameter
    },
    n : 10.,
    K : 10.,
    A : 1.,
    isotropic_hardening : "Voce" {
      R0 : 2.43305029349e+02, Rinf : 328.5922898572, b : 1.74240092312e+01},
    isotropic_hardening : "Voce" {
      R0 : 0., Rinf : 1.74583430632e+01, b : 2.62113021495e+02}
  },
  porosity_evolution : {
    algorithm : "staggered_scheme" {
      convergence_criterion : 1.e−10,
      maximum_number_of_iterations : 1000},
    nucleation_model : "PowerLaw (stress)" {
      fn : 2.92, sn : 500, m : 2, fmax : 0.0215, pmin : 0.0321}
  }
};
```

Applications

PhD title : Modelling of the irradiation effects on fracture toughness of precipitation hardened aluminum alloys in the JHR Nuclear Research Reactor (NRR)



Why AA6061 ?

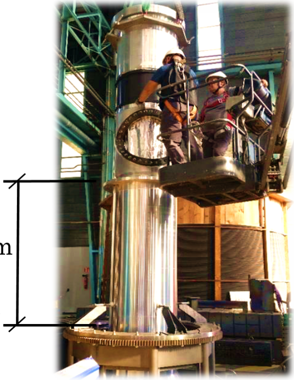
- Neutron transparency
- Corrosion resistance, Thermal conductivity
- Mechanical properties (35-70C)

PhD title : Modelling of the irradiation effects on fracture toughness of precipitation hardened aluminum alloys in the JHR Nuclear Research Reactor (NRR)

1400 mm

$\emptyset_{out}$= 740 mm

$\emptyset_{in}$= 720 mm



Why AA6061 ?

- Neutron transparency
- Corrosion resistance, Thermal conductivity
- Mechanical properties (35-70C)

Attention !

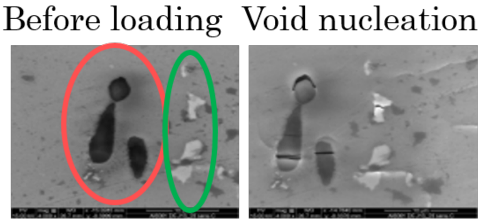
Neutron radiation alters the microstructure and deteriorates the ductility

Damage Mechanisms of AA6061

Mg	Si	Fe	Cu	Cr	Mn	Zn	Ti	Ni	Zr	Pb	Na	Al

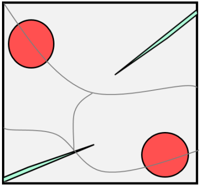
Precipitates

Size	Name	Morphology	Role
μm	Mg_2Si	Spherical	Pores
	Fe Intermetallics	Flakes	



(Shen12)

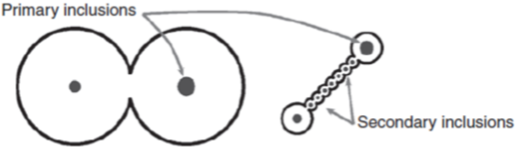
Microstructure



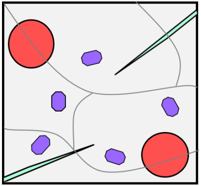
Mg	Si	Fe	Cu	Cr	Mn	Zn	Ti	Ni	Zr	Pb	Na	Al

Precipitates

Size	Name	Morphology	Role
μm	Mg_2Si	Spherical	Pores
	Fe Intermetallics	Flakes	
100 nm	$CrMn$	Octagonal	Smaller Pores



Microstructure

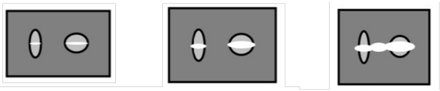


Plastic Flow

$$R_0 + Q_1\left(1 - e^{-b_1\,p}\right) + Q_2\left(1 - e^{-b_2\,p}\right)$$

Damage GTN Parameters (model 1)

Pre-existing Voids and Void Nucleation							Void Growth		Void Coalescence	
		Chu & Needl. nuc.		Power-Law nuc.						
f_0	f_{nuc}^{max}	ε_N	S_N	σ_N	p_N	f_N	q_1	q_2	f_c	f_r
%	%	%	%	MPa	%	%			%	%
0.35	2.15	10	10	500	3.21	2.92	2	1	4	5.6



Void nucleation

Void growth

Void coalescence

(ShenMorgeneyerGarnierAllaisHelfenCrepin13; PetitBessonRitterColasHelfenMorgeneyer19)

Power-Law Nucleation Stress Based

$$A_n = f_N \left\langle \frac{\sigma_I}{\sigma_N} - 1 \right\rangle^m \quad \text{if} \;\; \sigma_I \geq \sigma_N, \;\; p \geq p_N, \;\; \text{and} \;\; \int A_n dp \leq f_{\text{nuc}}^{max}$$

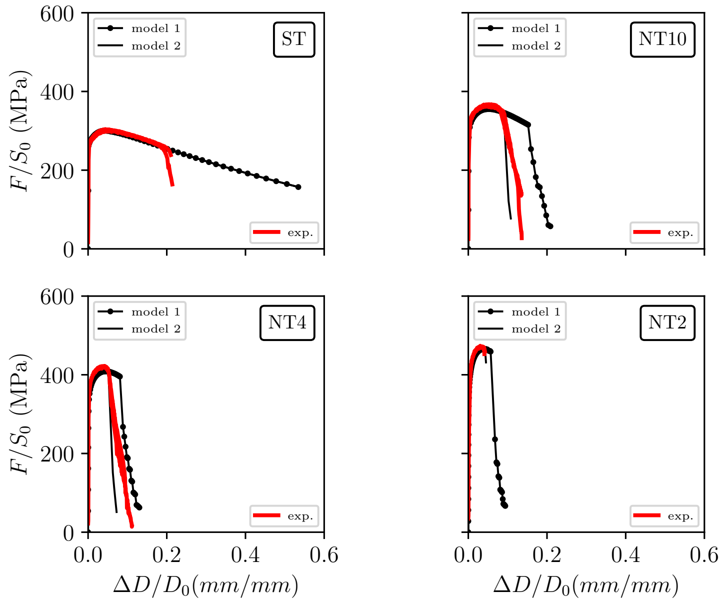
where $\{f_N, p_N, m, \sigma_N, f_{\text{nuc}}^{max}\}$ are material parameters, and σ_I is the maximum positive principal stress.

(**PetitBessonRitterColasHelfenMorgeneyer19**)

Damage GTN Parameters (model 1)

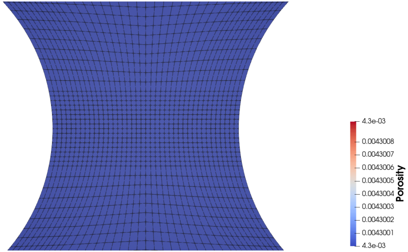
Pre-existing Voids and Void Nucleation							Void Growth		Void Coalescence	
f_0	f_{nuc}^{max}	Chu & Needl. nuc.		Power-Law nuc.			q_1	q_2	f_c	f_r
		ε_N	S_N	σ_N	p_N	f_N				
%	%	%	%	MPa	%	%			%	%
0.35	2.15	10	10	500	3.21	2.92	2	1	4	5.6

model 2 : f_c = 1% f_r = 3% q_1 = 3


600
400
200
0
F/S_0 (MPa)
model 1
model 2
ST
exp.
NT10
NT4
NT2
0.0
0.2
0.4
0.6
$\Delta D/D_0 (mm/mm)$

Porosity at GP

Average Porosity

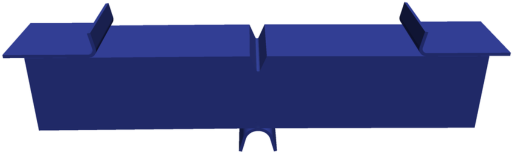


Conclusions

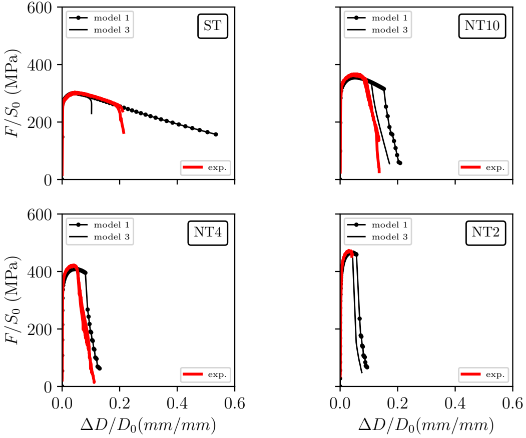
- In `TFEL/Math` :
  - A robust scalar Newton method with root-bracketing (bisection)
- In `TFEL/Material` :
  - 2 stress criteria : `Gurson-Tvergaard-Needleman` and `Rousselier-Tanguy-Besson`.
  - 4 nucleation laws : `Chu-Needleman` (stress and strain versions) and `Power-Law` (stress and strain versions).
- In `MFront` :
  - Extension of the `StandardElastoViscoPlasticity` brick to porous plasticity.
- Detailed documentation (under review).
- Tutorials :
  - http://tfel.sourceforge.net/ExtendingStandardElastoViscoPlasticityBrick--StressCriterion.html
  - http://tfel.sourceforge.net/ExtendingStandardElastoViscoPlasticityBrick--PorousStressCriterion.html

- Additional unit tests
- Better handling of almost hydrostatic loadings in the `Rousselier-Tanguy-Besson` stress criterion.
- Detailed performance comparisons between the standard implicit scheme and the proposed scheme.
- Extension of the `StandardElastoViscoPlasticityBrick` brick with new stress criteria :
  - Advanced GTN model : orthotropy, void shape, ...
  - Coalescence yield criteria : Thomason, ...
  - Easy coupling between void growth and void coalescence models

- Additional unit tests
- Better handling of almost hydrostatic loadings in the `Rousselier-Tanguy-Besson` stress criterion.
- Detailed performance comparisons between the standard implicit scheme and the proposed scheme.
- Extension of the `StandardElastoViscoPlasticityBrick` brick with new stress criteria :



- Extension of the `StandardElastoViscoPlasticityBrick` brick with new stress criteria :
  - Coalescence yield criteria : Thomason, ... (hereby "model 3")



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