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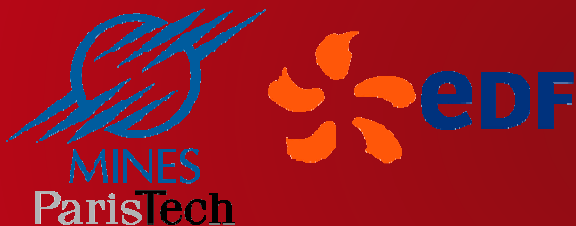
A reduced micromorphic single crystal plasticity model to study localization and void growth in ductile metals

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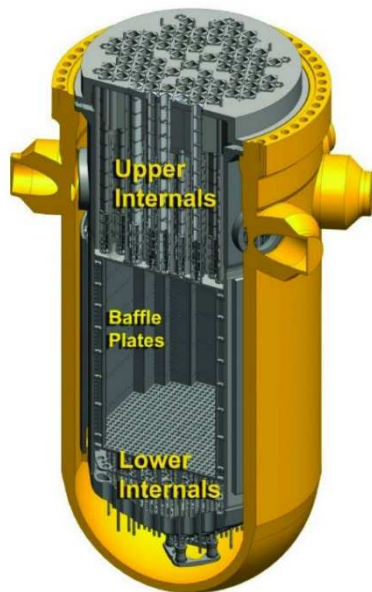
³EDF R&D les Renardières, France



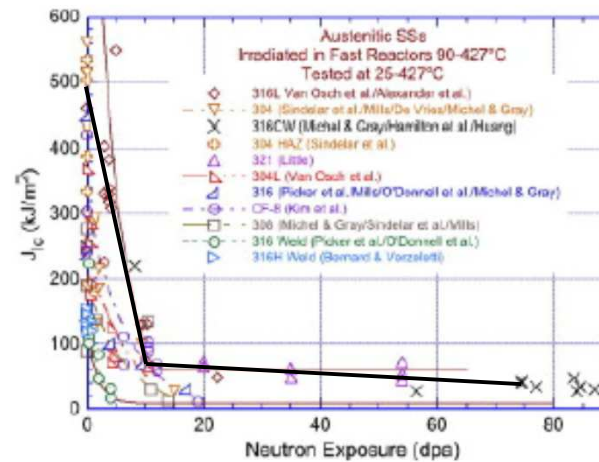
16th Edition of the European Mechanics of Material conference, Nantes,
France, March 26-28 2018

- ✓ Background: ductile fracture of irradiated stainless steels
- ✓ Void growth and coalescence study at micro-scale (conventional crystal plasticity)
- ✓ Enhanced crystal plasticity model to describe size effect
- ✓ Results on Void growth and coalescence study at micro-scale
- ✓ Conclusions and perspectives

PWR's internals structures made of austenitic stainless steel (300 series)



Fracture toughness

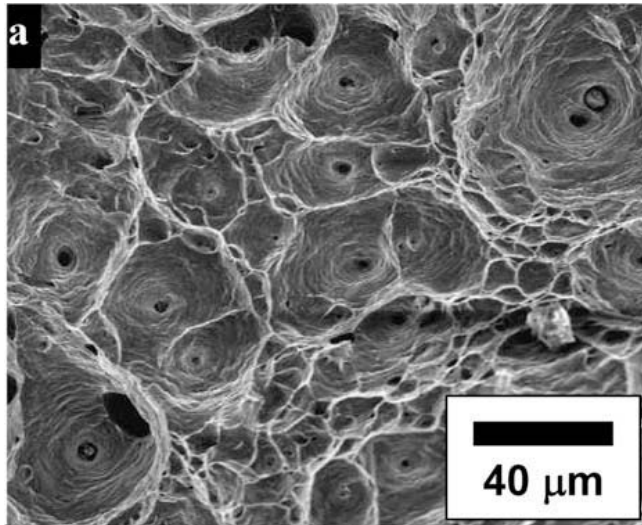


[Chopra & Rao (2011)]

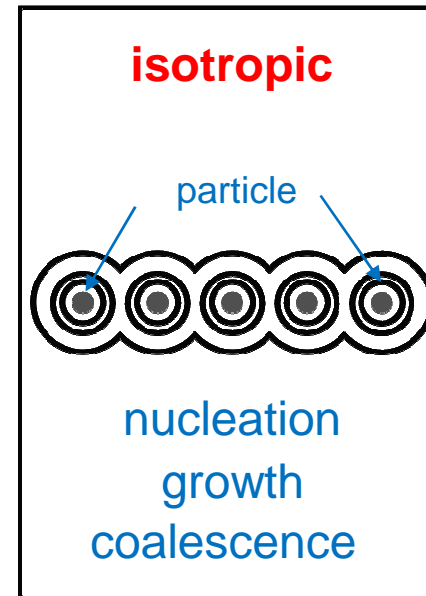
Strong decrease of fracture toughness with irradiation related (How?)
to evolution of mechanical properties (due to irradiation defects).

Physical mechanisms ?

[Das and Tarafder (2009)]



Dimples on fracture surface



Mechanism

[Pineau and Pardoën (2007),
Besson (2010),
Benzerga and Leblond (2010)]Pioneering modeling:

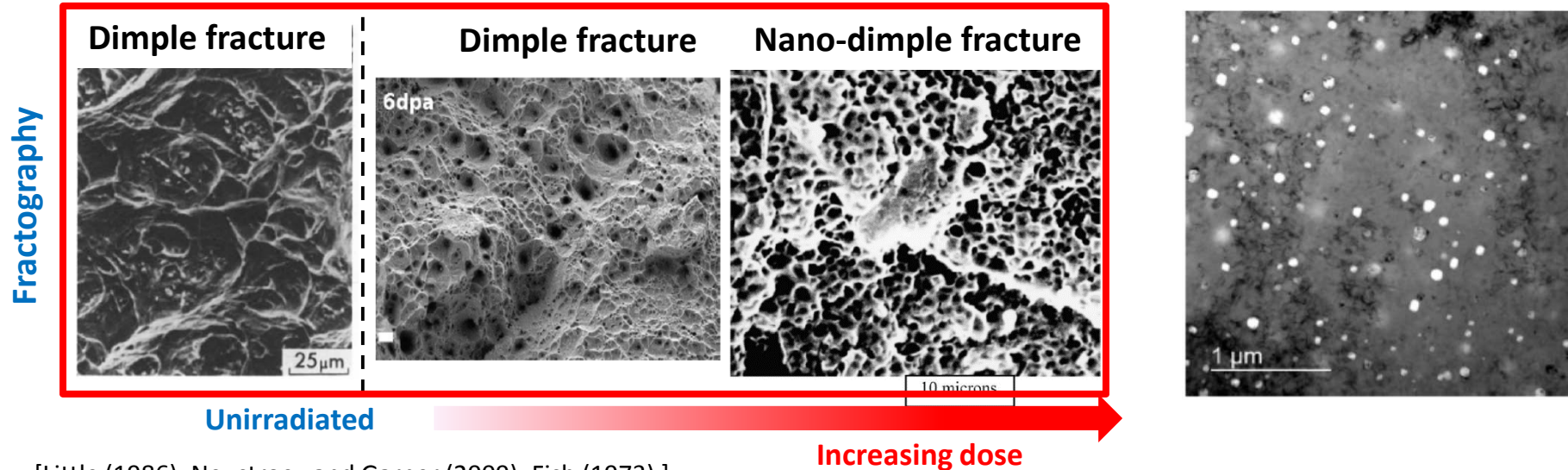
McClintock (1968), Rice and Tracey (1969)

Gurson (1977):

$$\frac{\sigma_{eq}^2}{\sigma_0^2} + 2f \cosh\left(\frac{3}{2} \frac{\sigma_m}{\sigma_0}\right) - 1 - f^2 = 0$$

Its extensions accounting for nucleation, coalescence, void shape, etc

Voids growth and coalescence at microscale on irradiated materials



Dimple-type Transgranular Fracture

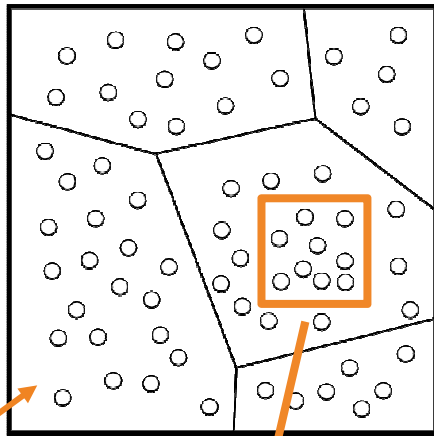
Some characteristics of the ductile fracture

- ❑ Intragranular voids
- ❑ Decreasing dimple size with irradiation
- ❑ Potential nano-dimple fracture at high irradiation levels



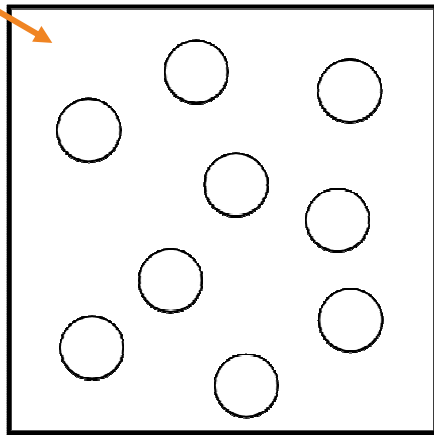
- ✓ Grain-scale modeling
- ✓ Nano-voids → size effects ?
- ✓ Experimental study : see Barrioz and al. (Monday, room KL, 11H30)
- ✓ Homogenized model : see Scherer and Hure (Wednesday, Audit 450,15h)

Polycrystal
with
intragranular
voids



hardening

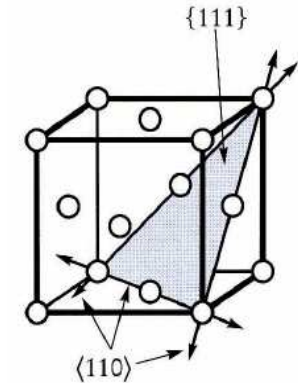
Voided
single crystal



➤ Crystal plasticity at finite strains

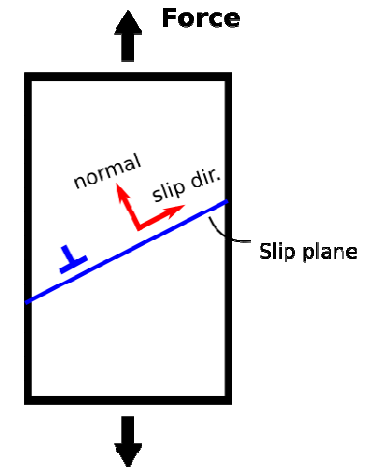
□ FCC crystal

- ✓ Plasticity: dislocation motion
- ✓ Slip planes $\{111\}$
- ✓ Slip directions $\langle \bar{1}10 \rangle$
- ✓ 12 slip systems
- ✓ Schmid tensor $\underline{N}^s = \underline{m}^s \otimes \underline{n}^s$



□ Schmid's law:

Plastic slip is initiated when the resolved shear stress τ^s on a slip plane reaches a critical value τ_c^s



✓ **Kinematics:**

Deformation gradient: $\tilde{\mathbf{F}} = \tilde{\mathbf{E}} \cdot \tilde{\mathbf{P}}$

✓ **Flow rule:**

Yield function: $\phi^s = \tau^{*s} - \tau_c^s \geq 0$

$$\tau^{*s} = |\tau^s| = |\tilde{\mathbf{M}} : \tilde{\mathbf{N}}^s| \quad \tilde{\mathbf{M}} = J_e \tilde{\mathbf{E}}^T \cdot \boldsymbol{\sigma} \cdot \tilde{\mathbf{E}}^{-T}$$

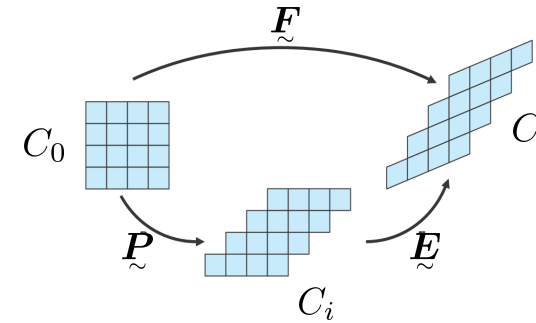
Plastic strain rate: $\dot{\tilde{\mathbf{P}}} \cdot \tilde{\mathbf{P}}^{-1} = \sum_{s=1}^{12} \dot{\gamma}^s \frac{\partial \phi^s}{\partial \tilde{\mathbf{M}}} = \sum_{s=1}^{12} \dot{\gamma}^s \text{sign}(\tau^s) \tilde{\mathbf{N}}^s$

Plastic slip rate: $\dot{\gamma}^s = \dot{\gamma}_{\text{ref}} \left\langle \frac{\phi^s}{\tau_{\text{ref}}} \right\rangle^n$

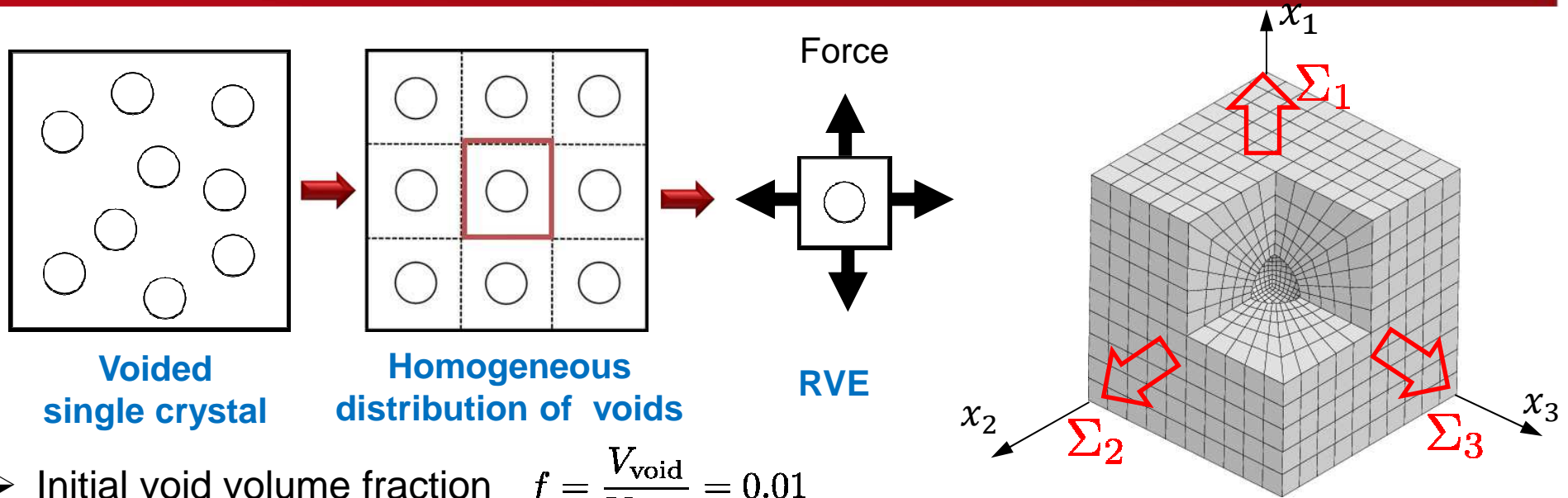
✓ **Hardening rule** $\tau_c^s = \tau_T^s + \mu b_D \sqrt{\sum_{u=1}^{12} a^{su} \rho_D^u}$ [Kubin (2008)]

✓ **Dislocation density** $\dot{\rho}_D^s = \frac{1}{b_D} \left(\frac{1}{L^s} - g_c \rho_D^s \right) \dot{\gamma}^s$ with $L^s = \kappa \left(\sum_{u=1}^{12} b^{su} \rho_D^u \right)^{-1/2}$

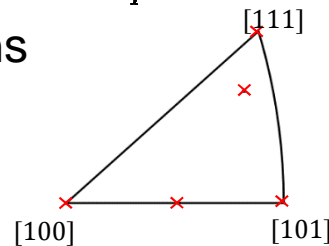
↙
↘
 Multiplication Annihilation



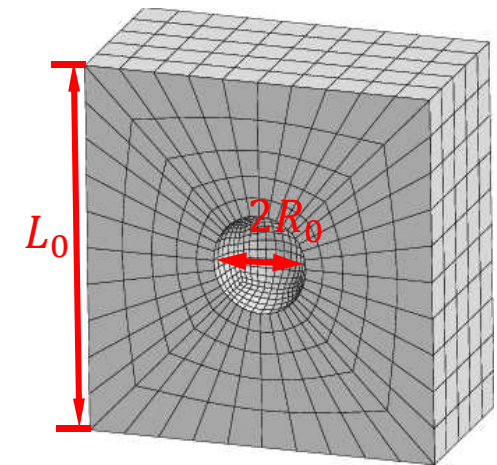
Study of growth and coalescence at microscale → FE Unit cell simulations: problem setup



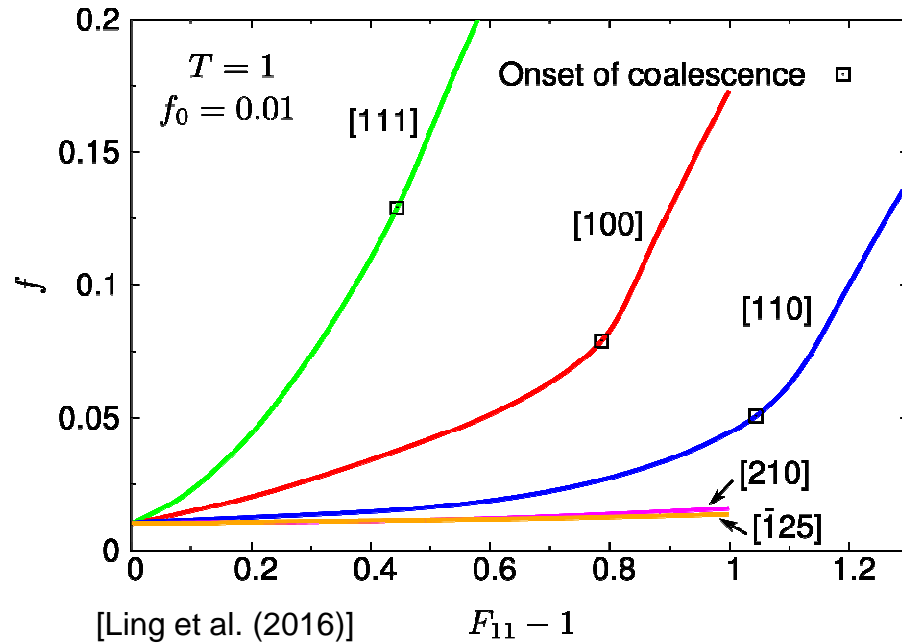
- Initial void volume fraction $f = \frac{V_{\text{void}}}{V_{\text{total}}} = 0.01$
- Periodic boundary conditions
- Axisymmetric loading $\Sigma_2 = \Sigma_3$
- Constant stress triaxiality $T = \frac{\Sigma_m}{\Sigma_{eq}} = 1 - 3$
- Different crystal orientations



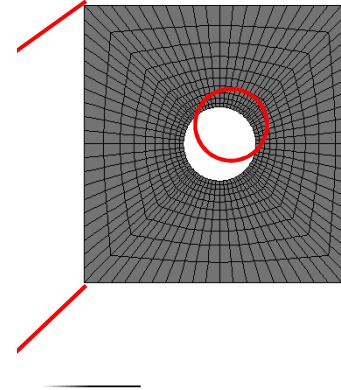
- $x_1 - x_2 - x_3$
- [100]-[010]-[001]
 - [110]-[1̄10]-[001]
 - [111]-[2̄11]-[01̄1]
 - [210]-[1̄120]-[001]
 - [1̄125]-[12̄1]-[210]



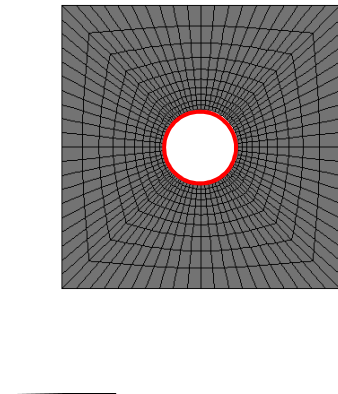
Study of growth and coalescence at microscale → Effect of crystal orientation



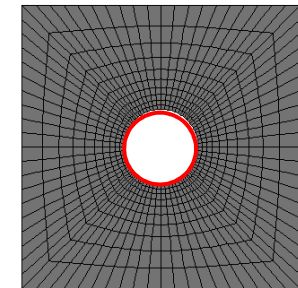
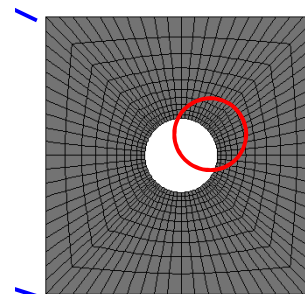
[100] $T = 1.0$



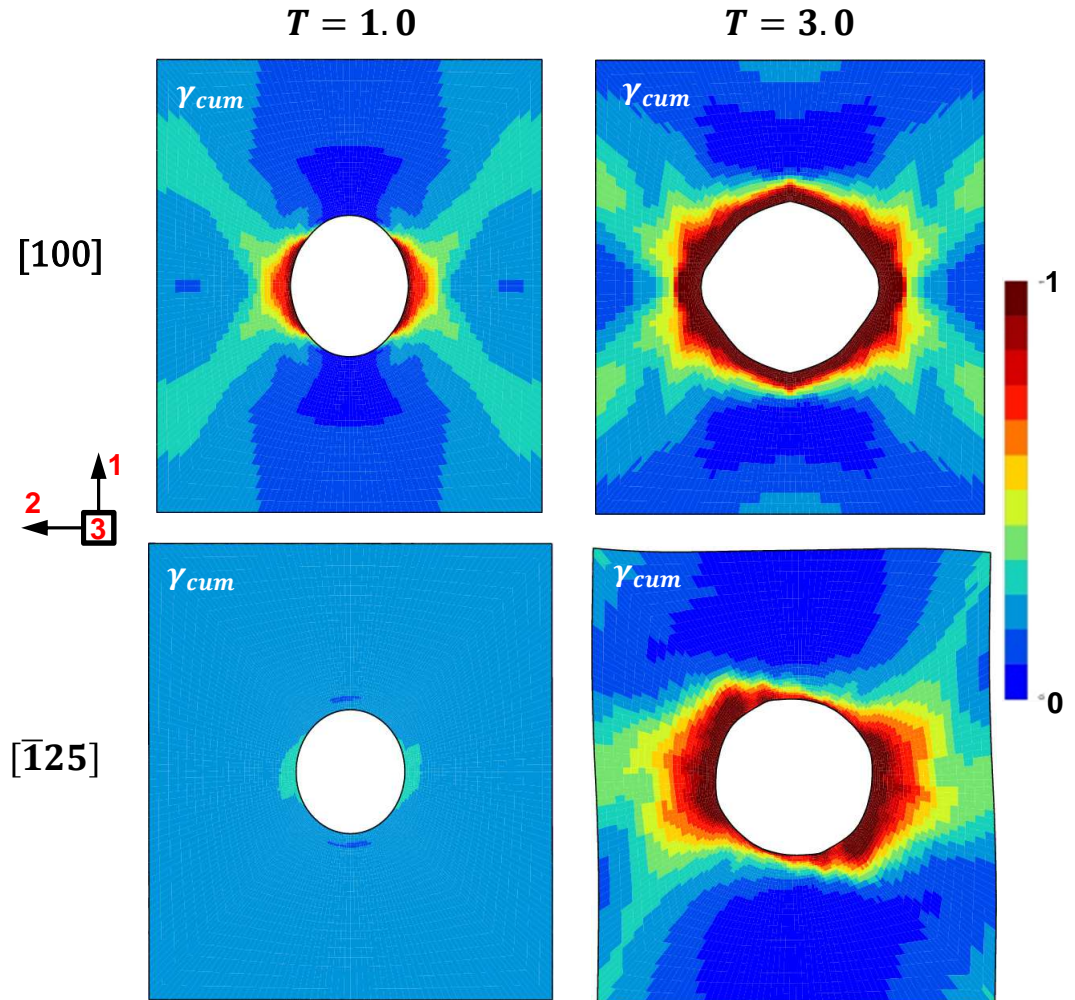
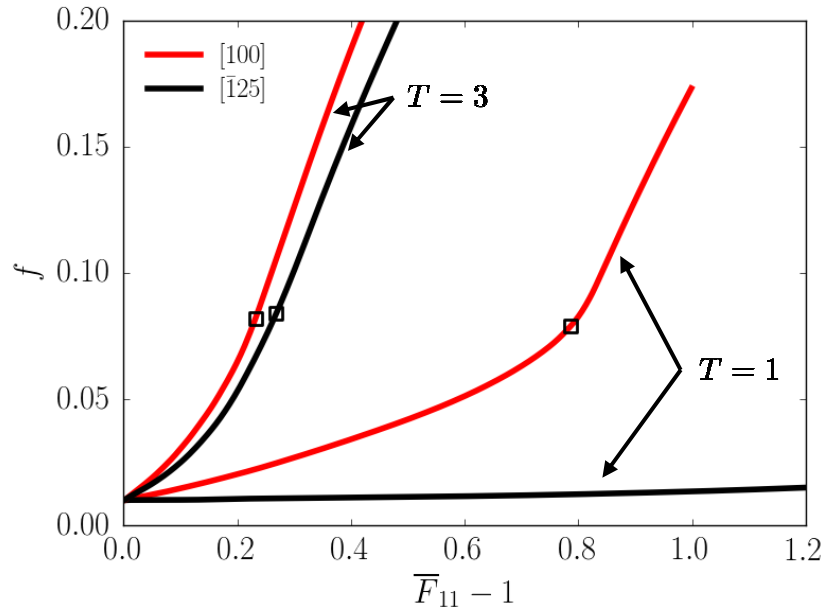
$[\bar{1}25]$ $T = 1.0$



- ✓ Effect of crystal orientation on the evolution of void shape
- ✓ Two stages: **growth** and **coalescence**
- ✓ Significant effect of the crystal orientation on void growth rate at $T=1$



Study of growth and coalescence at microscale → Effect of crystal orientation at different triaxialities

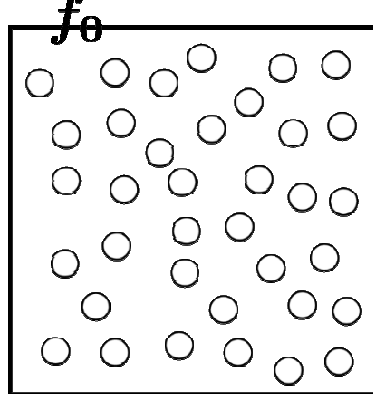
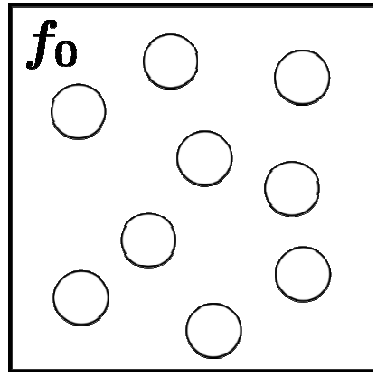


- ✓ Stronger effect of crystal orientation at $T=3$
- ✓ In agreement with Yerra et al. (2010) for BCC
- ✓ Why?

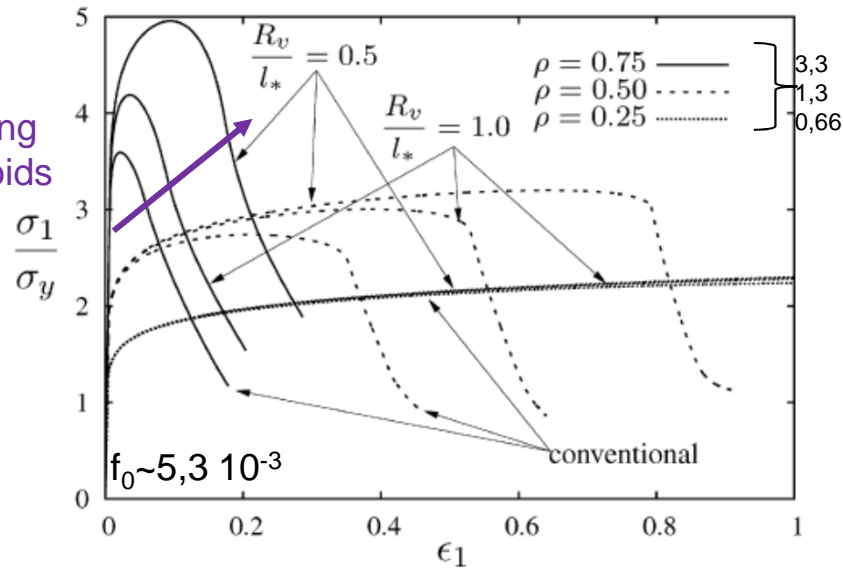
[Ling et al. (2016)]

$$\gamma_{cum} = \sum_s \gamma^s$$

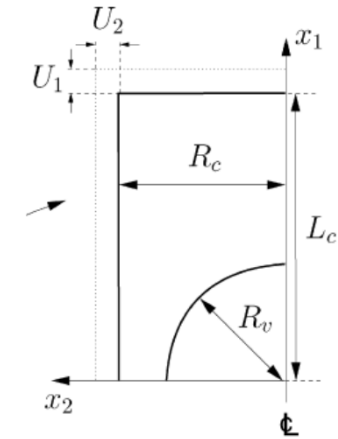
$$F_{11} - 1 = 0.1$$



Decreasing size of voids



Loading ratio



l_* : fixed length material parameter

C.F Niordson, Eur. J. Mech A/Solids2008

Size effect:

- Modify the attainable stress level
- Depend on stress ratio and initial volume fraction
- Modify the growth and coalescence
- Smaller is stronger !

✓ Need to enhance the crystal plasticity model

Study of growth and coalescence at microscale → Enhanced crystal plasticity models in the literature

Gradient terms	Additional DOFs in FEM	Number of the additional DOFs	Examples of references
$\nabla \gamma^s$	γ^s	12 DOFs (FCC)	(Gurtin, 2002) (Gurtin et al., 2007) (Borg, 2007)
$\nabla \nabla u$	∇u	9 DOFs	(Shu et Fleck, 1999)
Curl P_χ	P_χ	9 DOFs	(Cordero et al., 2010) (Aslan et al., 2011) (Cordero et al., 2012)
$\nabla \gamma_\chi$	γ_χ	1 DOF	(Wulfinghoff et Böhlke, 2012) (Wulfinghoff et Böhlke, 2013)

Our constraints:

- Implementation in Finite Element code in finite strain
- Application to fracture toughness modelling -> simulation of small structures (specimens)
- Future derivation of an elastoviscoplastic model for porous single crystals at finite strains including strain gradient effects



Aifantis-type model: numerically efficient

Aifantis, IJP, 1987

γ_χ : microslip variable

✓ **Kinematics**

Deformation gradient: $\underline{\underline{F}} = \underline{\underline{E}} \cdot \underline{\underline{P}}$

✓ **Power of internal forces** [Eringen, 1969; Germain, 1973]

$$P^i = \int_D \underline{\underline{\sigma}} : \text{grad } \underline{\underline{u}} \quad dV \quad \longrightarrow$$

One additional balance equation + boundary condition

✓ **Flow rule**

γ_{χ} is akin to: $\gamma_{cum} = \sum_{s=1}^{12} \gamma^s$

Yield function: $\phi^s = \tau^{*s} - (\tau_c^s) = \tau^{*s} - (\tau_c^s) \geq 0$

$$\begin{aligned} \text{div } \underline{\underline{\sigma}} &= 0 \\ \text{div } \underline{\underline{m}} - s &= 0, \\ &\forall \underline{\underline{x}} \in D, \end{aligned}$$

Generalized stress: $S = Js = H_{\chi}(\gamma_{\chi} - \gamma_{cum})$

$\tau^{*s} = |\tau^s| = |\underline{\underline{M}} : \underline{\underline{N}}^s|$ $\underline{\underline{M}} = J_e \underline{\underline{E}}^T \cdot \underline{\underline{\sigma}} \cdot \underline{\underline{E}}^{-T}$ Relative plastic slip

Plastic strain rate: $\dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} = \sum_{s=1}^{12} \dot{\gamma}^s \frac{\partial \phi^s}{\partial \underline{\underline{M}}} = \sum_{s=1}^{12} \dot{\gamma}^s \text{sign}(\tau^s) \underline{\underline{N}}^s$

$\underline{\underline{N}}^s = \underline{\underline{m}}^s \otimes \underline{\underline{n}}^s$,
the Schmid tensor

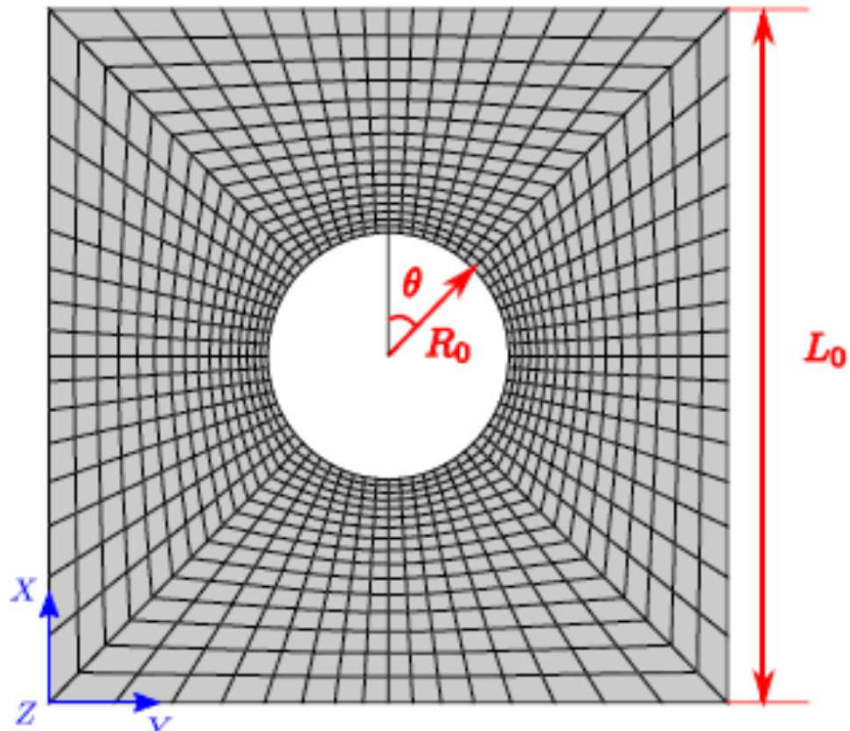
Plastic slip rate: $\dot{\gamma}^s = \dot{\gamma}_{ref} \left\langle \frac{\phi^s}{\tau_{ref}} \right\rangle^n$

Study of growth and coalescence at microscale → Unit cell simulations with micromorphic model

$$U_X(X=0) = 0, U_X(X=L_0) = U_1(t),$$

$$U_Y(Y=0) = 0, U_Y(Y=L_0) = U_2(t),$$

$$U_Z(Z=0) = 0, U_Z(Z=w_0) = 0.$$



Cylindrical void in a plate

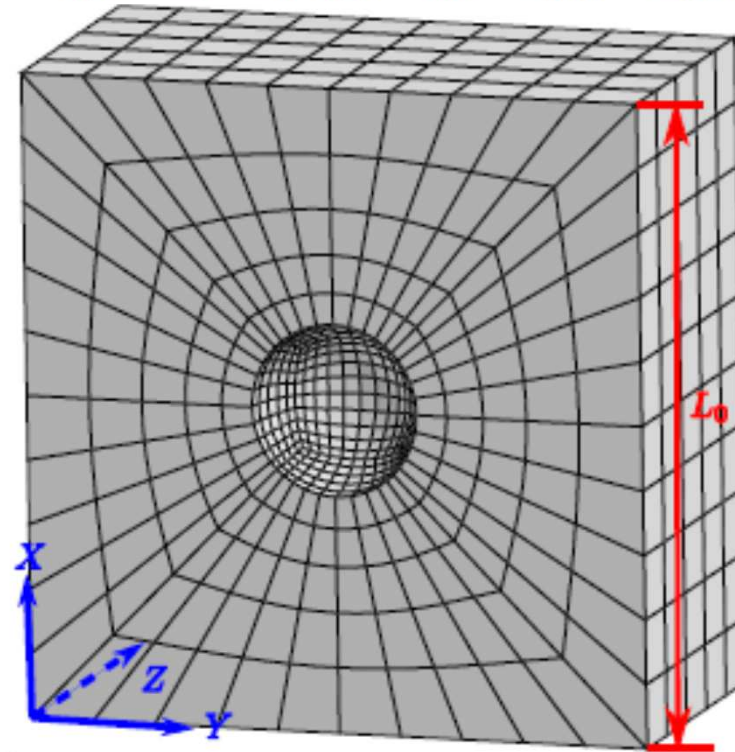
biaxial tensile loading in plane strain,
 $\sigma_{22}/\sigma_{11}=0,625$

FCC single crystal

$$U_X(X=0) = 0, U_X(X=L_0) = U_1(t),$$

$$U_Y(Y=0) = 0, U_Y(Y=L_0) = U_2(t),$$

$$U_Z(Z=0) = 0, U_Z(Z=L_0) = U_3(t) = U_2(t).$$

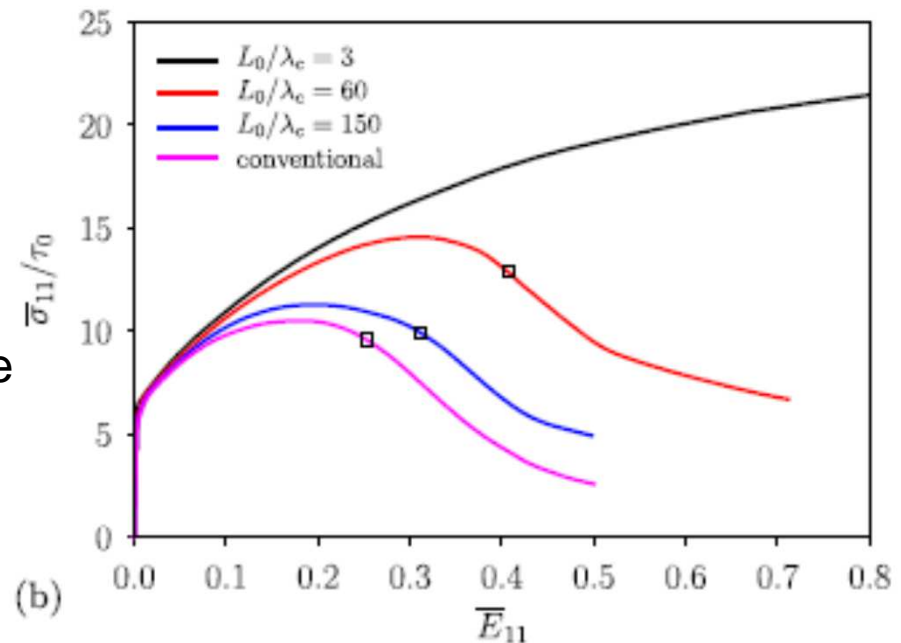
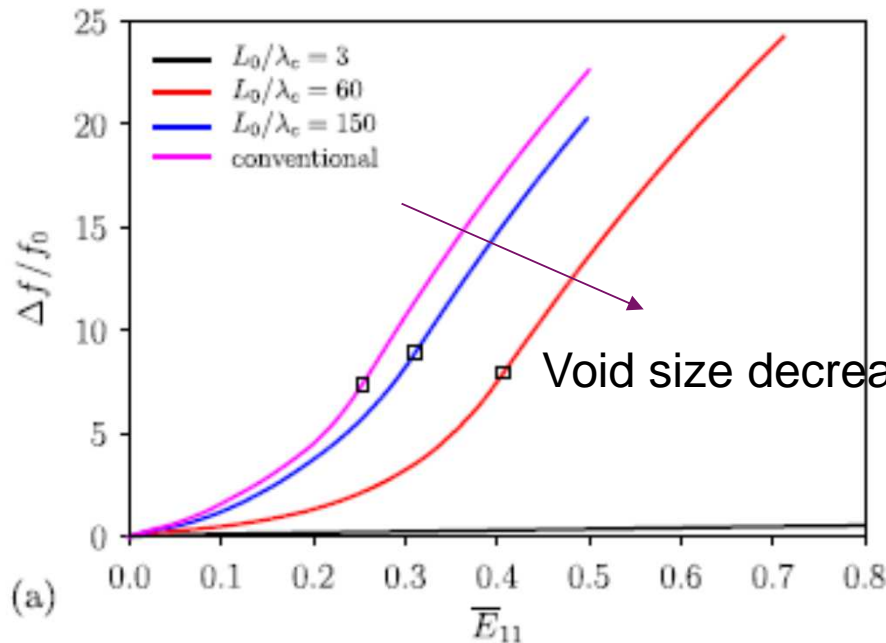


Spherical void in a cube

Stress triaxiality $T = \frac{\bar{\sigma}_m}{\bar{\sigma}_{eq}} = 2$

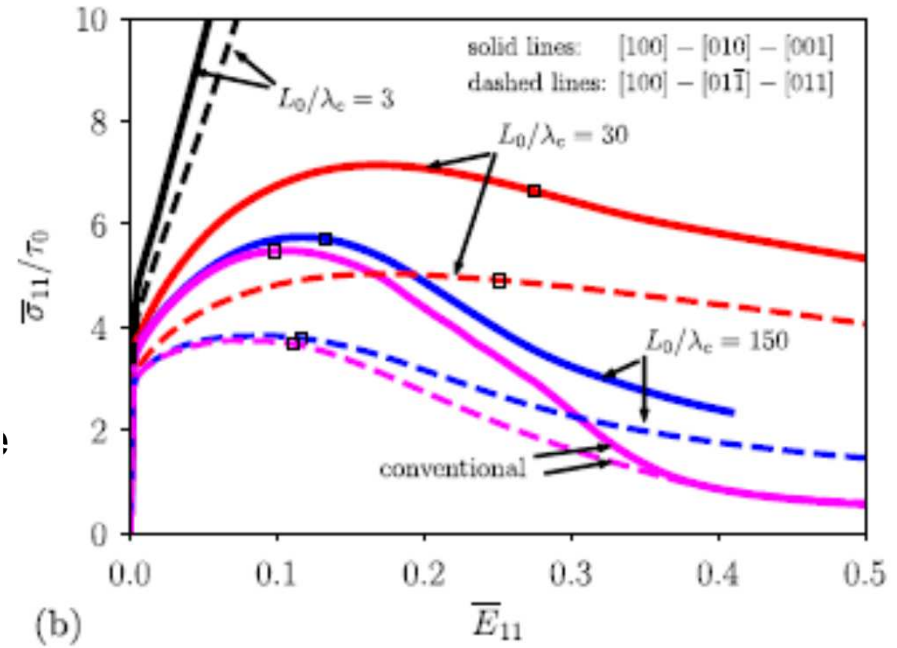
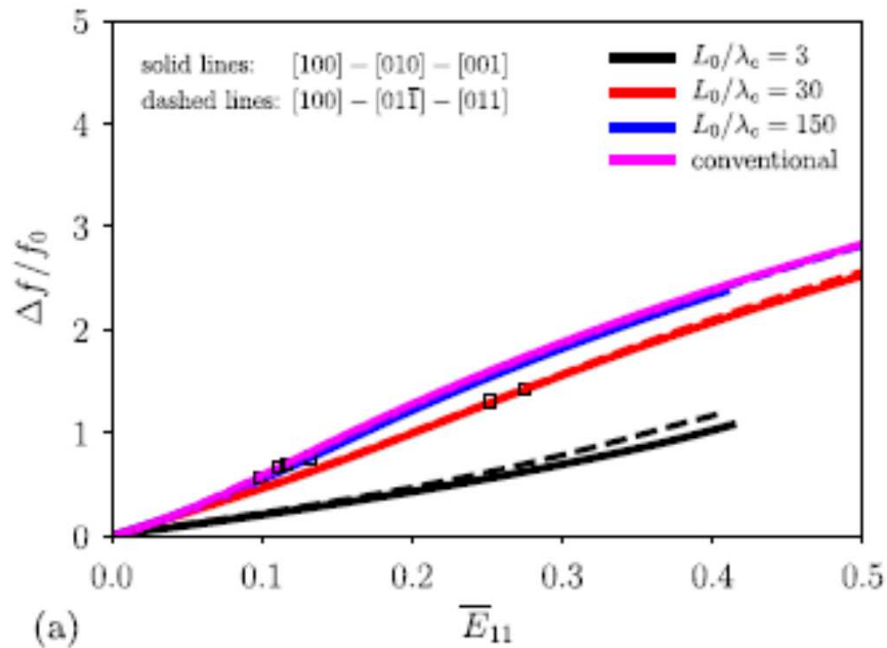
Crystal orientation : [100]-[010]-[001] $f_0=0.01$
 $H\chi=5 \cdot 10^4$ Mpa, $A=5$ N, L_0 variable

$$\lambda_c = \sqrt{\frac{A(H\chi + H)}{H\chi H}} = 0,06\text{mm}$$



- Void growth rate decreases with decreasing normalized unit cell size L_0/λ_c
- Overall stress : competition between hardening and softening due to void growth
- Decreasing L_0/λ_c : higher stress level due to strain gradient hardening and reduction of growth rate

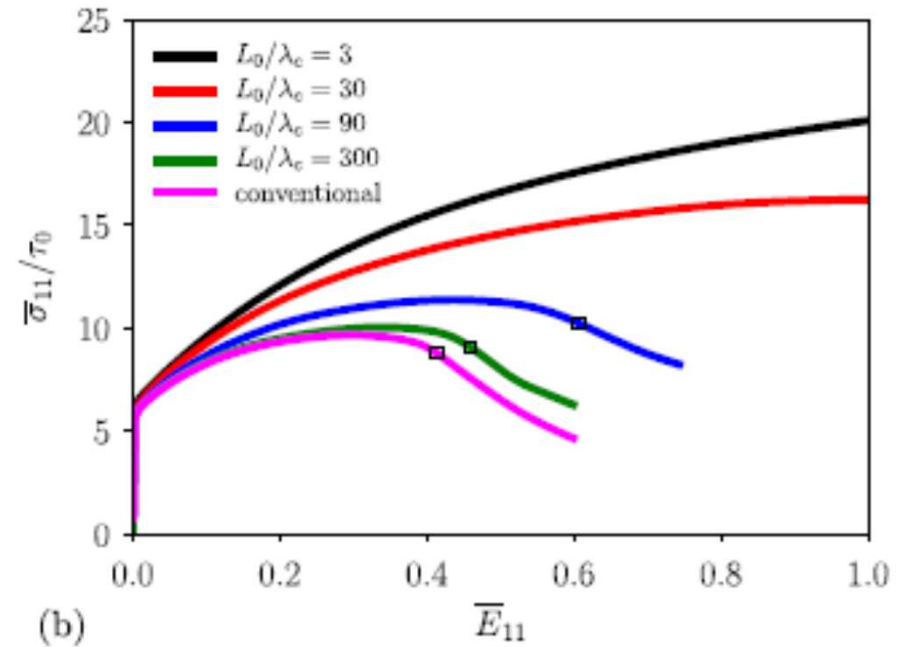
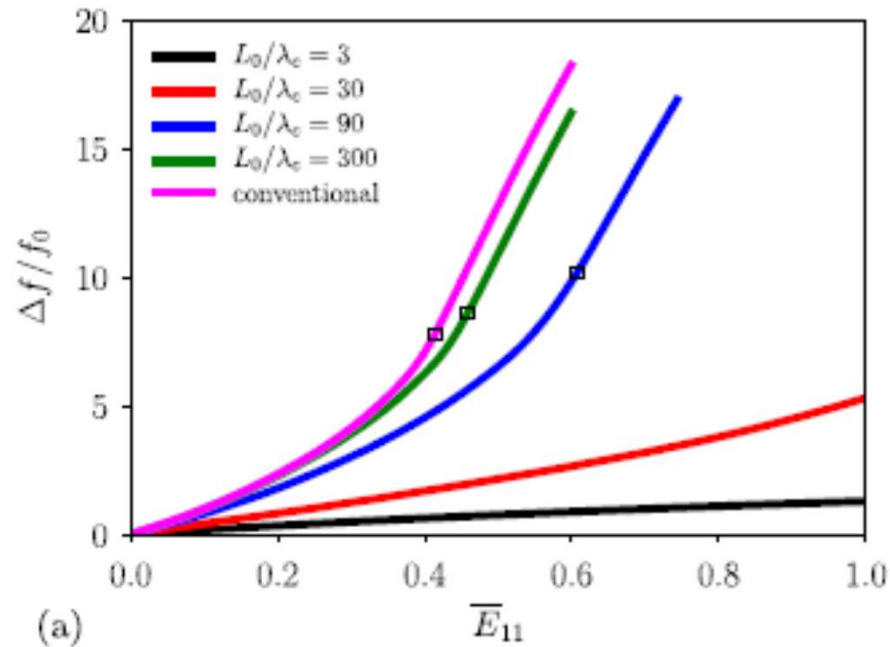
[100]-[010]-[001] [100]-[01-1]-[011] $f_0=0.1$



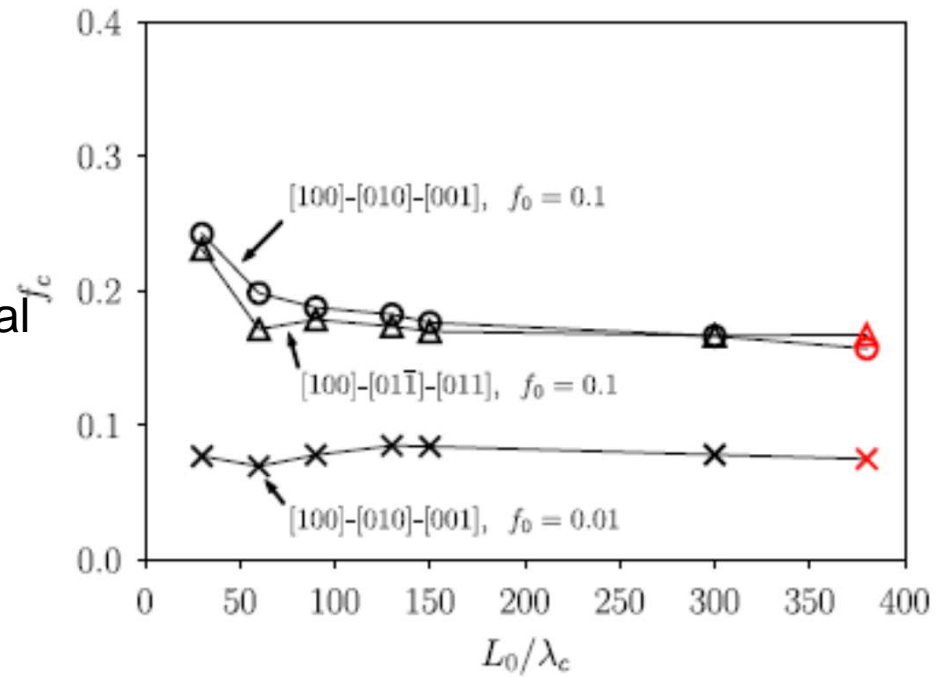
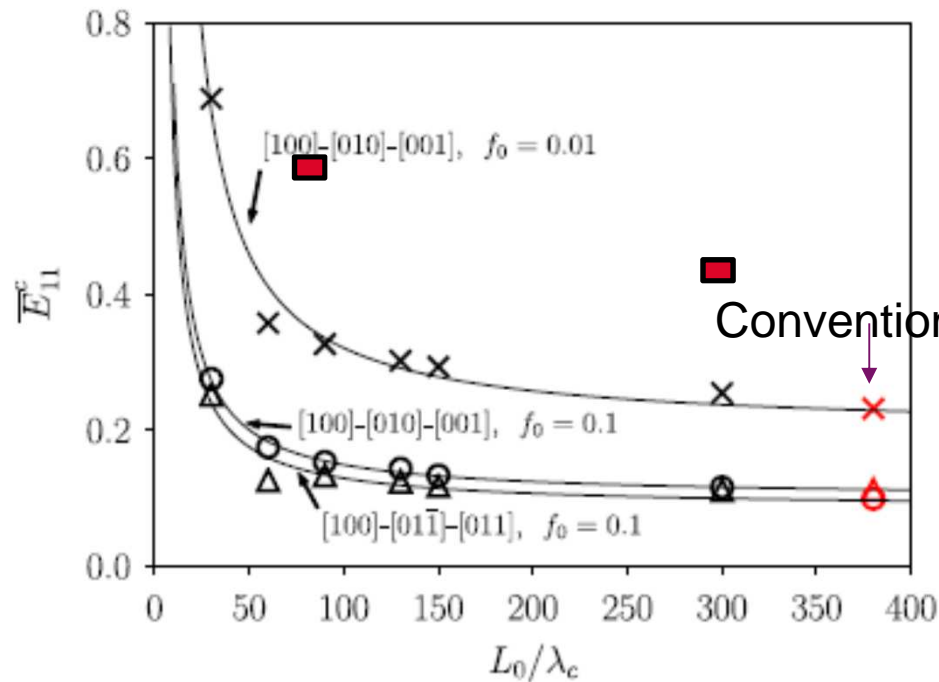
- For a given L_0/λ_c : Similar void growth rate but different stress-strain responses
- Related to the difference of active slip systems in the matrix
- Higher stress level for [100]-[010]-[001]
- Transition from growth to coalescence less marked than for $f_0=0,01$
- Void growth rate can not be neglected for $L_0/\lambda_c=3$

[100]-[010]-[001]

$f_0=0.01$



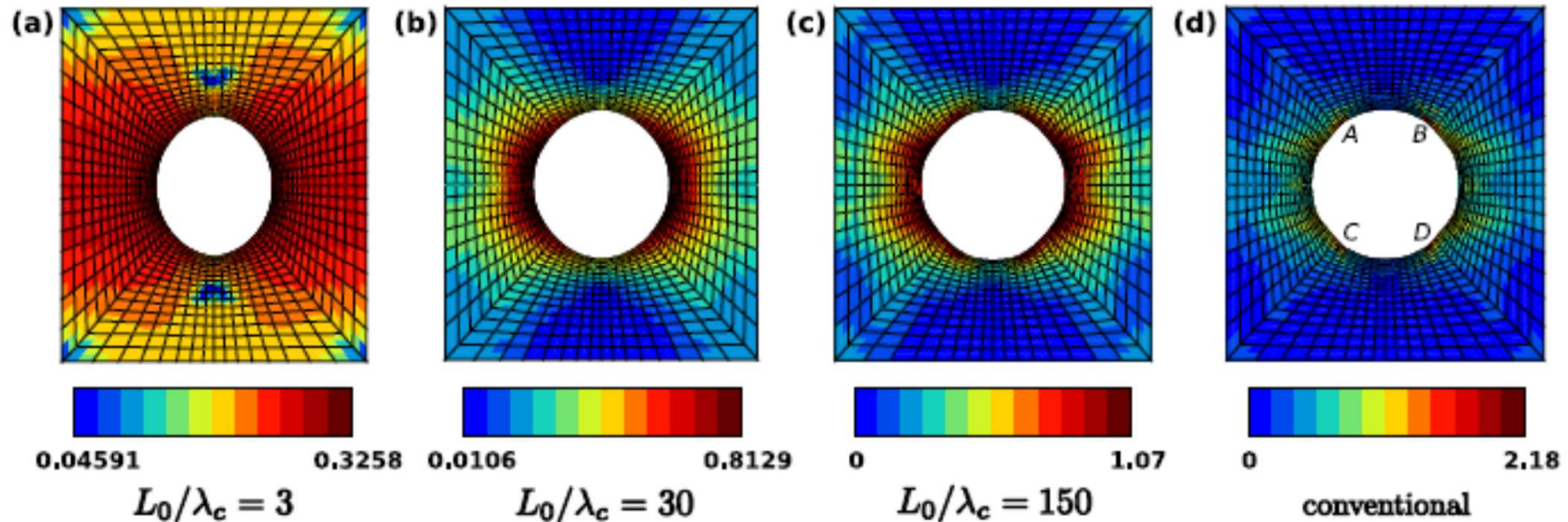
- Similar trends than for cylindrical void
- Softening occurs for larger strain for spherical void



- Onset of coalescence is delayed with decreasing L_0/λ_c
- Size effect can be neglected on f_c for $f_0=0,01$
- Increase in f_c when $L_0/\lambda_c < 60$ for $f_0=0,1$
- Critical strain at coalescence significantly larger for spherical void (■)

$E_{11}=0,1, f=0,1$ [100]-[010]-[001]

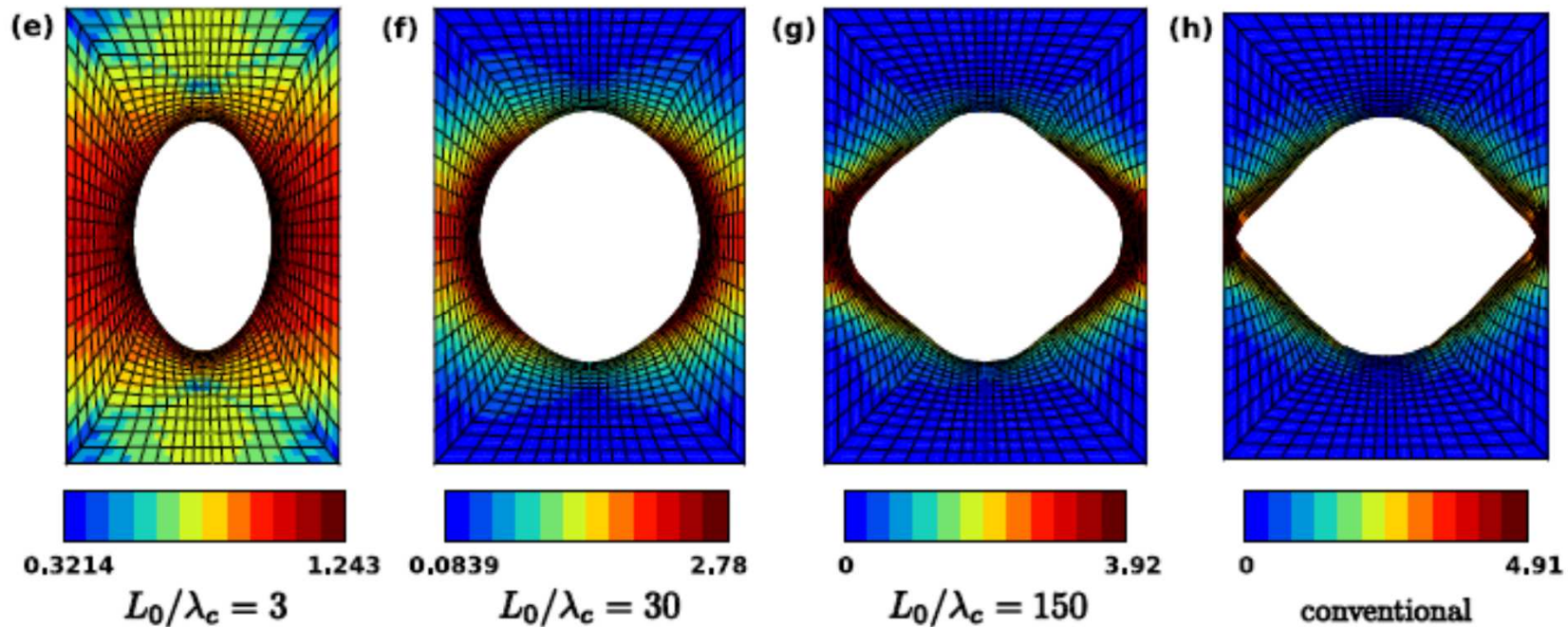
$$\gamma_{cum} = \sum_s \gamma^s$$



- 4 zones of plastic localization for the conventional theory
- Plastic deformation fields become more diffuse when L_0/λ_c decreases
- Maximum γ_{cum} lower based on micromorphic theory -> void growth is slowed down

$E_{11}=0,4$, $f=0,1$ [100]-[010]-[001]

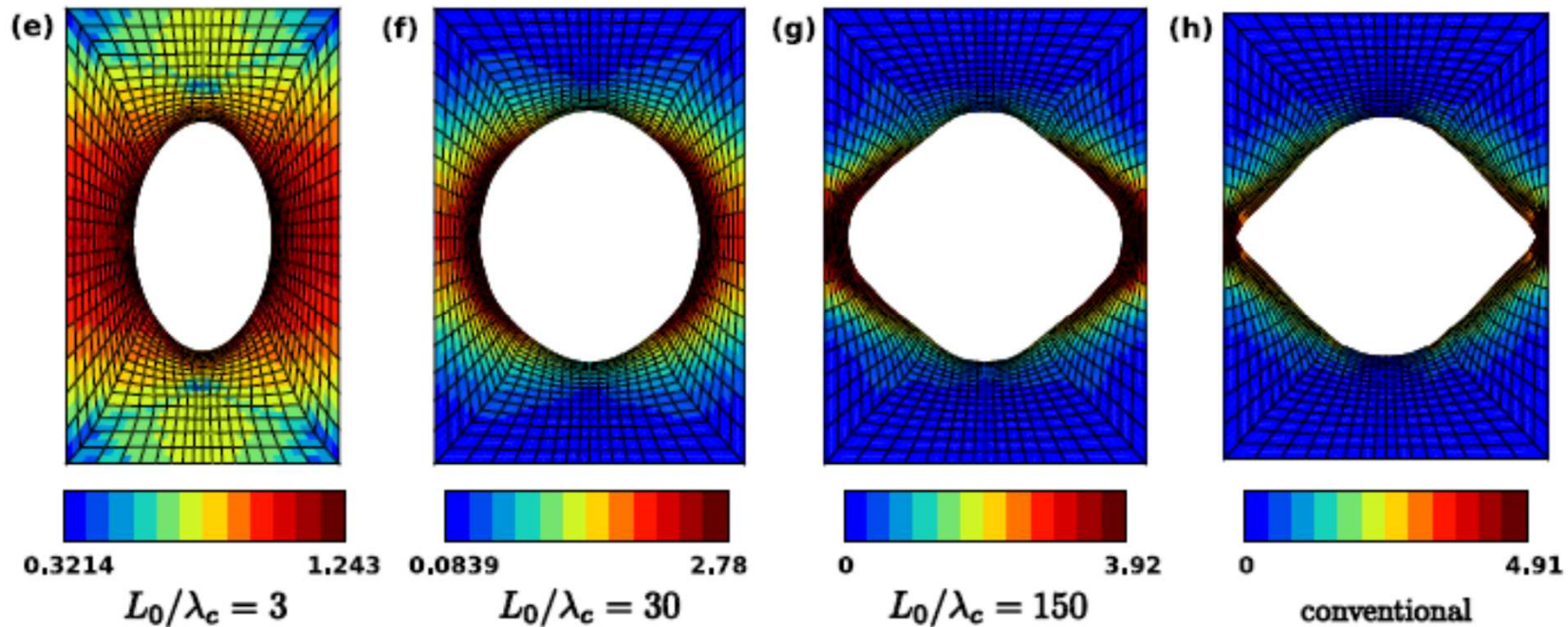
$$\gamma_{cum} = \sum_s \gamma^s$$



- Plastic deformation fields become more diffuse when L_0/λ_c decreases
- Maximum γ_{cum} lower based on micromorphic theory -> [Effect on the void shape](#)

$E_{11}=0,3$, $f=0,1$ [100]-[010]-[001]

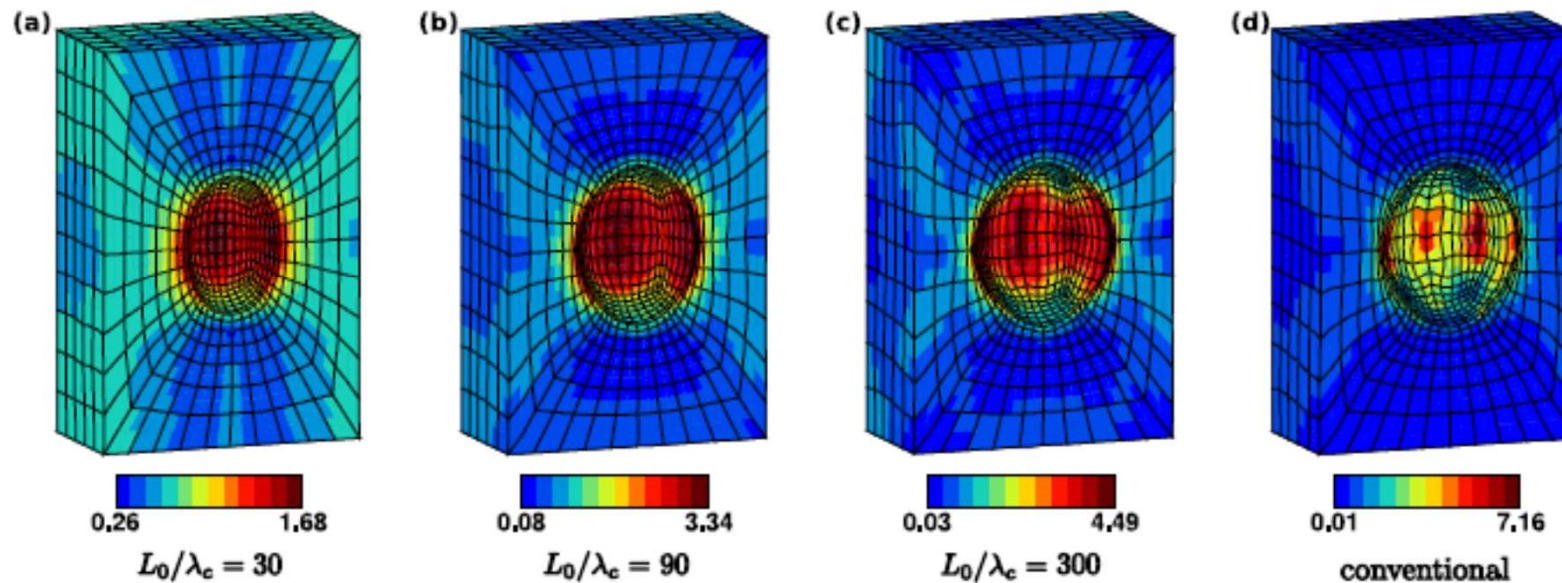
$$\gamma_{cum} = \sum_s \gamma^s$$



- Plastic deformation fields become more diffuse when L_0/λ_c decreases
- Maximum γ_{cum} lower based on micromorphic theory -> [Effect on the void shape](#)

$E_{11}=0,3$, $f=0,01$ [100]-[01-1]-[011]

$$\gamma_{cum} = \sum \gamma^s$$



- Plastic deformation fields become more diffuse when L_0/λ_c decreases
- Maximum γ_{cum} lower based on micromorphic theory
- Localisation of the plastic slip localization zones very different from the cylindrical case

- ❑ Void growth rate depends on crystal orientation and the effect is more significant at lower stress triaxialities.
 - ✓ This justifies the proposed approach for modeling ductile fracture at the scale of grain
- ❑ A micromorphic single crystal plasticity model has been proposed and implemented
- ❑ Size dependant overall behavior and void growth by the micromorphic model for voided single crystal
- ❑ Unit cells of smaller size exhibit a lower void growth rate compared with larger ones -> higher hardening rate and delayed onset of coalescence
- ❑ Future work: Modelling of the nanovoids growth (see Barrioz and al. for experimental work)
- ❑ The model will be coupled with the porous single crystal model of Ling et al. (2016)

Thank you for your attention!



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