
# Simulation des déformations de pièces mécaniques induites par des traitements de surface thermochimiques et mécaniques

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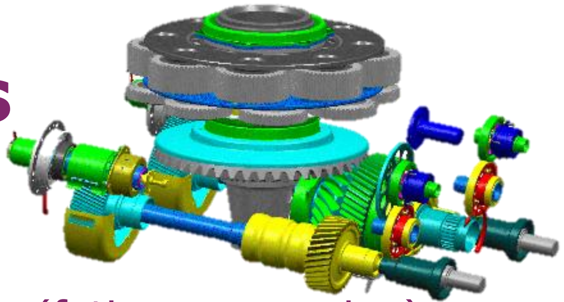
Arts et Métiers Sciences et Technologies

# Contexte et objectifs



Traitements de surface dans l'industrie:

- Utilité: Augmenter la durabilité des pièces métalliques (fatigue, corrosion), amélioration des propriétés de contact

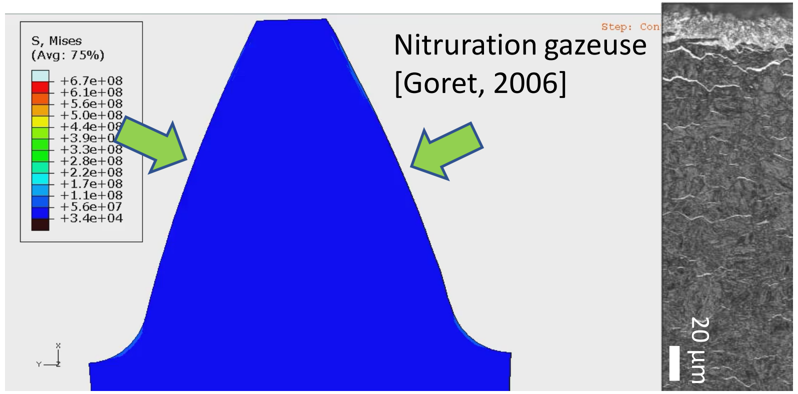
- Généralement via l'introduction de contraintes résiduelles s'opposant au chargement

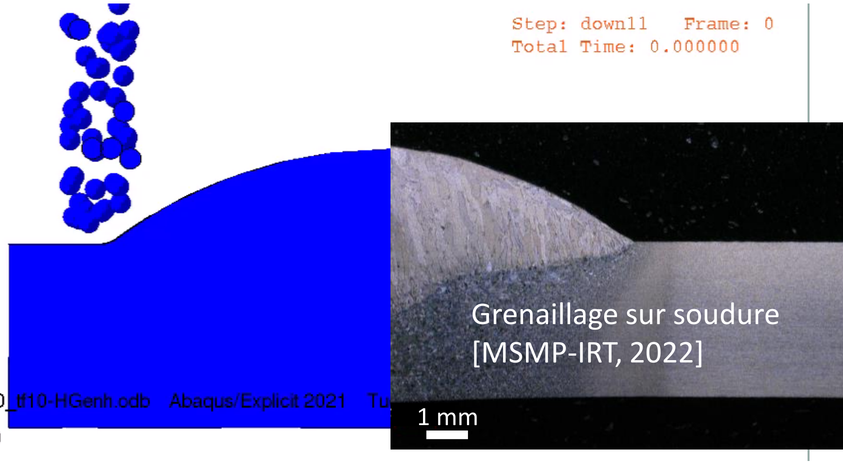
- Thermochimiques: **nitruration**, cémentation, carbonitruration, …

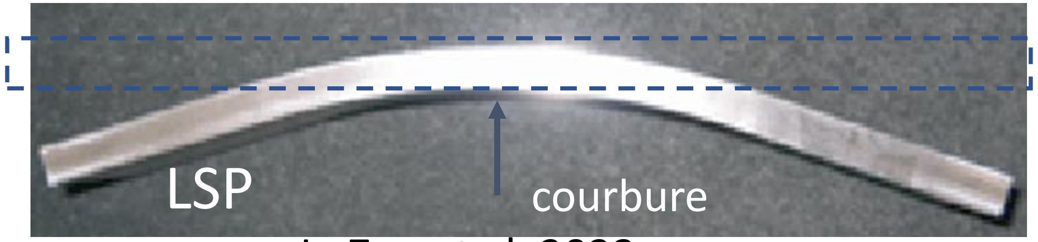
- Mécaniques: **grenaillage**, galetage, brunissage, martelage, LSP…

Mais il existe aussi conjointement des déformations. Exemples: Eprouvette Almen, mesure de contraintes par méthode du trou, méthode du contour, …

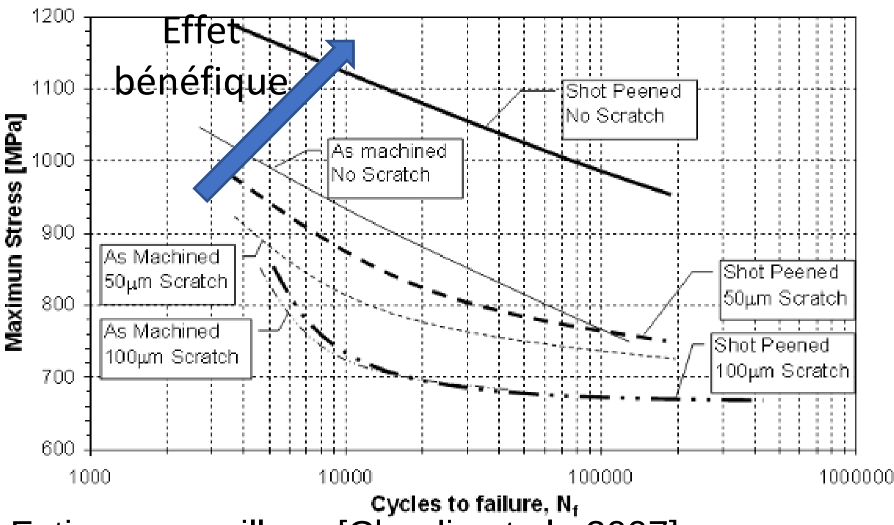
**Objectifs**: Proposer des outils de modélisation des traitements de surface pour la compréhension des mécanismes et pour l'assistance industrielle




In Zou et al, 2023




Fatigue grenaillage [Claudio et al., 2007]

# SOMMAIRE





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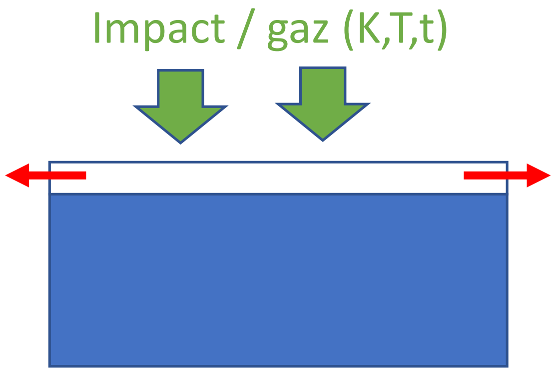
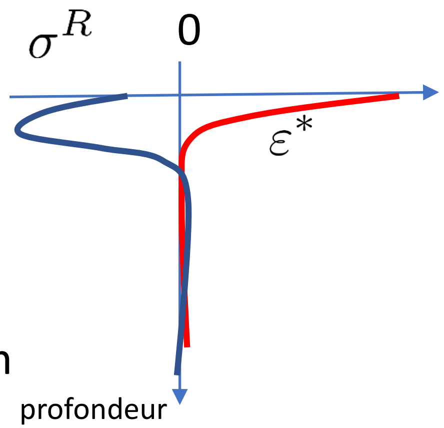
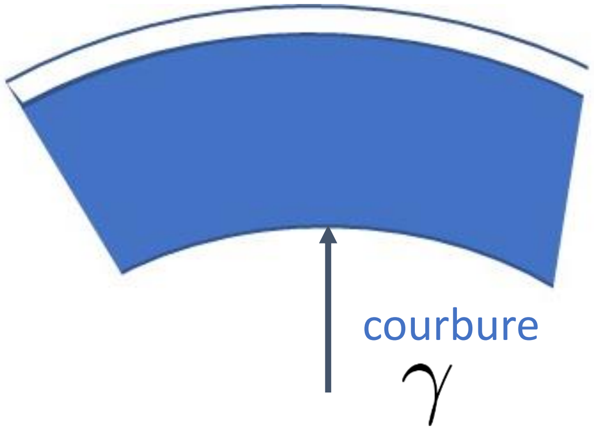
# Traitements de surface
## Principes généraux

1. Sous l'action d'un stimuli extérieur, les traitements de surface génèrent à partir de la surface des gradients de déformations incompatibles (plasticité, transformation de phases).
2. Ces déformations incompatibles $\varepsilon^*$ sont appelées libres de contrainte ou « eigenstrain » et sont rendues compatibles par la génération d'une déformation élastique
3. La déformation élastique permet le calcul des gradients de contrainte (milieu continu)
4. Les contraintes s'équilibrent dans la structure de la pièce. Ce sont les contraintes résiduelles $\sigma^R$ (ordre I).
5. Des distorsions de pièces peuvent apparaitre en fonction de la géométrie (courbure, déflexion)




Profondeur affectée: ~ 10 µm - ~ 1 mm




Courbure et contraintes différentes entre une tôle mince et un massif semi-infini (MSI)

# Déformation libre de contraintes - Eigenstrain

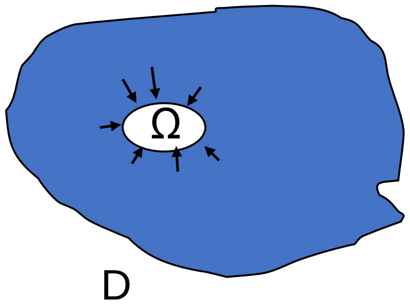
**Déformation inélastique dans Ω:**

Expansion thermique, transformation de phase, déformation initiale, déformation plastique, dislocation, misfit, …

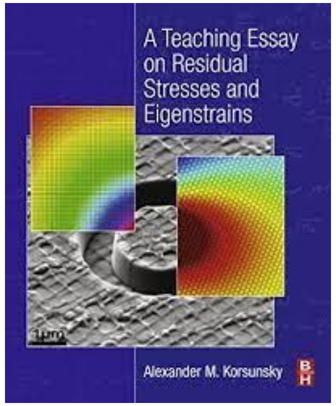
En HPP:

$$\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^{e} + \underset{\sim}{\varepsilon}^{*}$$

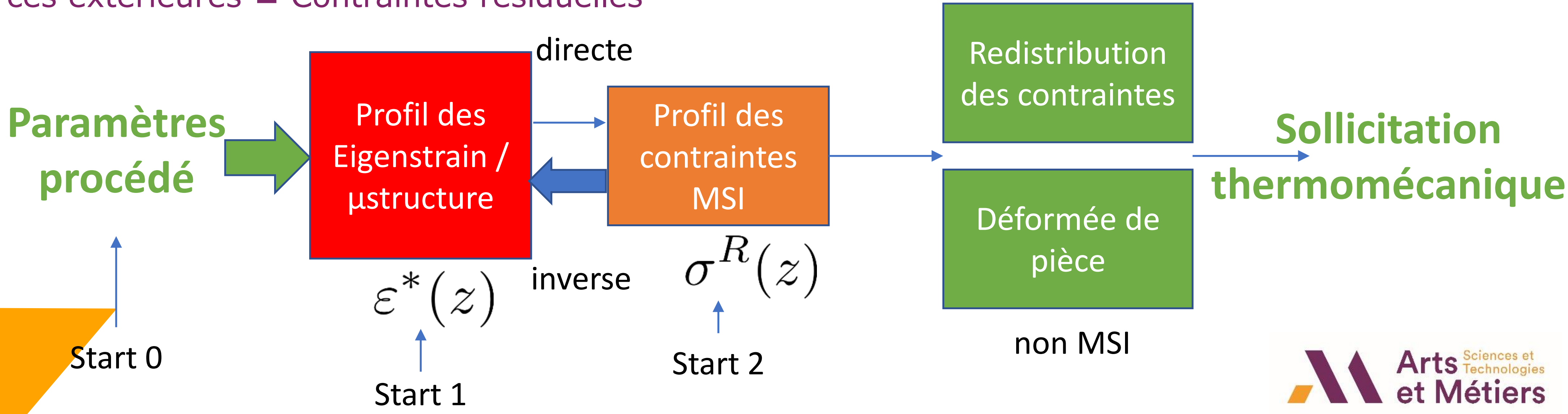
Ex: cas de l'inclusion d'Eshelby




[Korsunsky, 2017]
A teaching essay on residual stresses and Eigenstrains




**« Eigenstress »:** champ de contraintes internes autoéquilibrées créé par les « Eigenstrains » dans des corps libres de forces extérieures = Contraintes résiduelles



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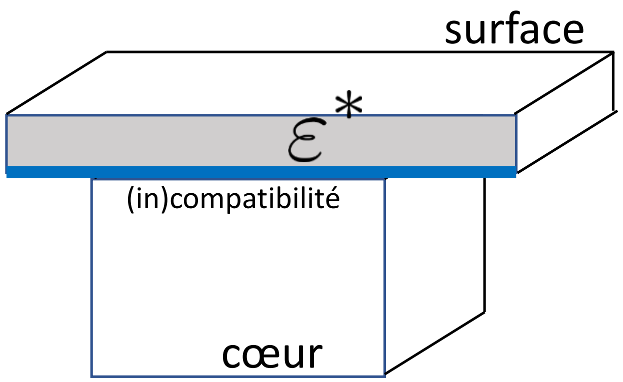
# Traitements de surface
# Principes généraux

**Cinématique et Comportement** $\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^*$ $\underset{\sim}{\sigma} = \underset{\approx}{C} : \underset{\sim}{\varepsilon}^e$

**Equilibre local** $div(\underset{\sim}{\sigma}) + \vec{F} = \rho\ddot{\vec{u}}$




**Equation de compatibilité (continuité de la matière)**

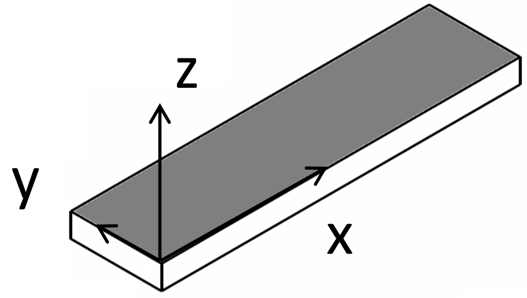
$$\frac{\partial^2 \varepsilon_{ij}}{\partial x_k \partial x_k} + \frac{\partial^2 \varepsilon_{kk}}{\partial x_i \partial x_j} - \frac{\partial^2 \varepsilon_{jk}}{\partial x_i \partial x_k} - \frac{\partial^2 \varepsilon_{ik}}{\partial x_j \partial x_k} = 0$$

**Equation d'équilibre de la structure – Conditions aux limites**

$$\int_{S_x} \sigma_{xx}(z)dydz = 0 \qquad \int_{S_x} z\sigma_{xx}(z)dydz = 0$$

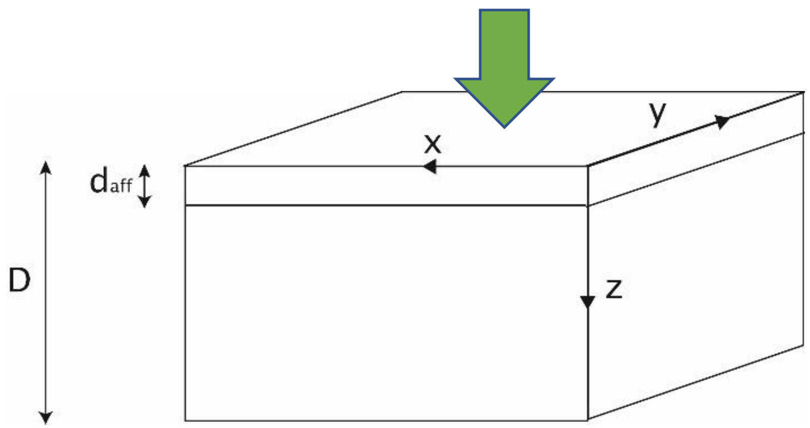
$$\int_{S_y} \sigma_{yy}(z)dxdz = 0 \qquad \int_{S_y} z\sigma_{yy}(z)dxdz = 0$$

Efforts normaux — Moments fléchissants



# Traitements de surface d'un MSI

# Principes généraux




- Traitement uniforme et isotrope plan sur la surface d'un Massif Semi-Infini (MSI)
- Massif semi-infini D>> $d_{aff}$
- Cadre HPP
- Elasticité isotrope
- Hyp: l'eigenstrain ne dépend pas de la géométrie (MSI, plaque mince, cylindre, …)

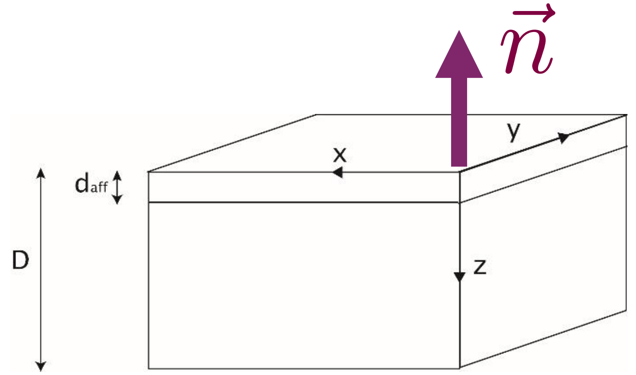
Contrainte statiquement admissible

$$\underset{\sim}{\sigma}(z) = \begin{pmatrix} \sigma_{xx}(z) & 0 & \sigma_{xz}(z) \\ 0 & \sigma_{xx}(z) & \sigma_{yz}(z) \\ \sigma_{zx}(z) & \sigma_{zy}(z) & \sigma_{zz}(z) \end{pmatrix}$$

Déformation totale cinématiquement admissible

$$\underset{\sim}{\varepsilon}(z) = \begin{pmatrix} \varepsilon_{xx}(z) & 0 & \varepsilon_{xz}(z) \\ 0 & \varepsilon_{xx}(z) & \varepsilon_{yz}(z) \\ \varepsilon_{zx}(z) & \varepsilon_{zy}(z) & \varepsilon_{zz}(z) \end{pmatrix}$$

# Traitements de surface
# Principes généraux




## ❑ Equilibre

$$\begin{cases} \dfrac{\partial \sigma_{xz}(z)}{\partial z} = 0 \\ \dfrac{\partial \sigma_{yz}(z)}{\partial z} = 0 \\ \dfrac{\partial \sigma_{zz}(z)}{\partial z} = 0 \end{cases} \qquad \begin{cases} \sigma_{xz}(z) = C_1 \\ \sigma_{yz}(z) = C_2 \\ \sigma_{zz}(z) = C_3 \end{cases}$$

## ❑ Conditions aux limites

$$\underset{\sim}{\sigma}(z).\vec{n} = \vec{0} \qquad \vec{n} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_{x,y,z}$$

$$\begin{cases} \sigma_{xz}(z) = C_1 = 0 \\ \sigma_{yz}(z) = C_2 = 0 \\ \sigma_{zz}(z) = C_3 = 0 \end{cases}$$

$$\underset{\sim}{\sigma}(z) = \begin{pmatrix} \sigma_{xx}(z) & 0 & 0 \\ 0 & \sigma_{xx}(z) & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



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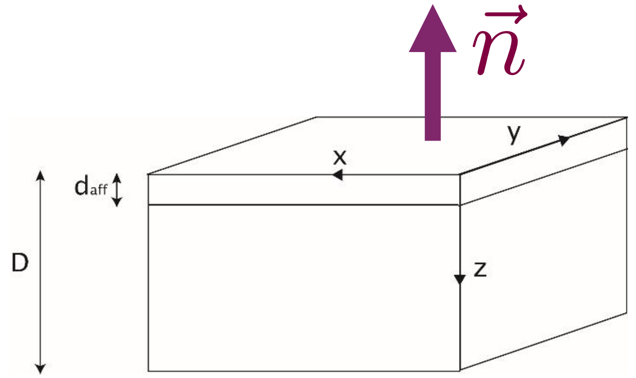
# Traitements de surface
# Principes généraux




- Loi de comportement

$$\varepsilon_{xx}(z) = \frac{1-\nu(z)}{E(z)}\sigma_{xx}(z) + \varepsilon^*_{xx}(z)$$

$$\varepsilon_{zz}(z) = \frac{-2\nu(z)}{E(z)}\sigma_{xx}(z) + \varepsilon^*_{zz}(z)$$

- Compatibilité des déformations totales

$$\varepsilon_{xx,zz}(z) = 0 \quad \Longrightarrow \quad \varepsilon_{xx}(z) = A.z + B$$

- Conditions aux limites MSI

$$z \rightarrow \infty \qquad \varepsilon_{xx}(z \rightarrow \infty) = 0$$

$$\varepsilon^*_{xx}(z \rightarrow \infty) = 0 \quad \Longrightarrow \quad \varepsilon_{xx}(z) = 0$$

$$\underset{\sim}{\varepsilon}(z) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \varepsilon_{zz}(z) \end{pmatrix}$$

Relation entre la déformation libre et la contrainte résiduelle [Zarka, 1980]

$$\varepsilon^*_{xx}(z) = \frac{\nu(z)-1}{E(z)}\sigma^R_{xx}(z)$$

$$\underset{\sim}{\varepsilon}^*(z) = \begin{pmatrix} \varepsilon^*_{xx} & 0 & 0 \\ 0 & \varepsilon^*_{xx} & 0 \\ 0 & 0 & -2.\varepsilon^*_{xx} \end{pmatrix}$$

Déf. plastique

E= 200 GPa
$\nu = 0.3$
$\sigma_{xx} = -1000\ MPa$

$$\Longrightarrow \varepsilon^p_{xx} = 0,35\%$$



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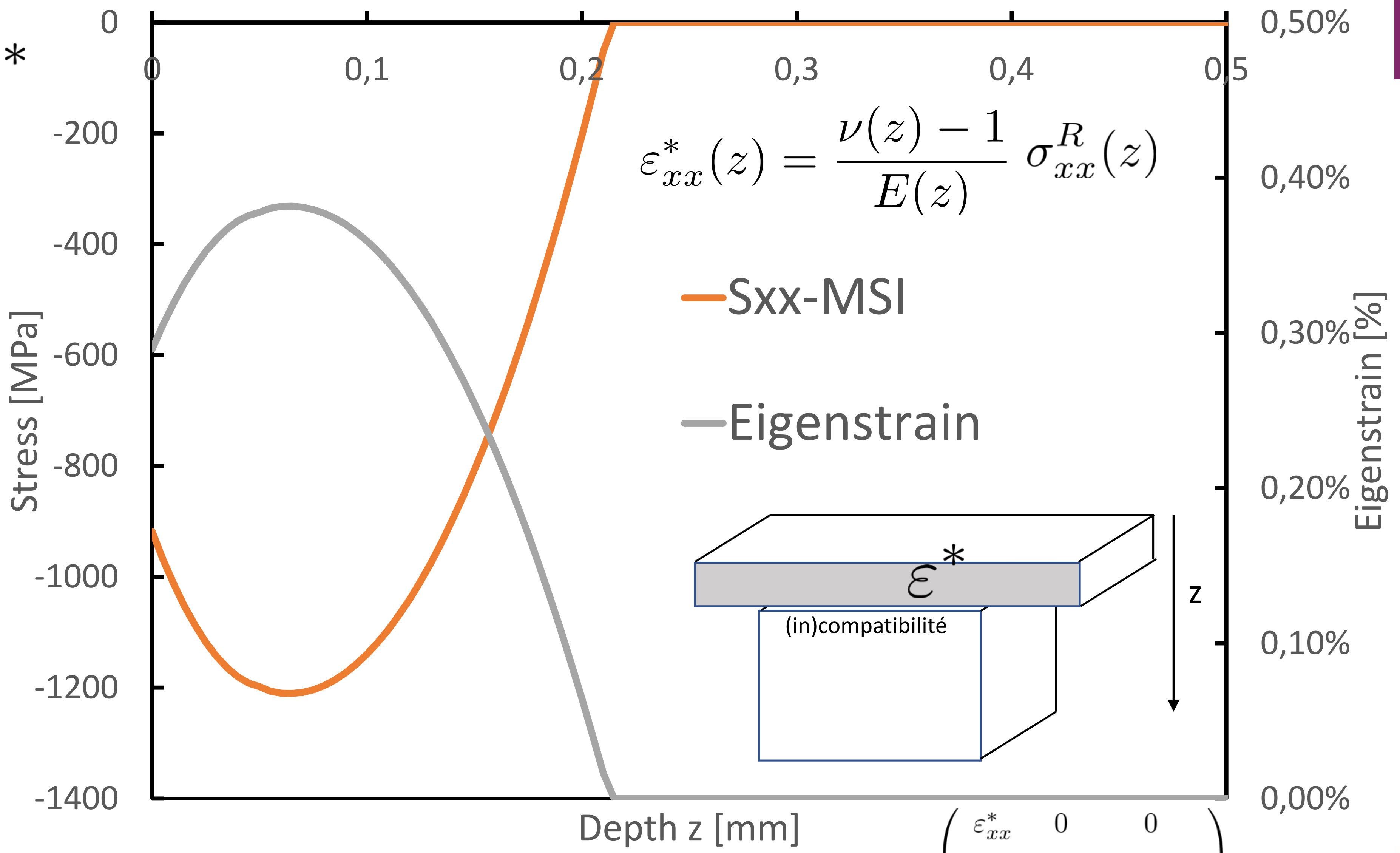
reconstruction inverse

$\sigma^R \rightarrow \varepsilon^*$

# Profils sur Massif Semi Infini



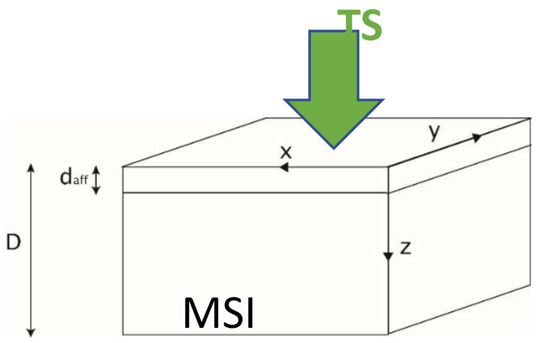

$$\varepsilon^*_{xx}(z) = \frac{\nu(z) - 1}{E(z)} \sigma^R_{xx}(z)$$

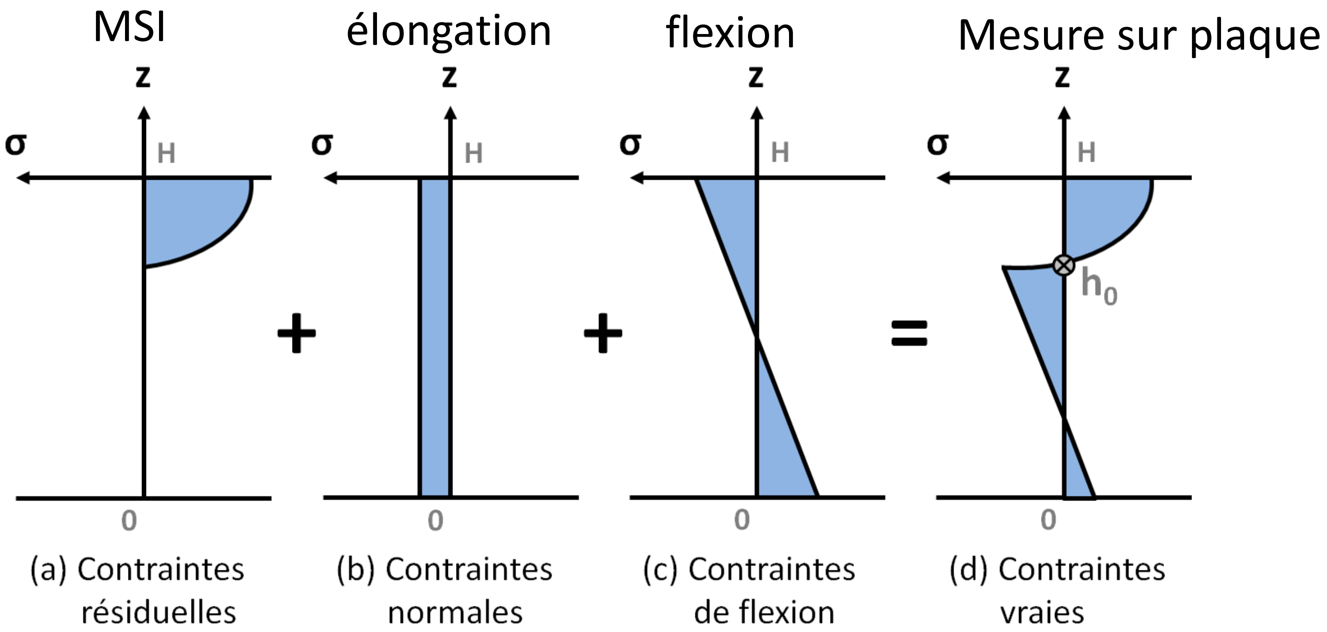
$$\begin{pmatrix} \varepsilon^*_{xx} & 0 & 0 \\ 0 & \varepsilon^*_{xx} & 0 \\ 0 & 0 & -2.\varepsilon^*_{xx} \end{pmatrix}$$

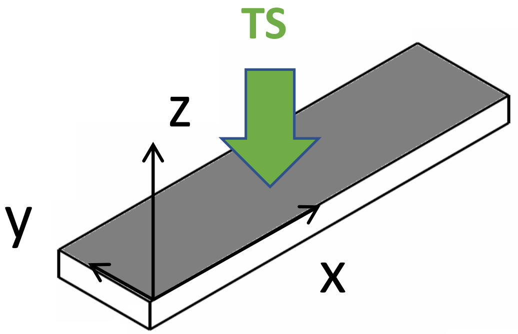
# Cas analytique d'une plaque d'épaisseur finie H

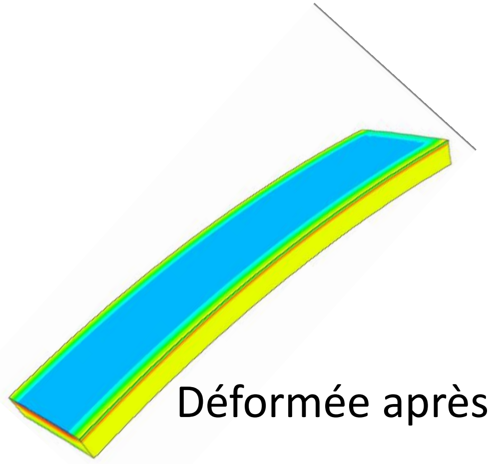
Traitement de surface (TS) – Eigenstrain identique au MSI
Redistribution des contraintes dans une plaque plane (Castex 1984)

Décomposition:




$$\sigma^R(z) + \sigma^N(z) + \sigma^F(z) = \sigma^V(z)$$

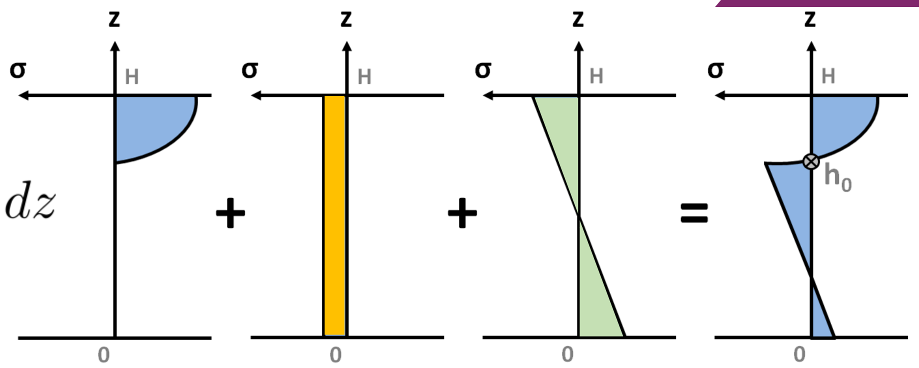
$$\sigma^N(z) = -\frac{1}{H} \cdot \int_{h_0}^{H} \sigma^R(z) \cdot dz$$

$$\sigma^F(z) = -\frac{6(2z - H)}{H^3} \cdot \int_{h_0}^{H} \sigma^R(z) \cdot \left(z - \frac{H}{2}\right) \cdot dz$$

# Cas analytique d'une plaque d'épaisseur finie H

## Moment fléchissant

$$M_x = \int_0^H \sigma^R(z) \cdot z \cdot dz = \int_{h_0}^H \sigma^R(z) \cdot z \cdot dz$$



(a) Contraintes résiduelles (b) Contraintes normales (c) Contraintes de flexion (d) Contraintes vraies

## Courbure

$$\gamma = \frac{M_x}{(1+\nu) \cdot D} \qquad D = -\frac{E \cdot H^3}{12 \cdot (1-\nu^2)}$$

$$\sigma^N(z) = -\frac{1}{H} \cdot \left( \frac{\eta A - \delta B}{\rho} \right)$$

$$\sigma^F(z) = -\frac{6(2z-H)}{H^3} \cdot \left( \frac{\beta B - \gamma A}{\rho} \right)$$

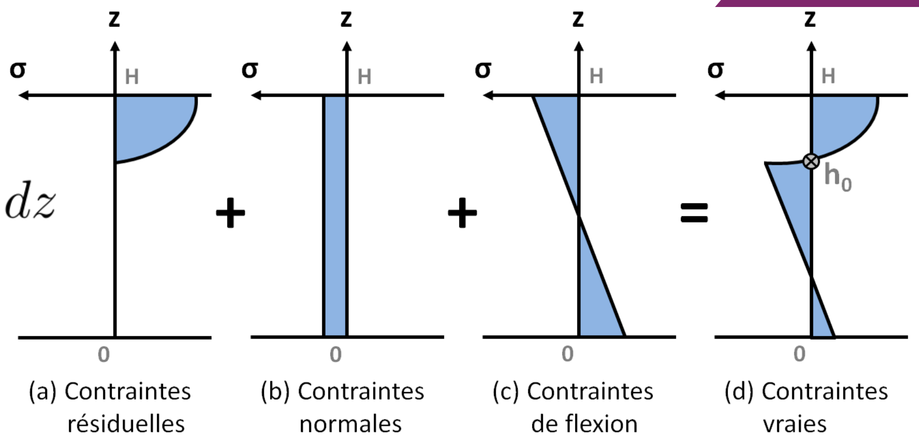
$$\begin{cases} \eta = \dfrac{3H^2 h_0 - 6h_0^2 H + 4h_0^3}{H^3} \\ \delta = \dfrac{6h_0 \cdot (h_0 - H)}{H^3} \\ \beta = \dfrac{h_0}{H} \\ \gamma = \dfrac{h_0 \cdot (h_0 - H)}{2H} \\ \rho = \beta\eta - \gamma\delta \end{cases}$$

$$\begin{cases} A = \displaystyle\int_{h_0}^H \sigma^V(z) \cdot dz \\ B = \displaystyle\int_{h_0}^H \sigma^V(z) \cdot \left(z - \frac{H}{2}\right) \cdot dz \end{cases}$$

# Cas analytique d’une plaque d’épaisseur finie H

## Moment fléchissant induit par les CR

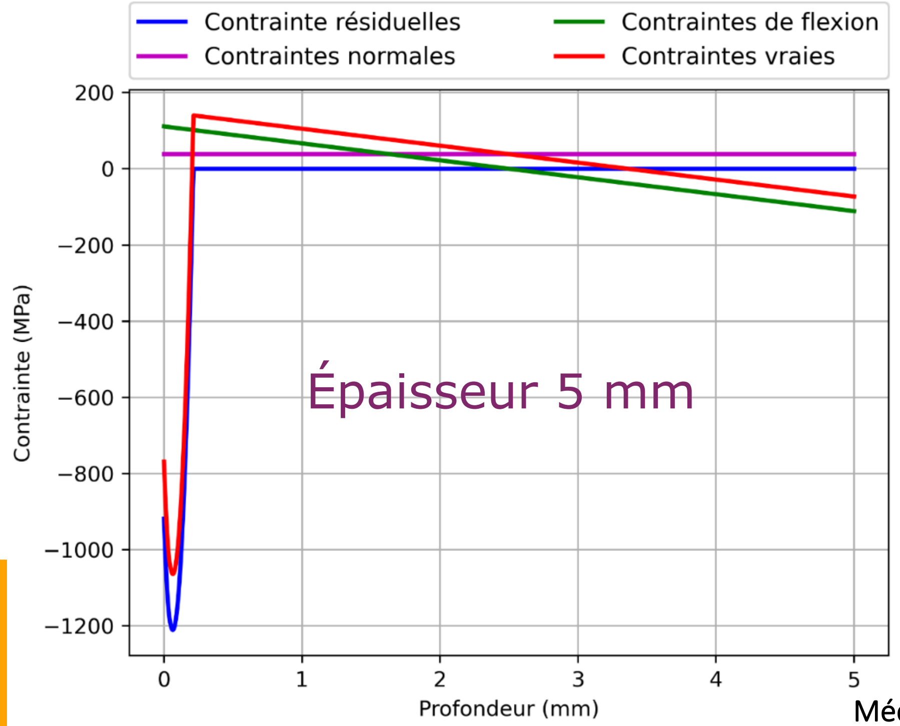
$$M_x = \int_0^H \sigma^R(z) \cdot z \cdot dz = \int_{h_0}^H \sigma^R(z) \cdot z \cdot dz$$

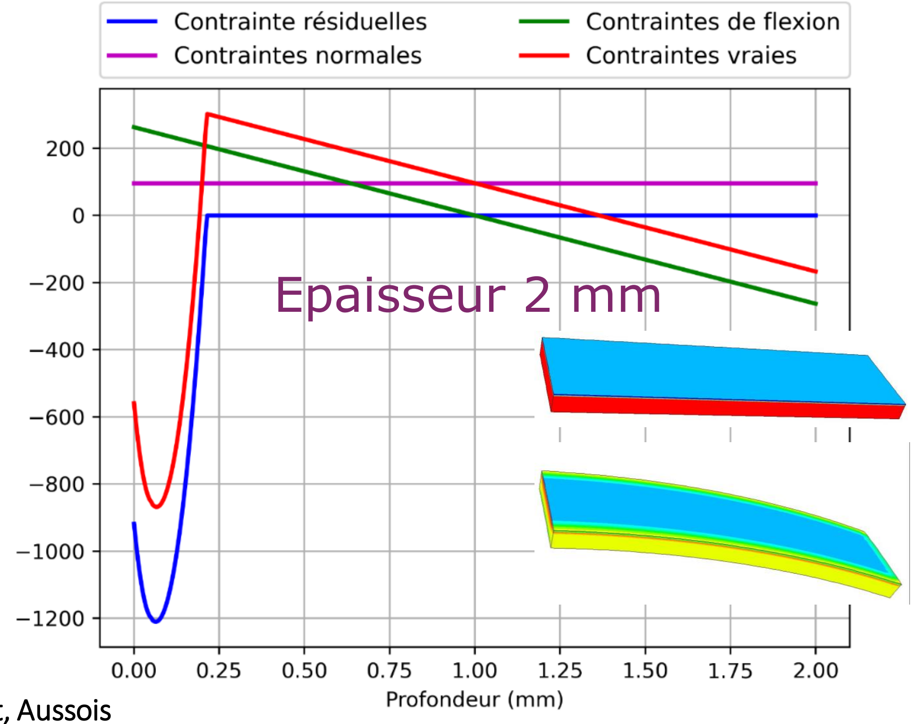



## Courbure induite

$$\gamma = \frac{M_x}{(1+\nu) \cdot D} \qquad D = -\frac{E \cdot H^3}{12 \cdot (1-\nu^2)}$$

Redistribution des contraintes dépend de la géométrie

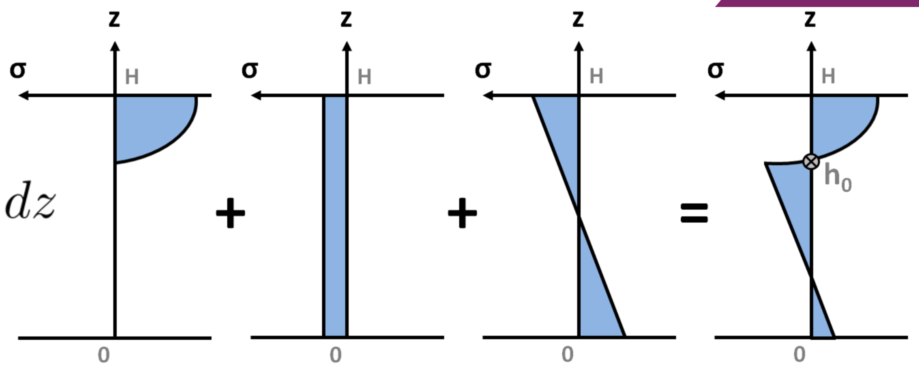


# Cas analytique d'une plaque d'épaisseur finie H

Moment fléchissant induit par les CR

$$M_x = \int_0^H \sigma^R(z) \cdot z \cdot dz = \int_{h_0}^H \sigma^R(z) \cdot z \cdot dz$$

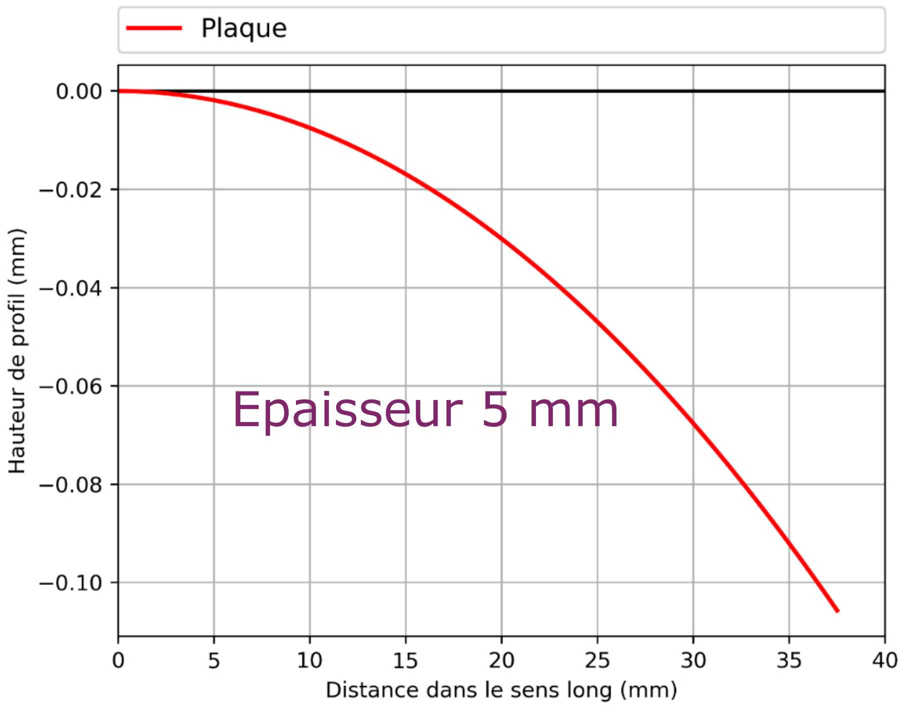


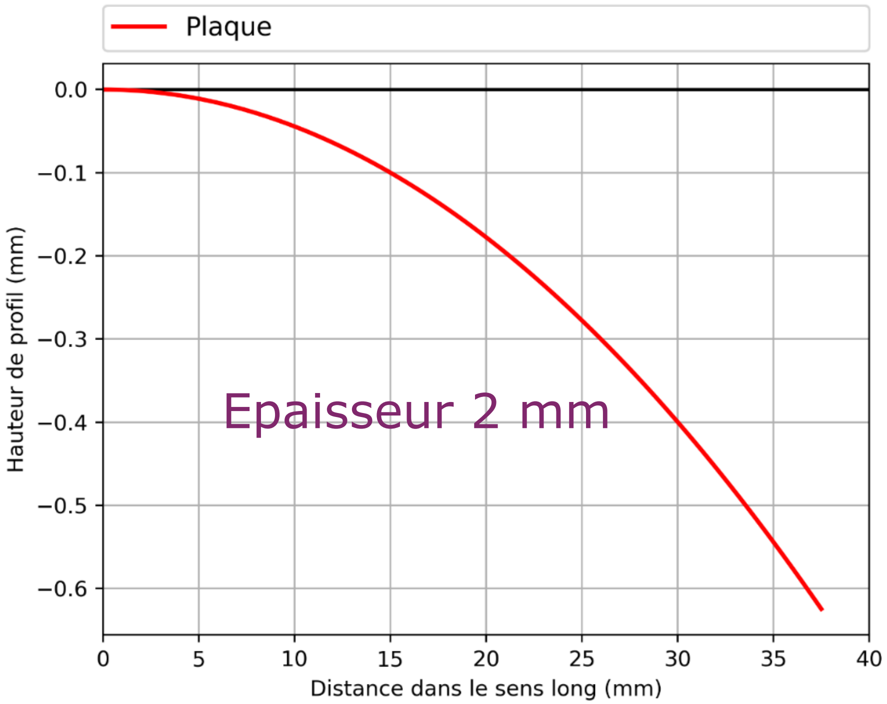
(a) Contraintes résiduelles (b) Contraintes normales (c) Contraintes de flexion (d) Contraintes vraies

Courbure induite

$$\gamma = \frac{M_x}{(1+\nu) \cdot D} \qquad D = -\frac{E \cdot H^3}{12 \cdot (1-\nu^2)}$$

Flèche dépend de la géométrie





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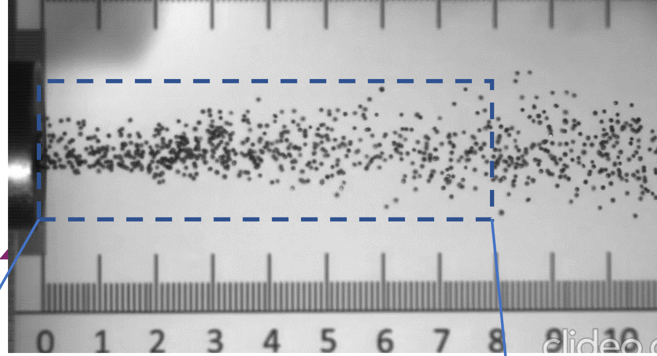
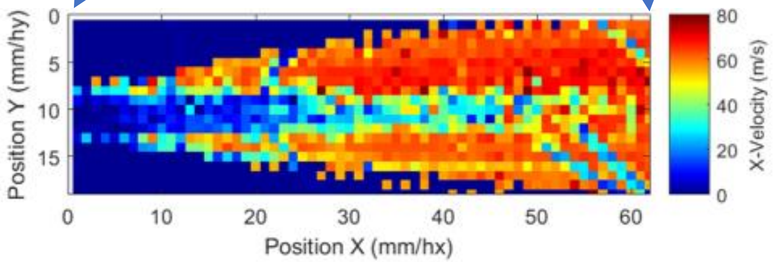
# Grenaillage de précontrainte


- ❑ Impact de grenailles en surface
  Paramètres procédé: media, vitesse (10-100 m/s), angle, recouvrement
- ❑ Déformation plastique en proche surface (10-~100 µm)
- ❑ Gradient de déformation plastique et de contraintes résiduelles
- ❑ Redistribution élastique sur structure




PT and DIC, [Kubler, Rotinat, Badreddine et al., 2020]




Plusieurs méthodes de modélisation du grenaillage:

- *Simulation de l'impact multibilles répété : couteux et, souvent, sur VER (ENSAM, UTT, INSA, KIT, PolyMtl…)*
- *Analyse élastoplastique simplifiée (Zarka, Inglebert 84)*
- Simulation par plaquage de champs par EF et rééquilibrage élastique

Au laboratoire MSMP: 13 Thèses « Grenaillage » depuis 1986:
Guechichi 86, Desvignes 87, Khabou 89, Cao 89, Masmoudi 90, Fathallah 94, Ahdad 96, Lillamand 98, Renaud 2011, Guiheux* 2016, Gelineau** 2018, Mauduit* 2018, Eschard 2024
Collaborations UTT** et LEM3*

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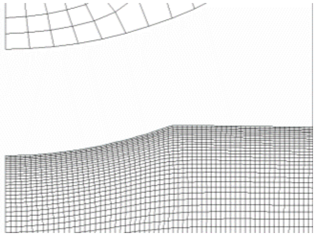
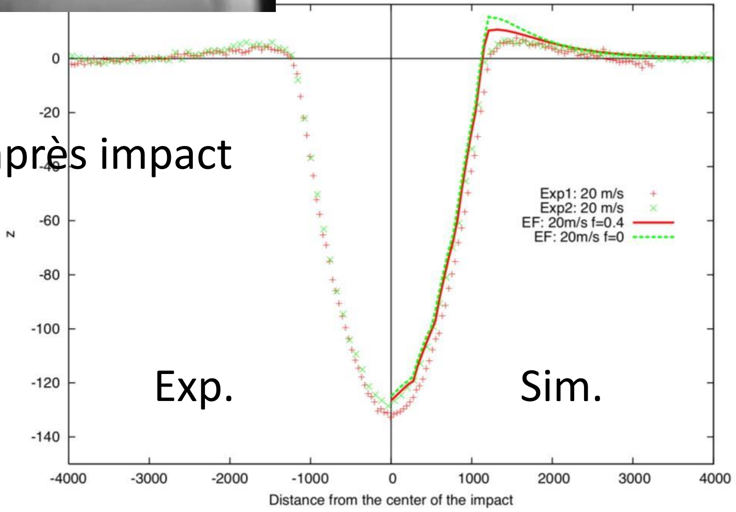
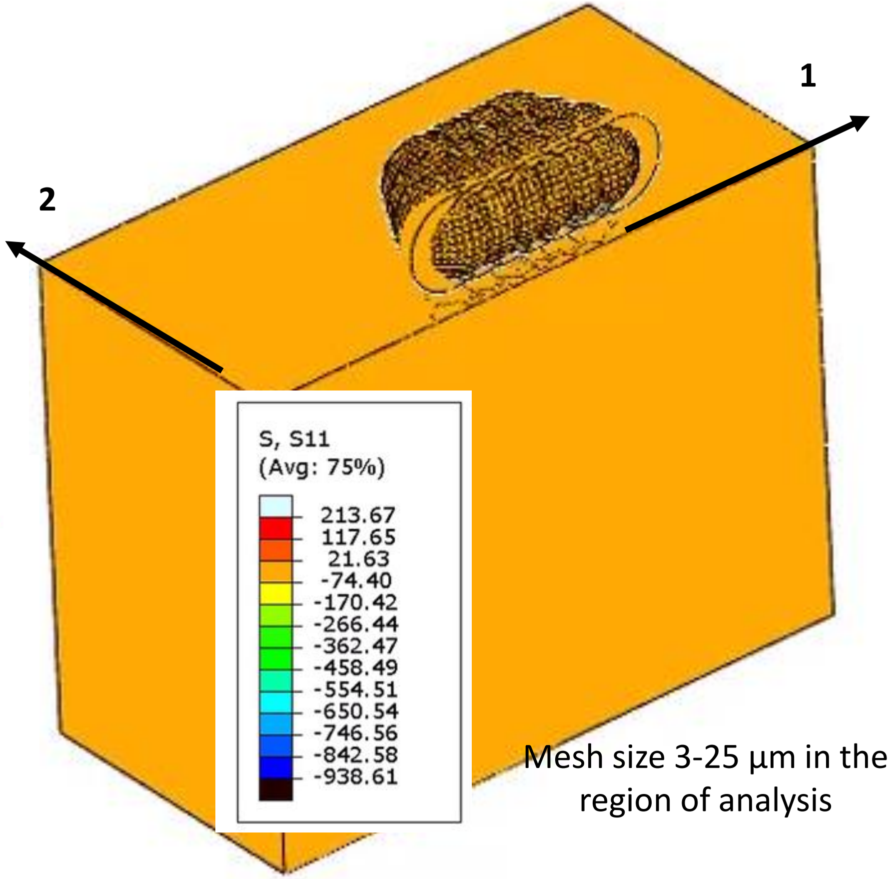
# Modèle Eléments Finis du grenaillage sur MSI:

- Impacts multiples sur MSI Multiple Abaqus Explicit (Renaud 2011, Kubler et al. 2019)
- Paramètres procédé – media ∅D, vitesse V, angle α, recouvrement C
- Comportement élasto(visco)plastique de la cible. Calibration des paramètres d'écrouissage cyclique

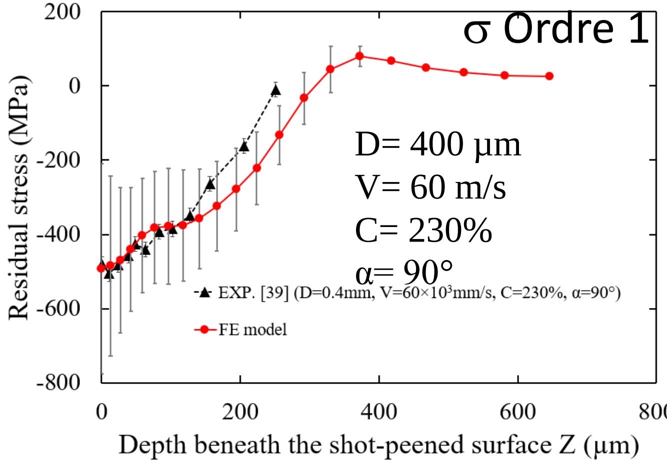
Calibration sur mono-impact

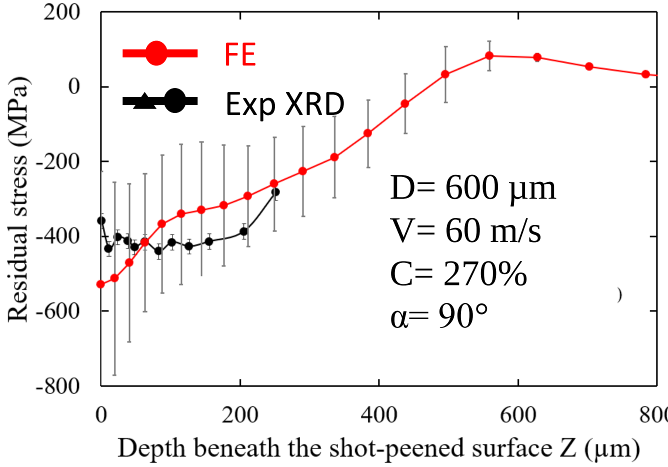





Mesh size 3-25 μm in the region of analysis




Guiheux, Kubler, Berveiller et al., Shot peening of TRIP780 steel, 2019
Modèle TRIP multiphasé évolutif (α, B, γ-> α')

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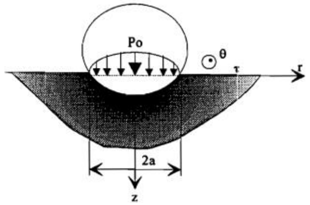
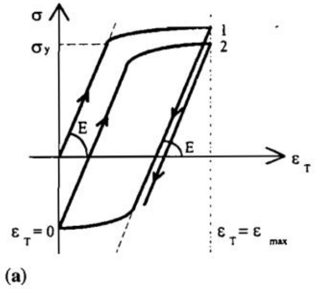
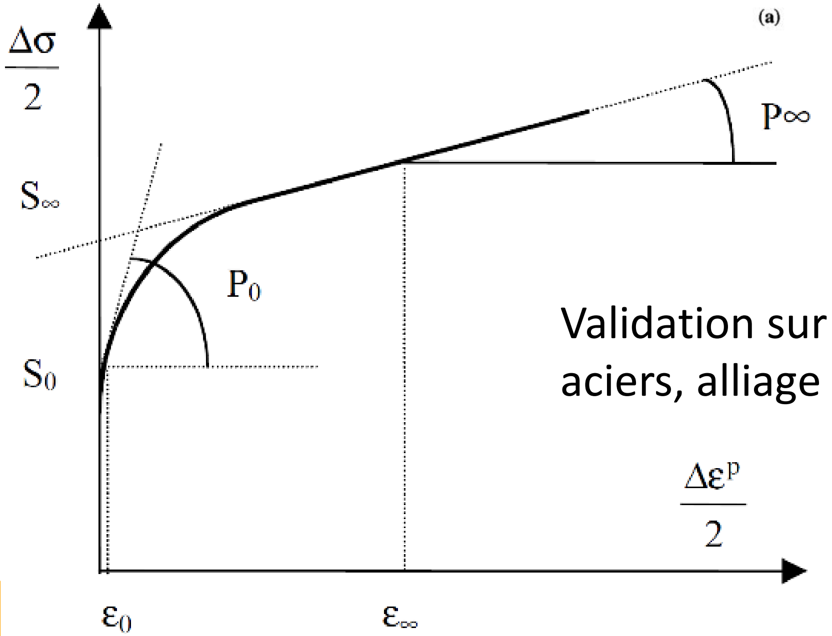
# Analyse élastoplastique simplifiée
# Grenaillage sur MSI


- Modèle de Zarka, Inglebert, 1984 / Implémentation industrielle PEENSTRESS (MIC)
- Similitude entre comportement cyclique et impacts répétés sur une structure (grenaillage)
- Grenaillage = chargement de Hertz + comportement élastoplastique cyclique du matériau



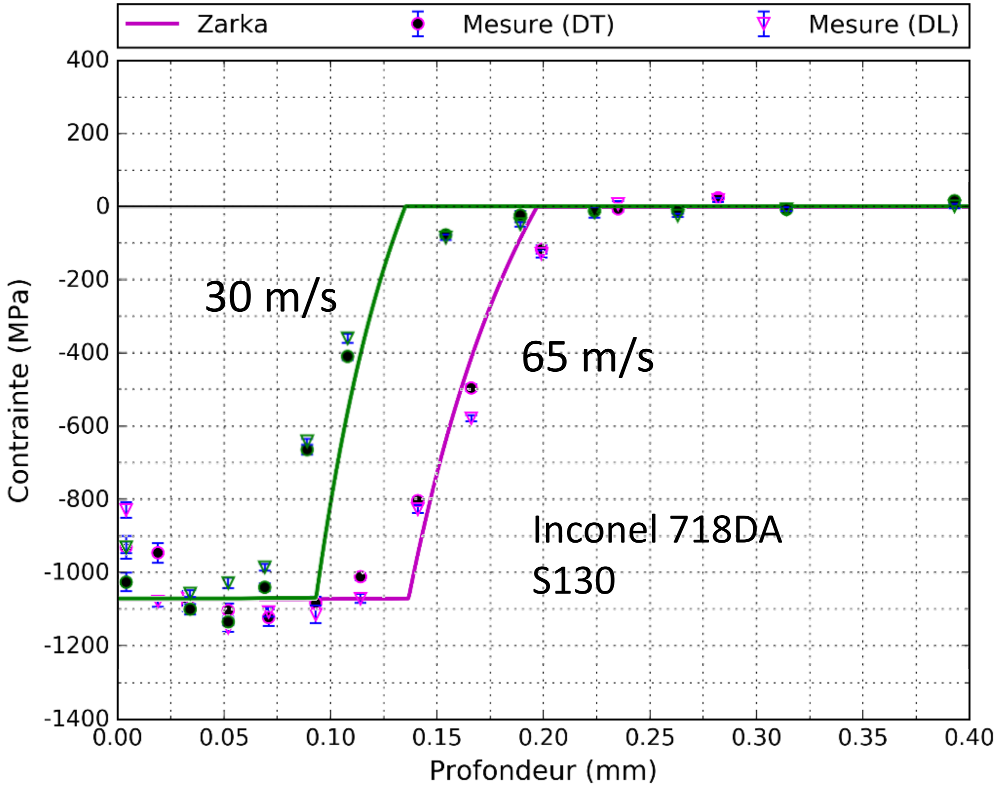

$$\underset{\sim}{\Sigma}^H = \begin{bmatrix} \Sigma^H_{rr}(z) & 0 & \Sigma^H_{rz}(z) \\ 0 & \Sigma^H_{\theta\theta}(z) & 0 \\ \Sigma^H_{rz}(z) & 0 & \Sigma^H_{zz}(z) \end{bmatrix}$$




Validation sur TiAl6V, aciers, alliage Al

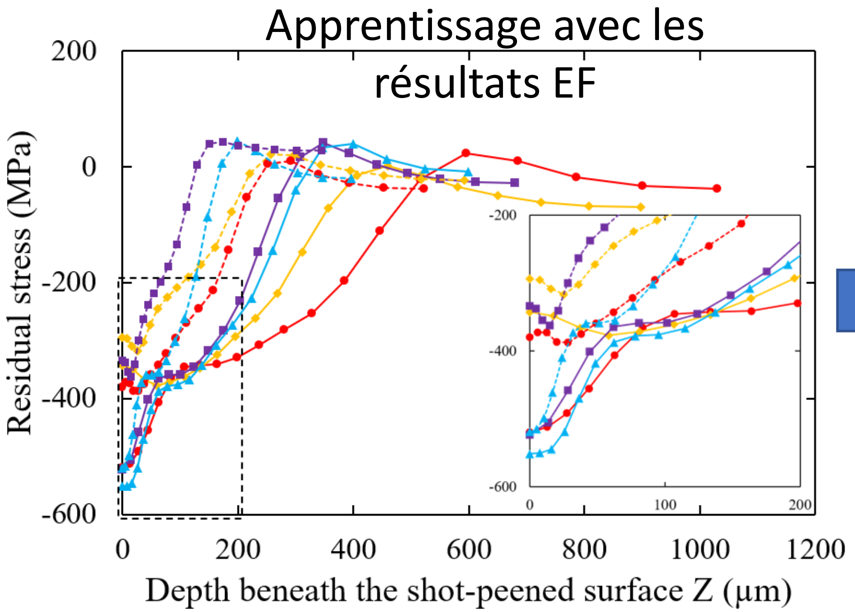
5 paramètres simplifiés de la loi d'écrouissage cyclique

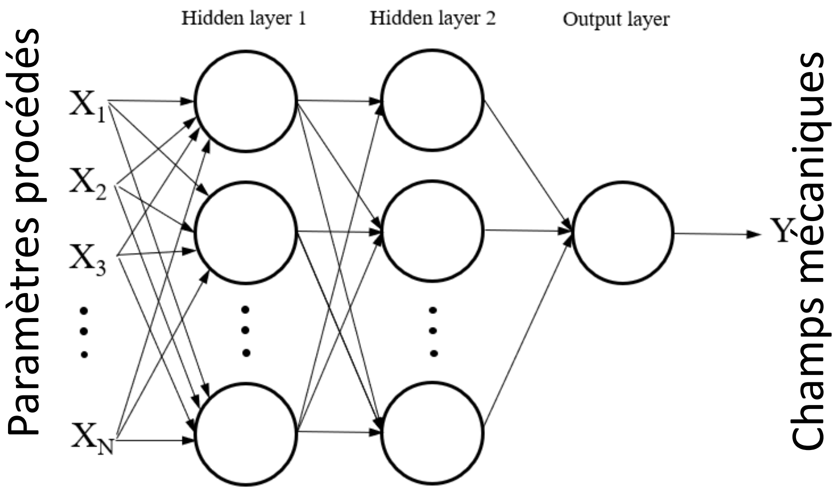


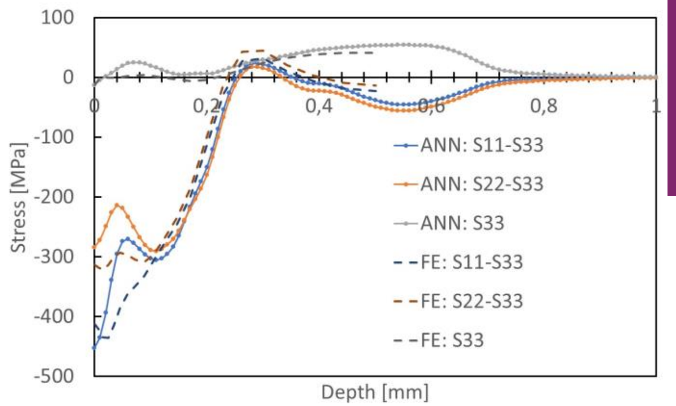

[PhD Gelineau 2018] ENSAM-UTT

# IA: Modèle Réseau de Neurones basé sur la simulation EF

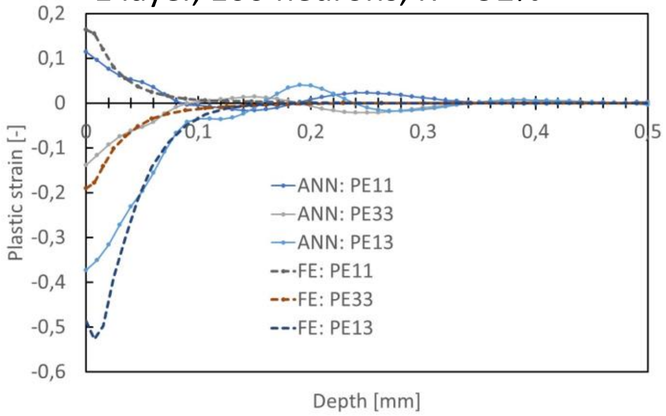
- Champs complets $\sigma_{ij}^R$, PEEQ, écrouissage

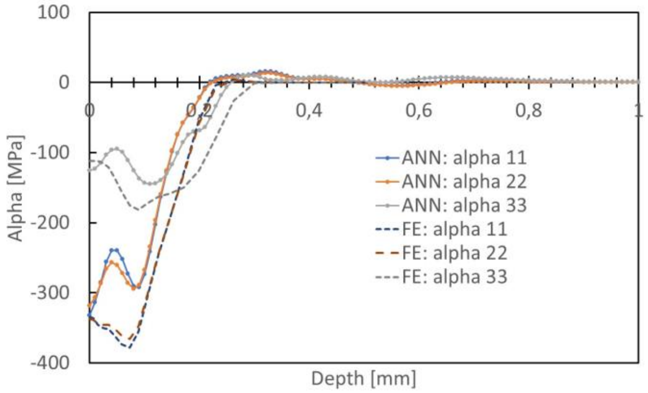



1 layer, 100 neurons, $R^2$= 92%




D= 300 µm, V= 80 m/s, C= 210%, α= 55°

- Cela fonctionne si ANN bien entrainé
- Perspectives:
  - ANN contraint
  - Respect des équations d'équilibre, de compatibilité
  - Cas non MSI

Daoud, M., Kubler, R. et al, 'Prediction of residual stress fields after shot-peening of TRIP780 steel with second-order and artificial neural network models based on multi-impact finite element simulations', Journal of Manufacturing Processes, 2021.

# Grenaillage de précontrainte et déformée

Automatisation dans Abaqus
(PYGINI, projet CONDOR, 2019)

Intégration d'un champ de contrainte autoéquilibré dans un code de calcul EF
- Méthode 1: champ thermique fictif
- **Méthode 2: initialisation des pseudo contraintes $\sigma^0$et rééquilibrage [Rouhaud 1997] [Gelineau 2018]**

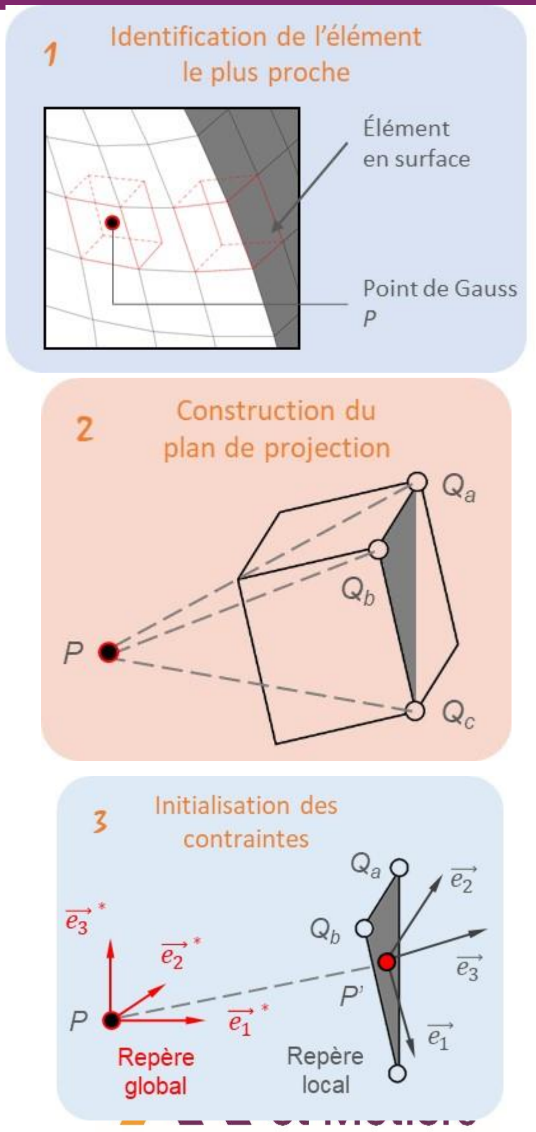
$$\underset{\sim}{\sigma}^0 = 2\mu \cdot \underset{\sim}{\varepsilon}^e + \lambda \cdot tr\left(\underset{\sim}{\varepsilon}^e\right) \cdot \underset{\sim}{I}$$

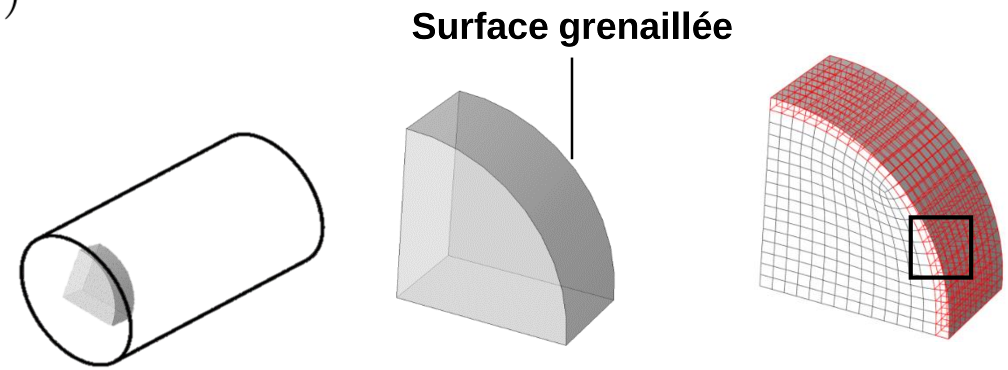
$$\underset{\sim}{\sigma}^0 = -2\mu \cdot \underset{\sim}{\varepsilon}^p = \begin{bmatrix} \sigma^0(z) & 0 & 0 \\ 0 & \sigma^0(z) & 0 \\ 0 & 0 & -2\sigma^0(z) \end{bmatrix}$$

$$\varepsilon^p_{xx}(z) = \frac{\nu - 1}{E} \cdot \sigma^R_{xx}(z)$$

- ❑ Pseudo contraintes à introduire avant équilibrage

$$\sigma^0_{xx}(z) = \frac{1-\nu}{1+\nu} \cdot \sigma^R_{xx}(z)$$



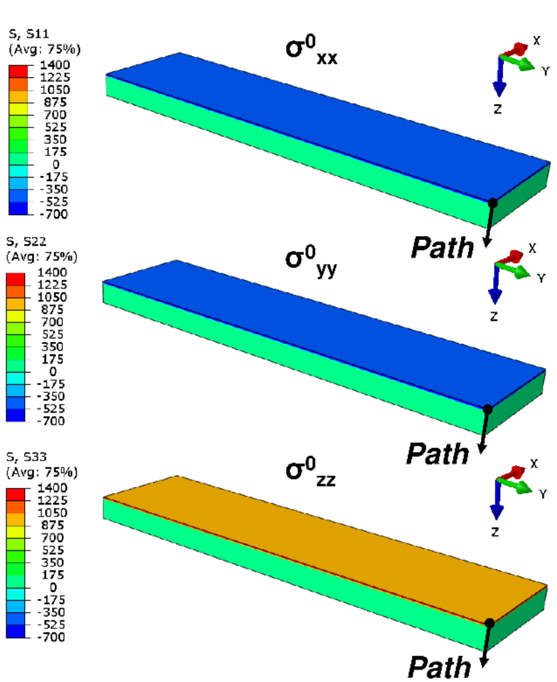




PhD Gelineau 2018, ENSAM - UTT

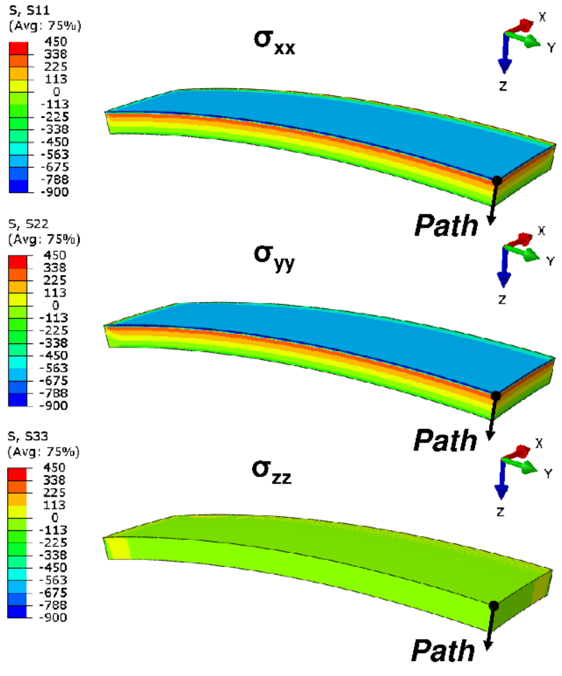
# Initialisation des $\sigma$ par EF sur plaque mince grenaillée (e=2 mm)

$$\sigma^0(z) = \frac{1-\nu}{1+\nu} \cdot \sigma(z)$$

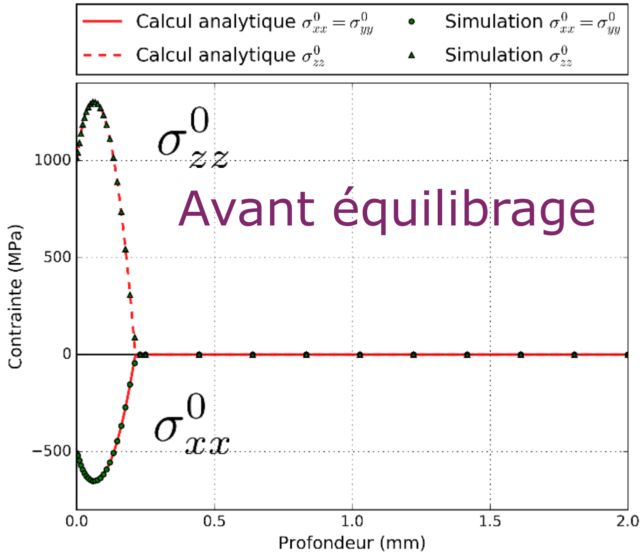
Analyse Exp.

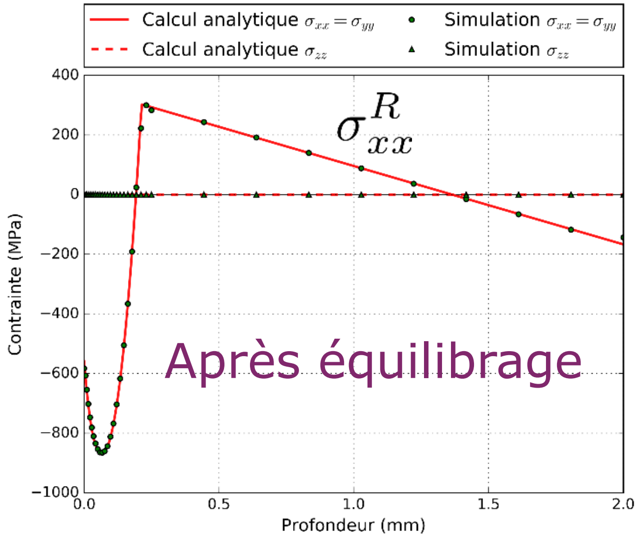


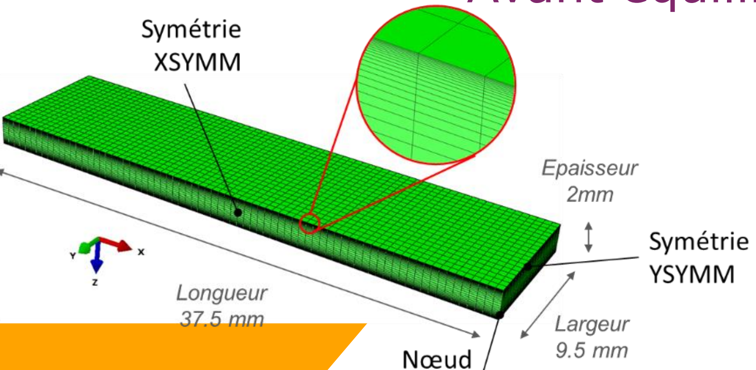

Avant équilibrage




Après équilibrage

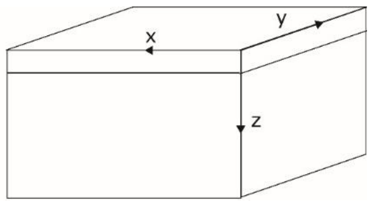


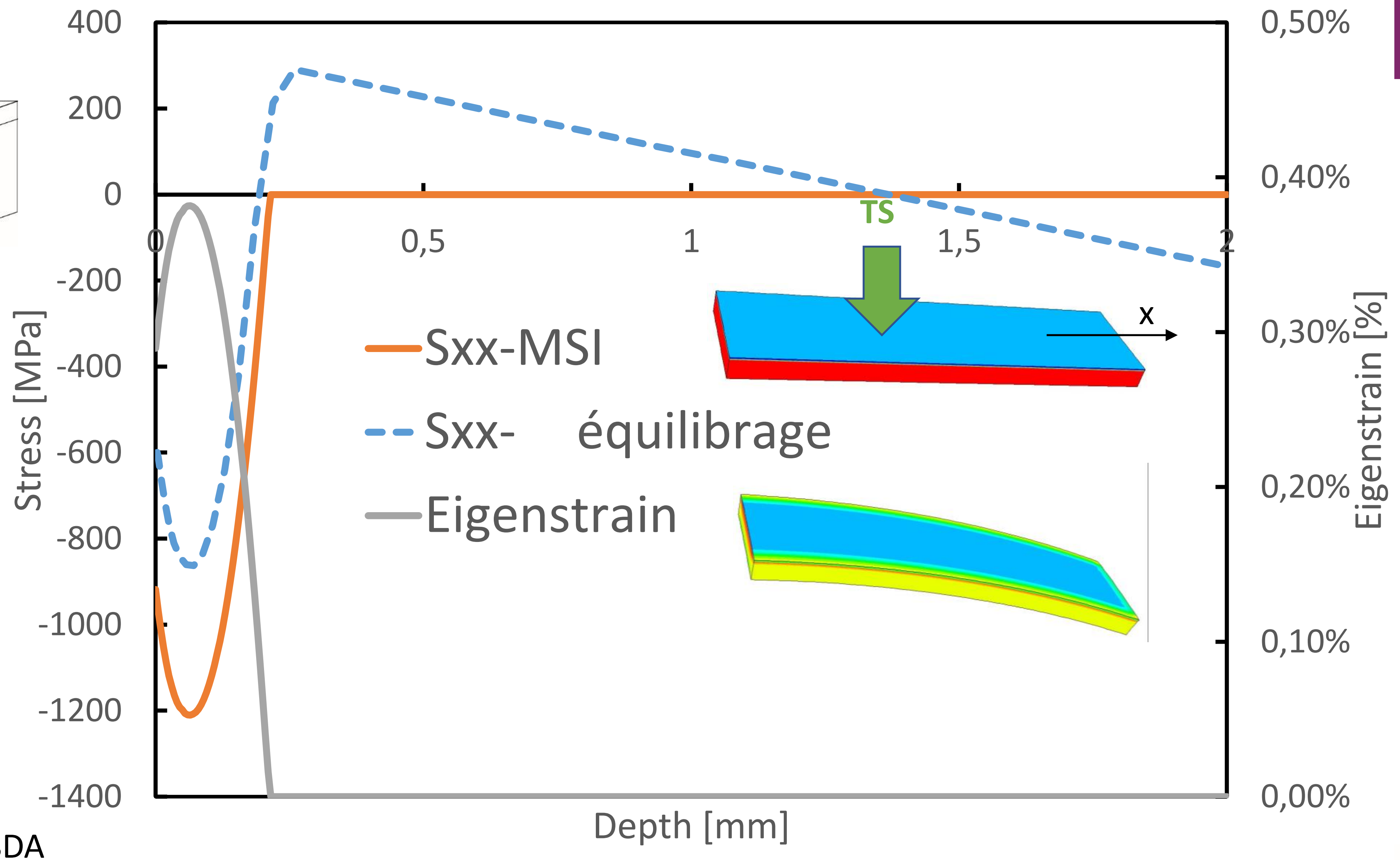




[PhD Gelineau 2018] ENSAM-UTT, Matériau Inco 718DA

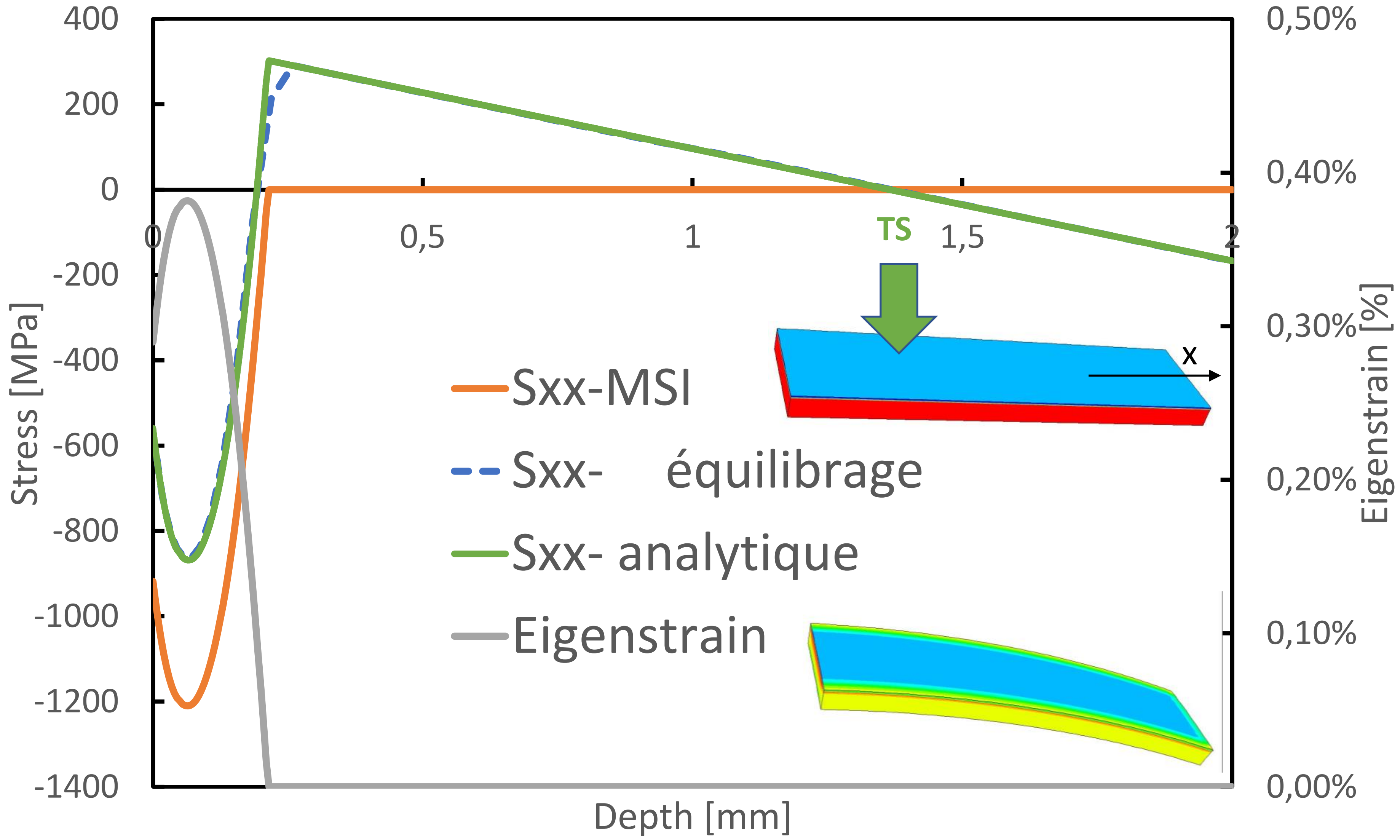
# CR sur plaque mince grenaillée (e=2 mm)




Matériau Inco 718DA

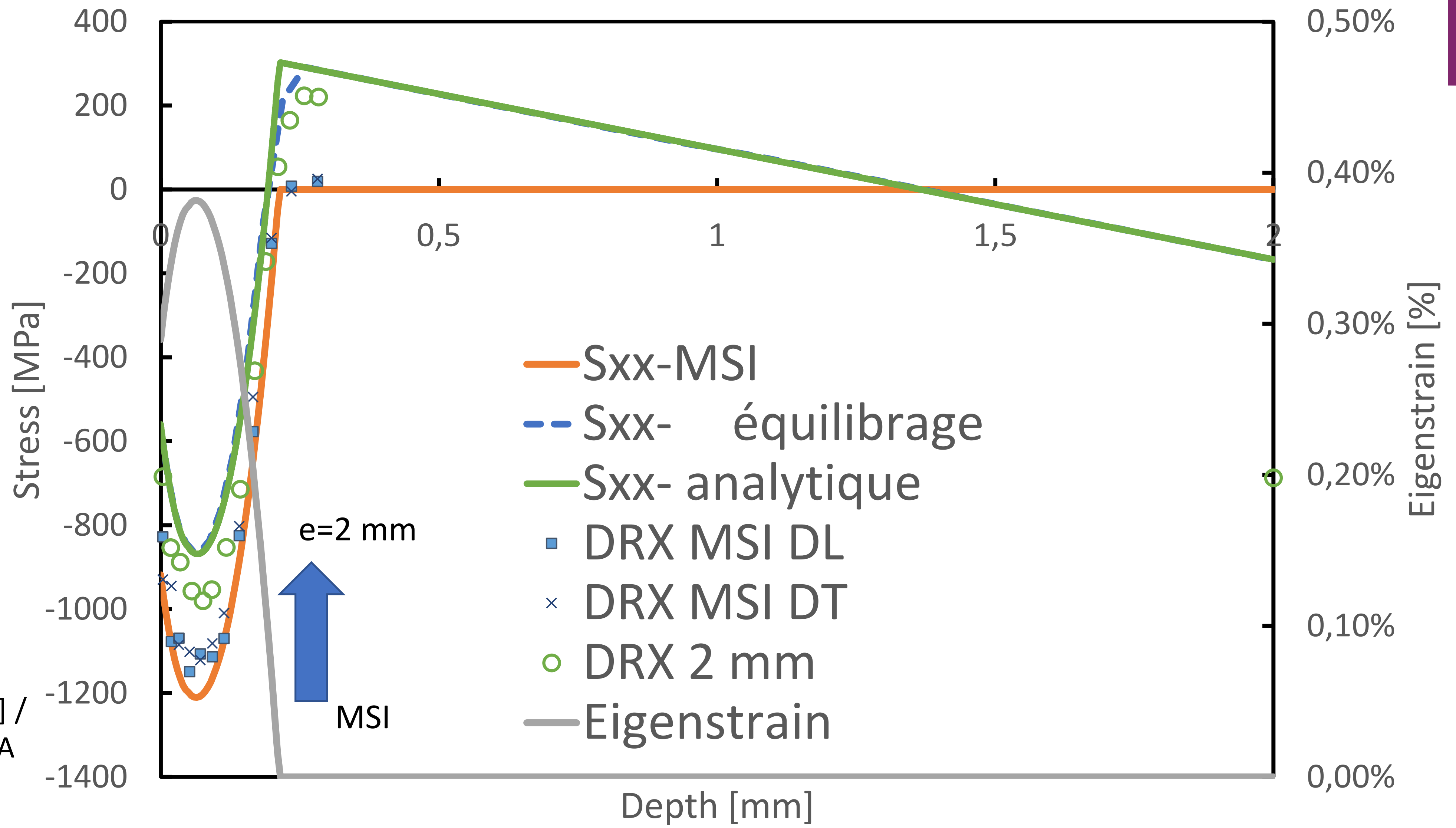
# CR sur plaque mince grenaillée (e=2 mm)




Matériau Inco 718DA

Modèle EF identique au modèle analytique

# CR sur plaque mince grenaillée (e=2 mm)



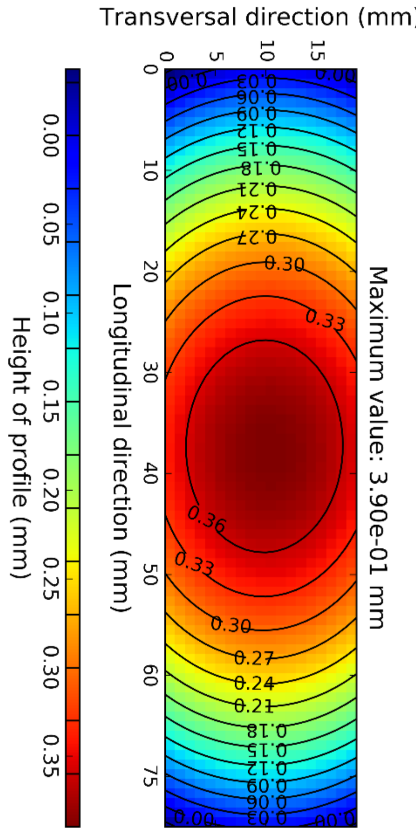

Data
[PhD Gelineau 2018] /
Matériau Inco 718DA

Modèles en bon accord avec l'expérience

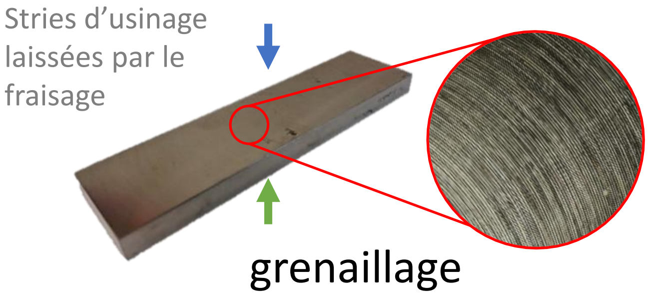
# Déformée sur plaque mince grenaillée (e=2 mm)

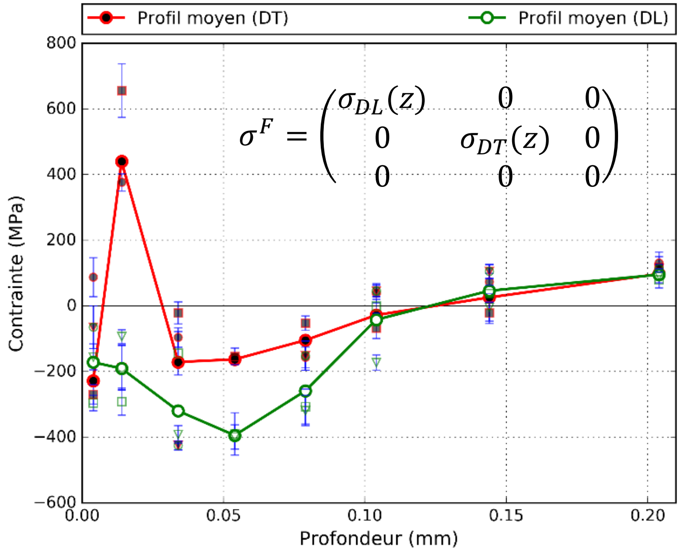
- Déformée d'une plaque mince grenaillée (e= 2 mm)

## Mesure MMT

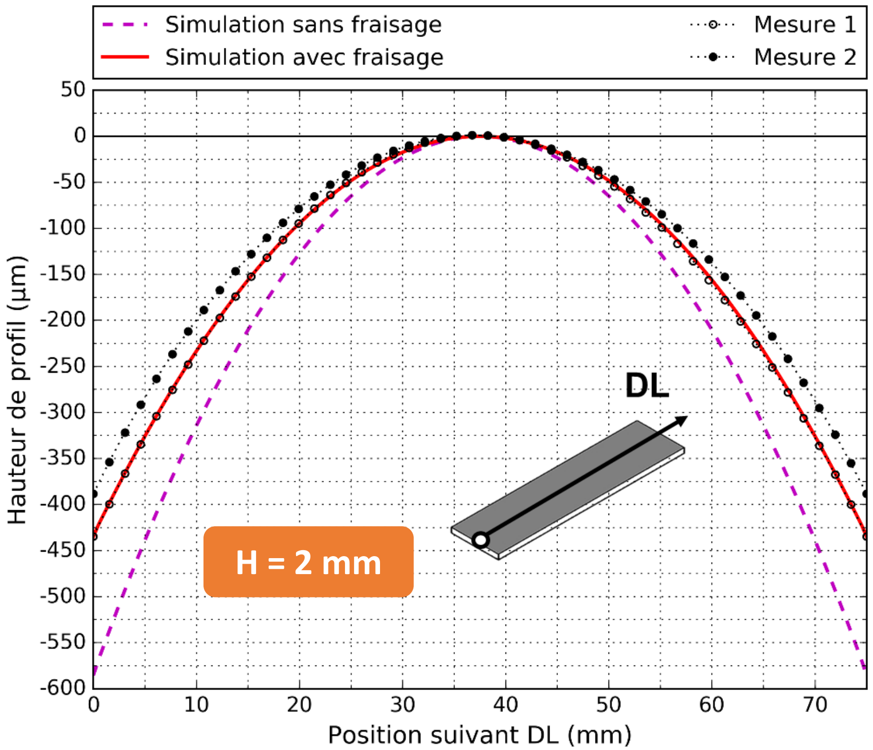



## Fraisage

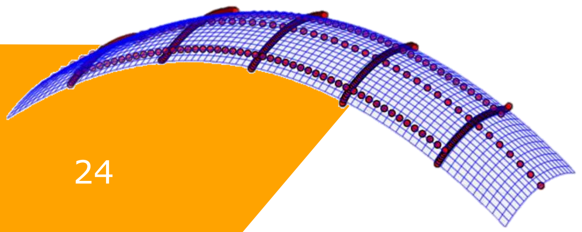



## Mesure vs modèle EF



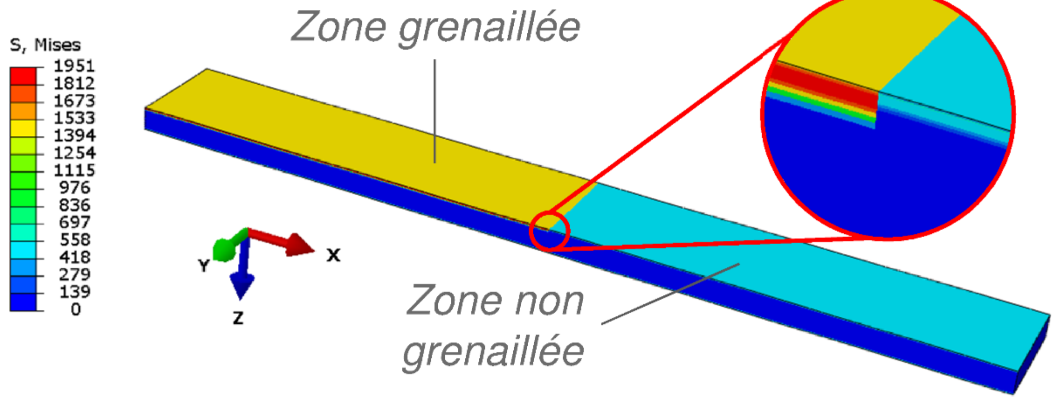

Prise en compte des CR issues du fraisage sur la face opposée

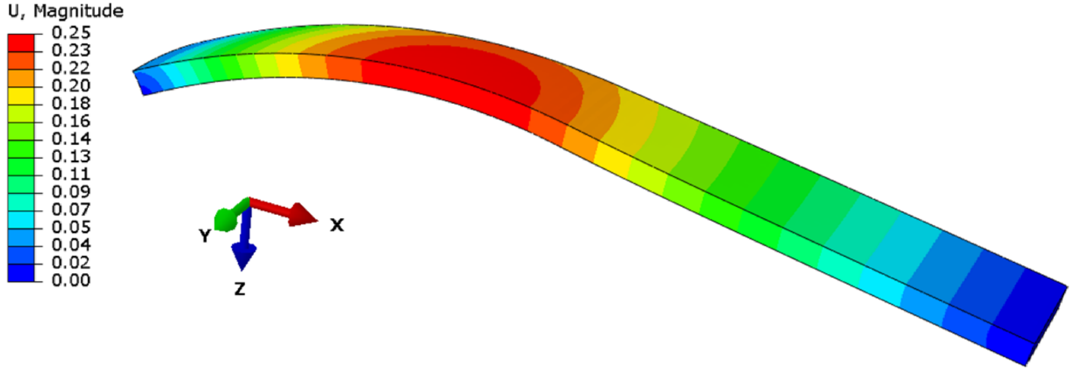


[PhD Gelineau 2018], ENSAM-UTT

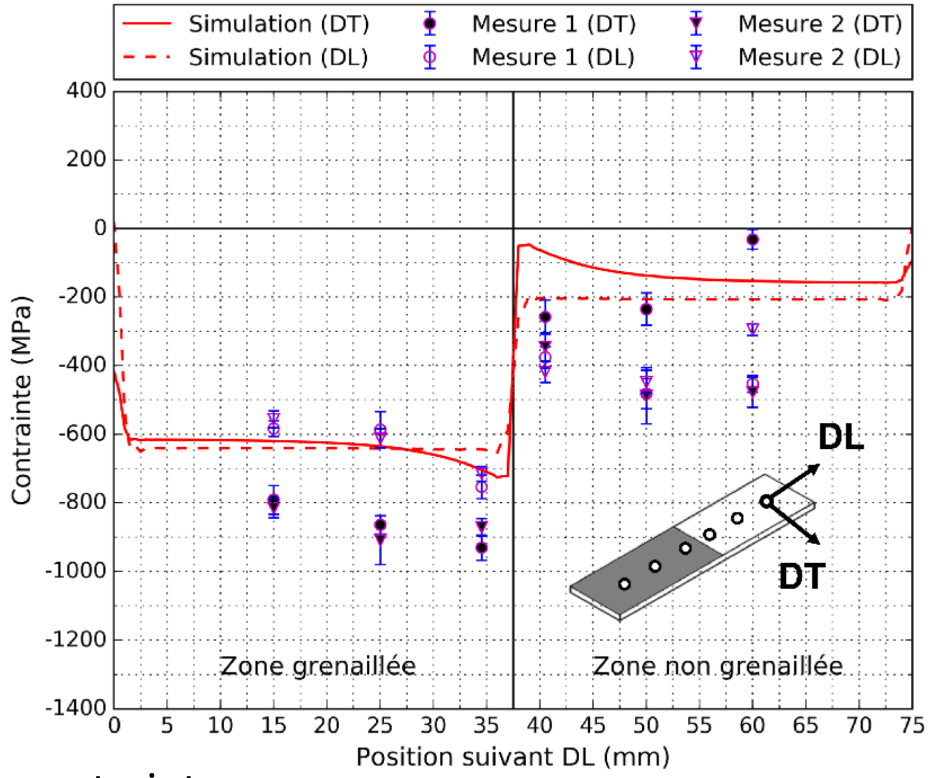
# Déformée sur plaque mince grenaillée (e=2 mm)

- plaque mince grenaillée **partiellement** (e= 2 mm)




Comparaison Expérience
Modélisation CR en surface



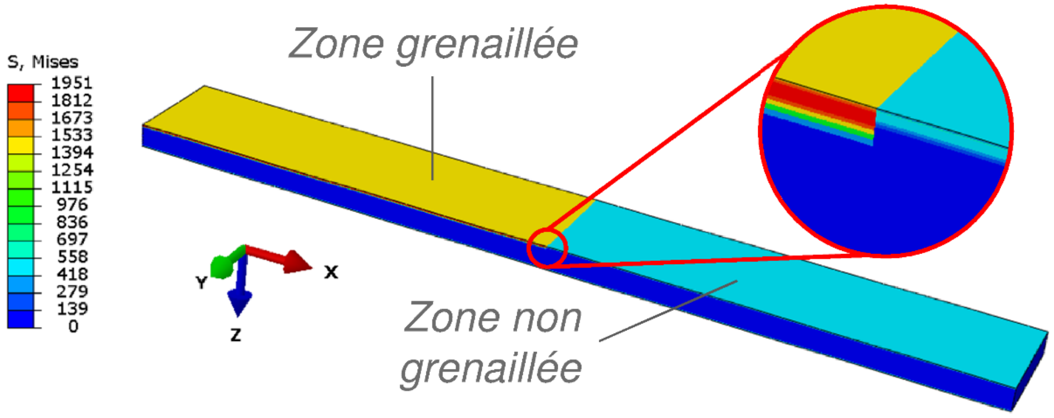

[PhD Gelineau 2018]

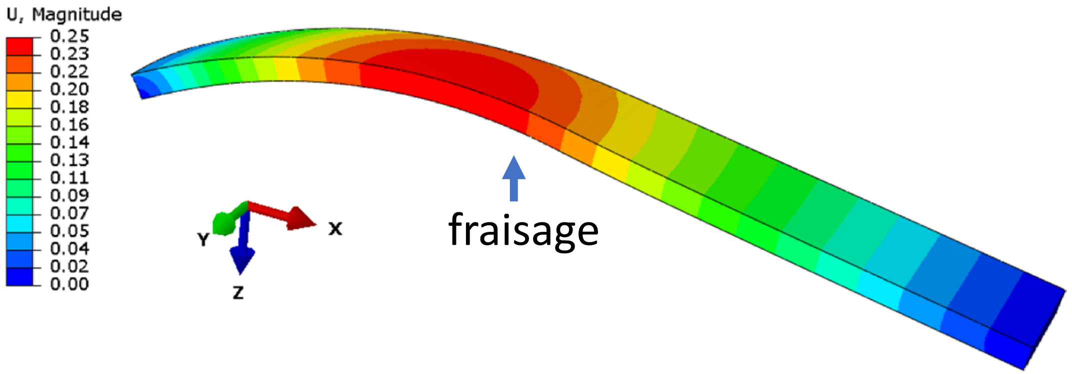
Zone non grenaillée affectée par les contraintes

Matériau Inco 718DA

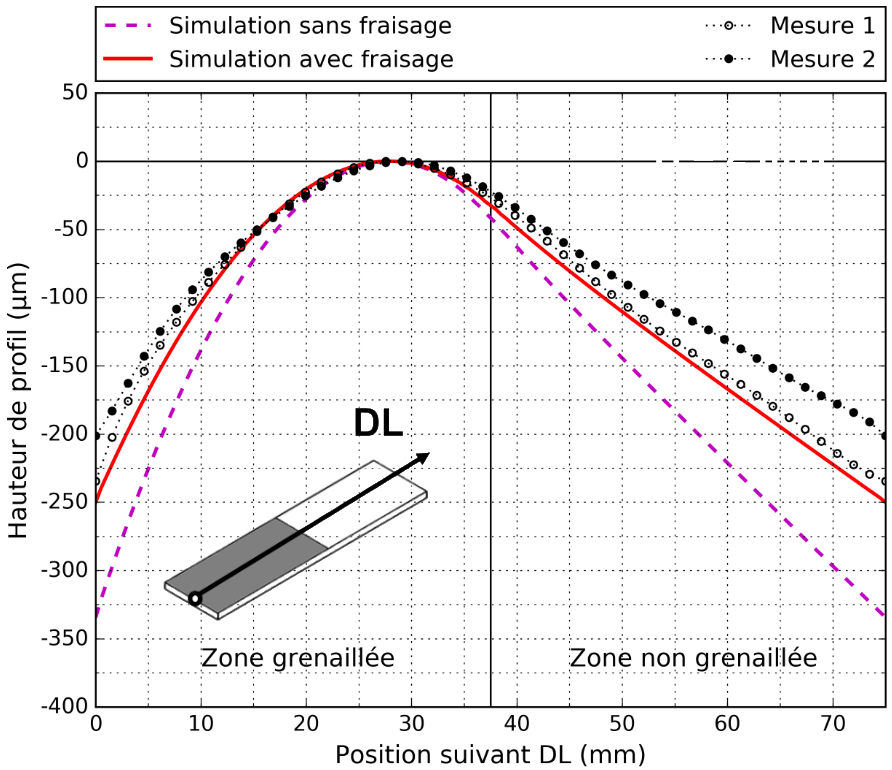
# Déformée sur plaque mince grenaillée (e=2 mm)

- plaque mince grenaillée **partiellement** (e= 2 mm)




Comparaison Expérience Modélisation Déformée



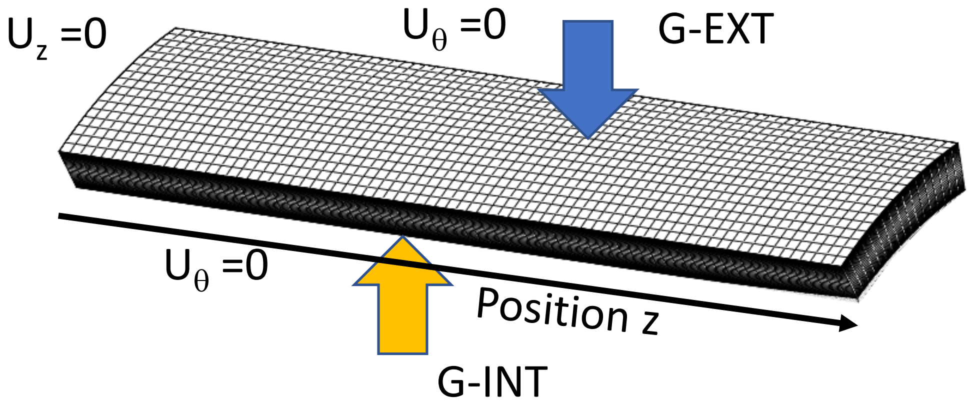

Prédiction de la déformée en tenant compte du fraisage sur la face opposée

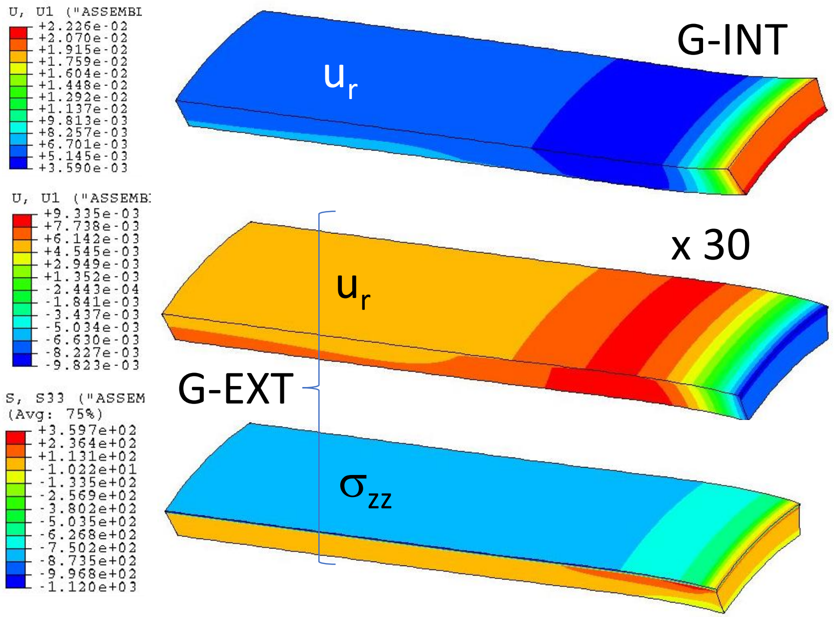
[PhD Gelineau 2018]

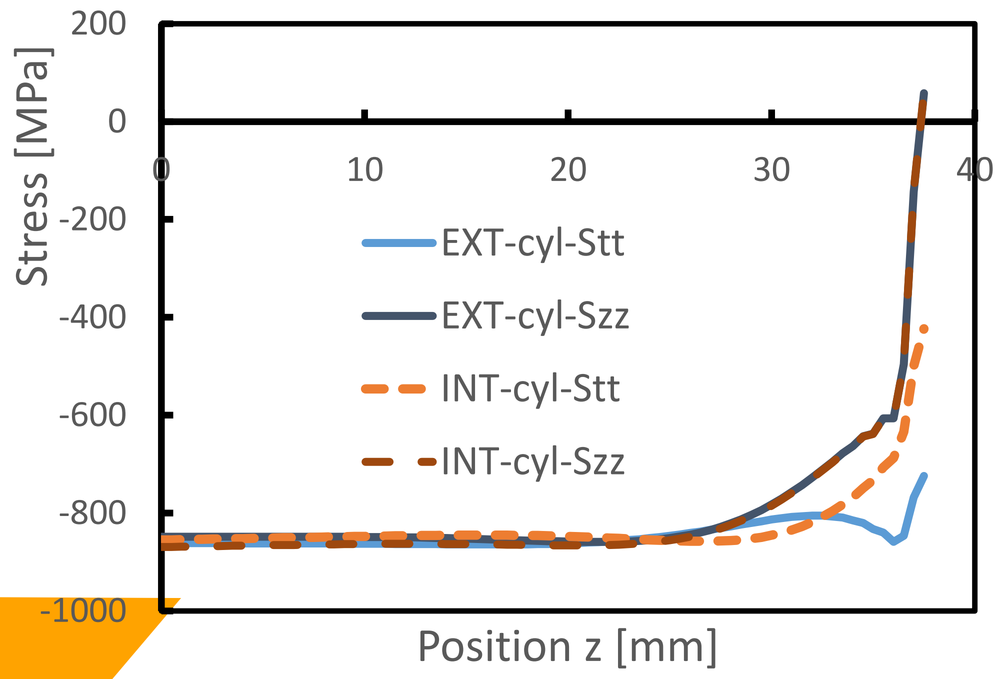
Matériau Inco 718DA

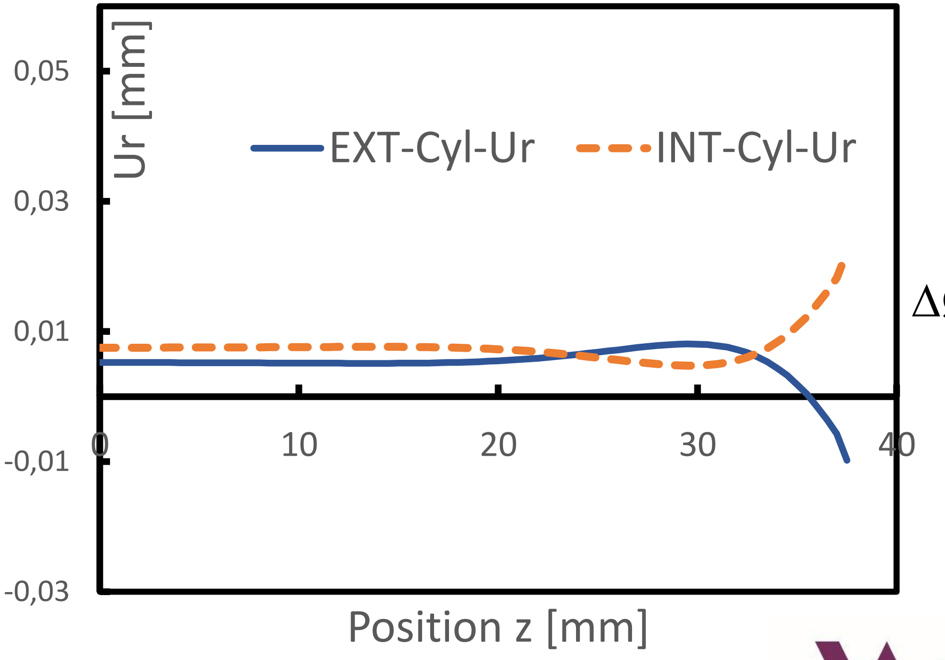
# Application à la déformée d'un tube circulaire grenaillé

Tube $\varnothing_{int}$= 40 mm, e= 2 mm, L= 37.5 mm



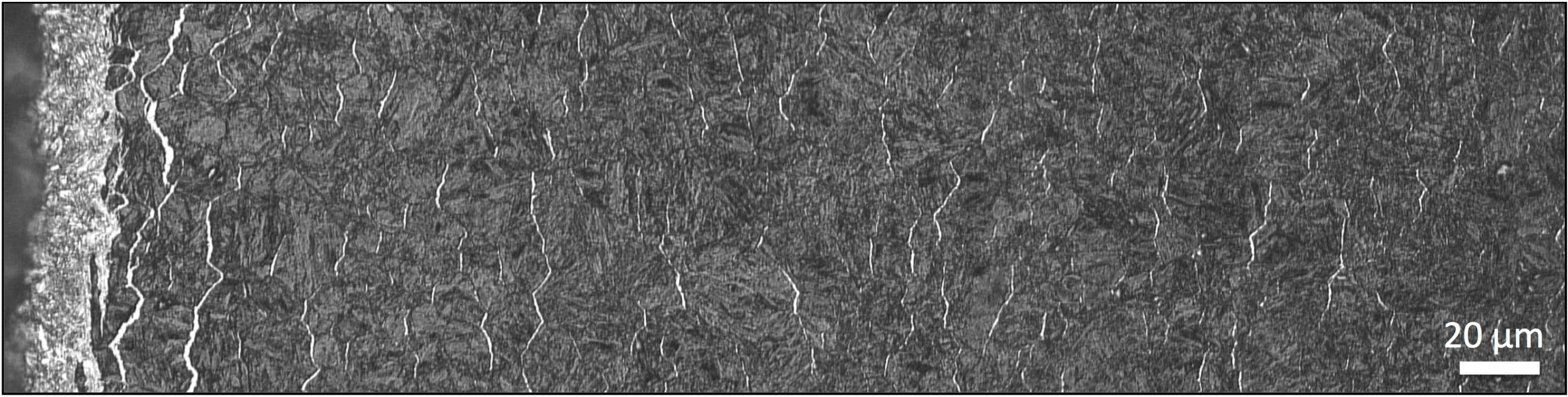




$\Delta\varnothing$= 20-40 µm

# Nitriding surface treatment



- Metallurgy of nitriding carbon steels (gas nitrided of 32CrMoV13)
- Mechanical properties of nitriding layers
- Residual stress generation mechanisms and evolution during complex thermocanical loadings
- Modeling of diffusion/precipitation and stress generation using multiphysic and multiscale approaches (and AI)
- Numerical tools
- Goal : integrated approach from the nitriding parameters to the durability and fatigue life



# Nitriding @ MSMP Lab.

## 13 PhD thesis

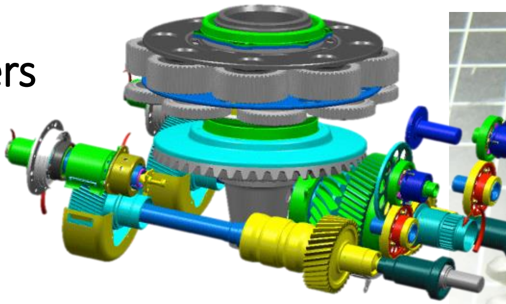
- 2025 – **P.Razafimahefa**, 4.0 nitring (or using AI), AERONIT IRT M2P
- 2024 – **F.Delabre**, Nitriding used in OG electric steel processing
- 2023 – **Y.Zhang**, Gas nitriding of tool steels
- 2022 – **L.Germain**, Stress influences of diffusion, case of gas nitriding surface treatment
- 2018 – **F.Godet**, Relations microstructure/behavior at the fatigue crack initiation – multiscale approach for the33CrMoV12-9 steel, NITRU project IRT M2P
- 2017 – **H.Weil**, Fatigue life of nitriding layers, optimization of process parameters
- 2016 – **B.Guillot**, Étude de procédés de préparation de surface avant nitruration, FUI DEFINIT
- 2015 – **G.Fallot**, Rôle du carbone lors de la nitruration d'aciers de construction et influence sur les propriétés mécaniques
- 2009 – **S.Jégou**, Influence des éléments d'alliage sur les contraintes résiduelles
- 2006 – **V.Goret**, Modélisation du traitement de nitruration
- 2000 – **M.Chaussumier**, Modèle de calculs en fatigue multiaxiale
- 1998 – **J-N.Loquet**, Caractérisations métallurgique et mécanique
- 1992 – **L.Barrallier**, Genèse des contraintes résiduelles

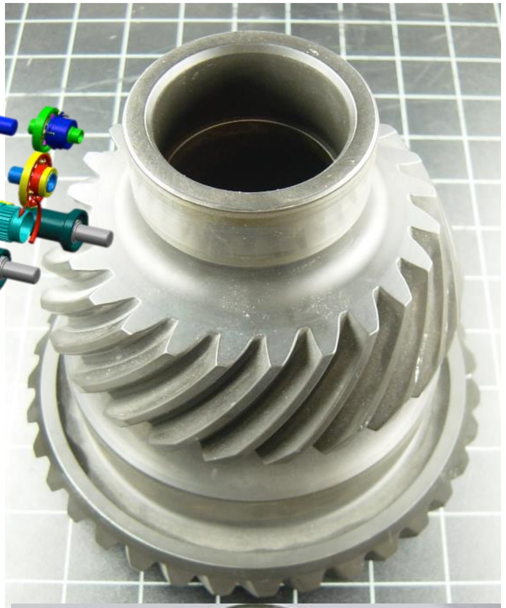
## Industrial partners

- Airbus
- Safran
- Naval Group
- NTN-SNR
- ALD
- Bodycote
- Renault Sport F1
- Transvalor
- LISI Automotive
- ThyssenKrupp Electrical Steel

## Academic, institutional partners

- Lorraine University, IJL
- INSA Lyon, LAMCOS
- DTU, Pr. M.A.J. Somers
- IRT M2P





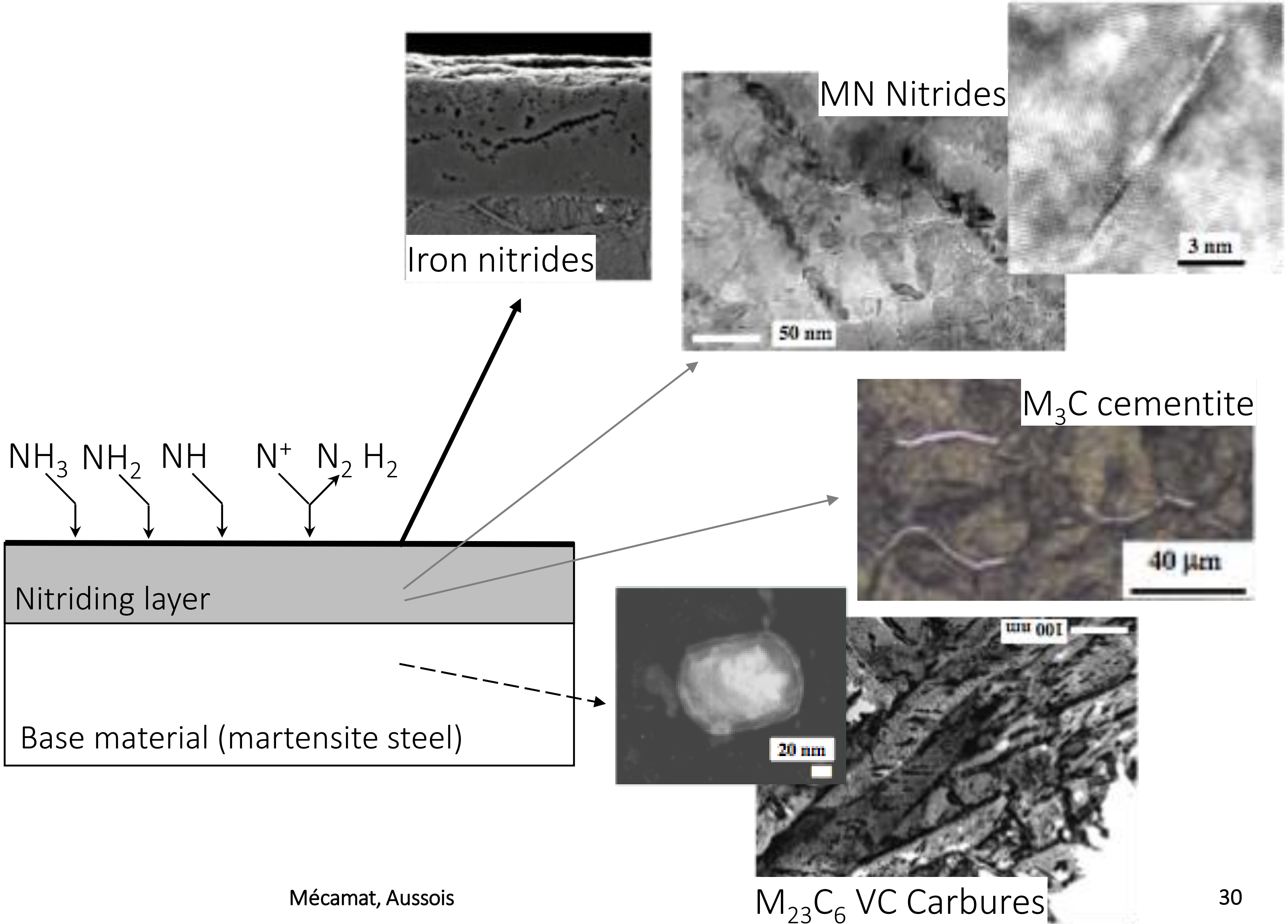
# Microstructure of nitriding carbon steels

- Gaz nitriding
- $T_N$ : 450-550°C
- $t_N$ : 10-100 h
- $K_N$ : nitrogen potential

- Increasing fatigue life, wear and corrosion resistance

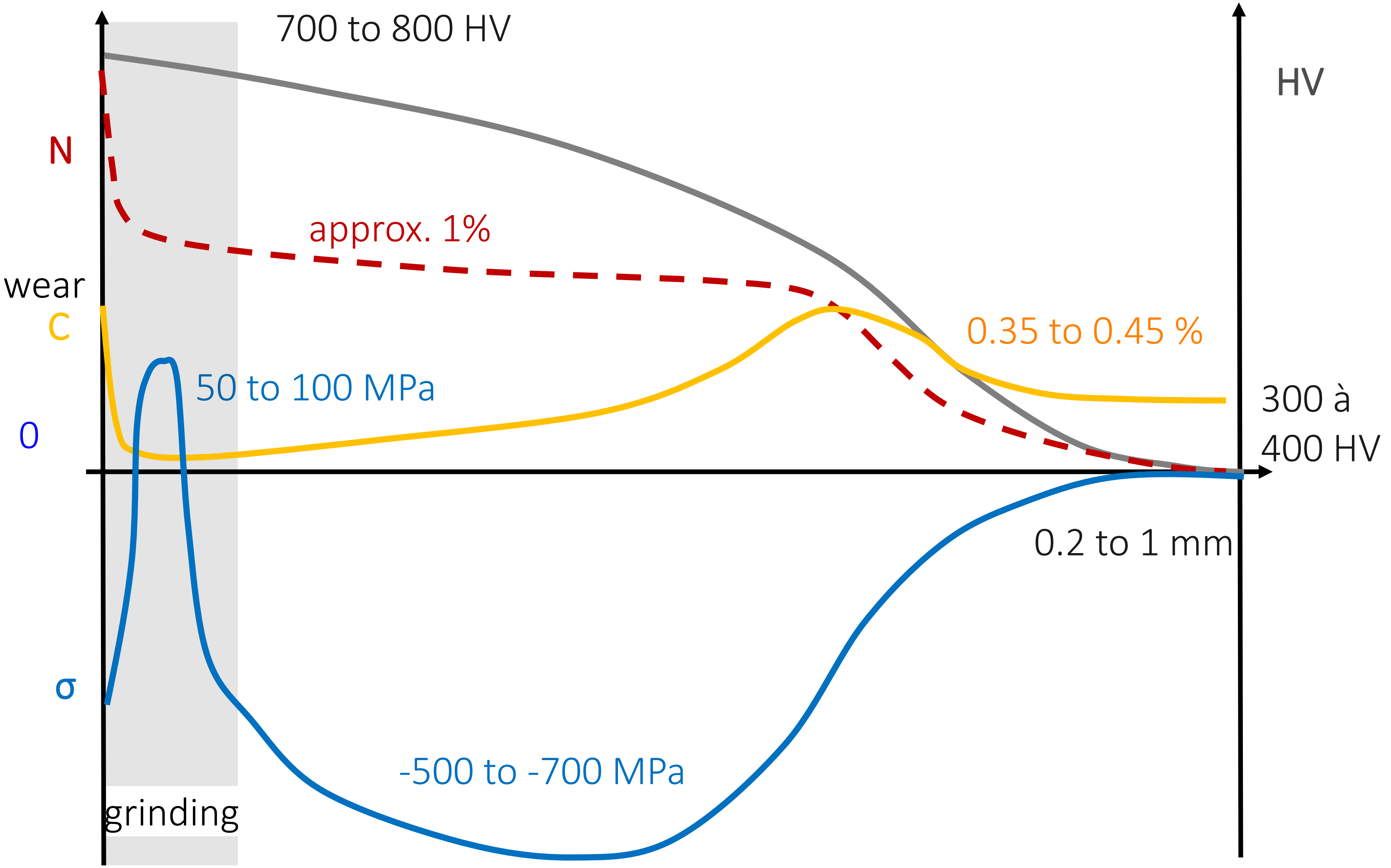
**Adsorption effect**

**Microstructure gradient generation**



# Microstructure of nitriding carbon steels

- Nitrogen and carbon co-diffusion
- Hardness
- Residual stresses
- Improvement of fatigue life, wear and corrosion resistance



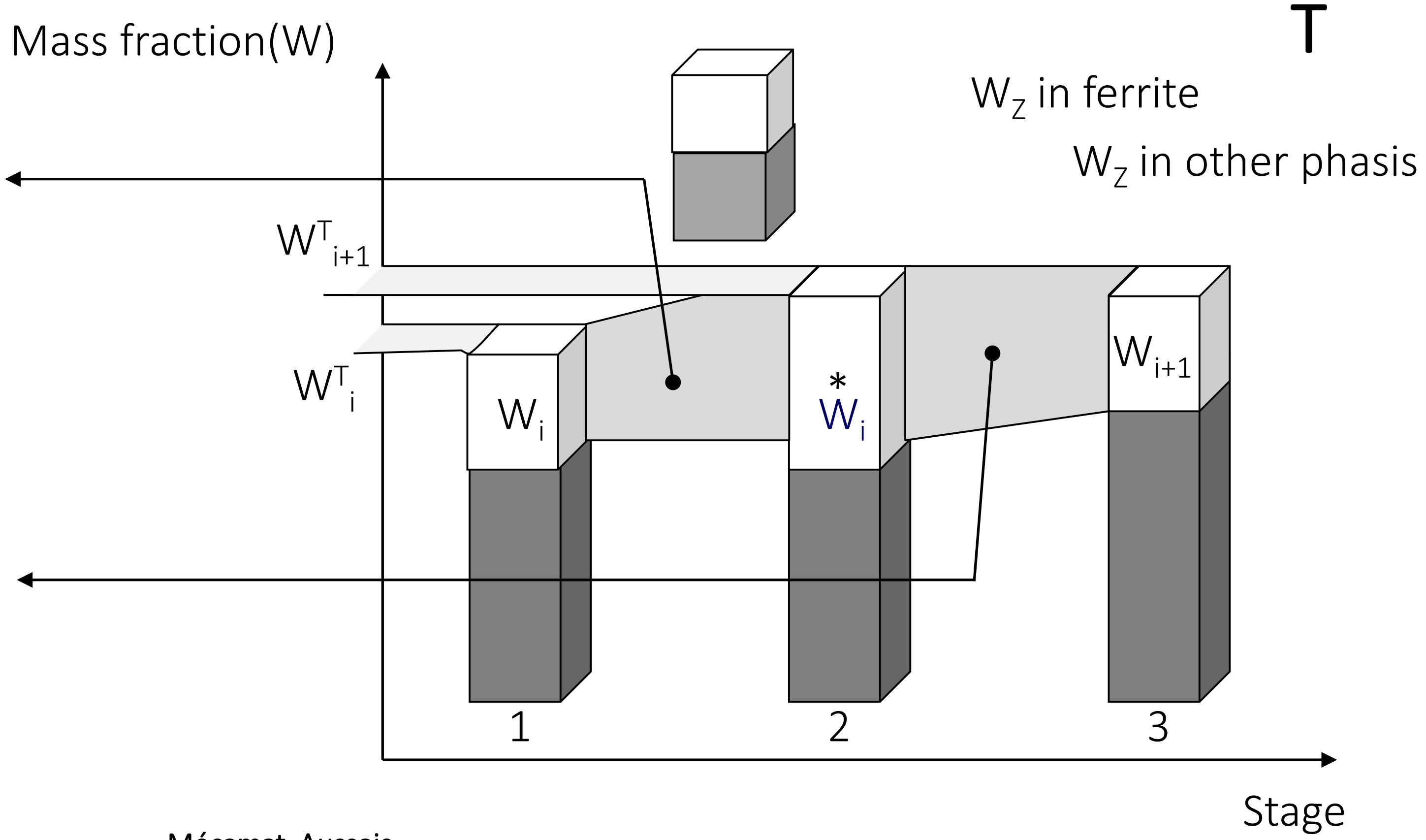
# Nitriding simulation
## Metallurgy

- Nitrogen and carbon co-diffusion
- Superficial decarburizing effect

Now DICTRA ?

Diffusion equation: long distance
Azote and carbone
Effective Diffusion Coefficients
Boundary conditions: N inflow, C outflow?
Mechanic?

Thermodynamique software: short distance
Material composition
Thermodynamique equilibrum?



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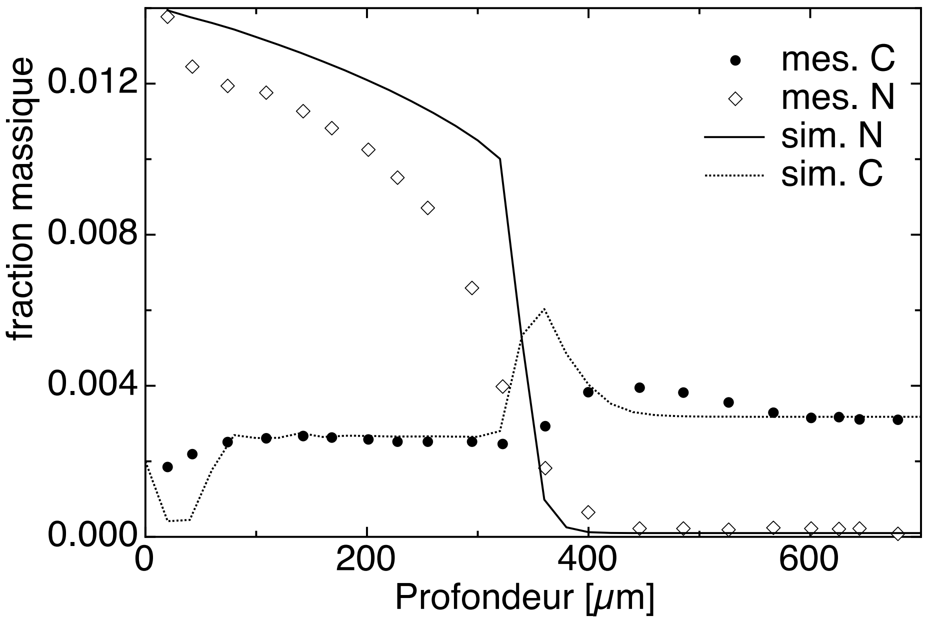
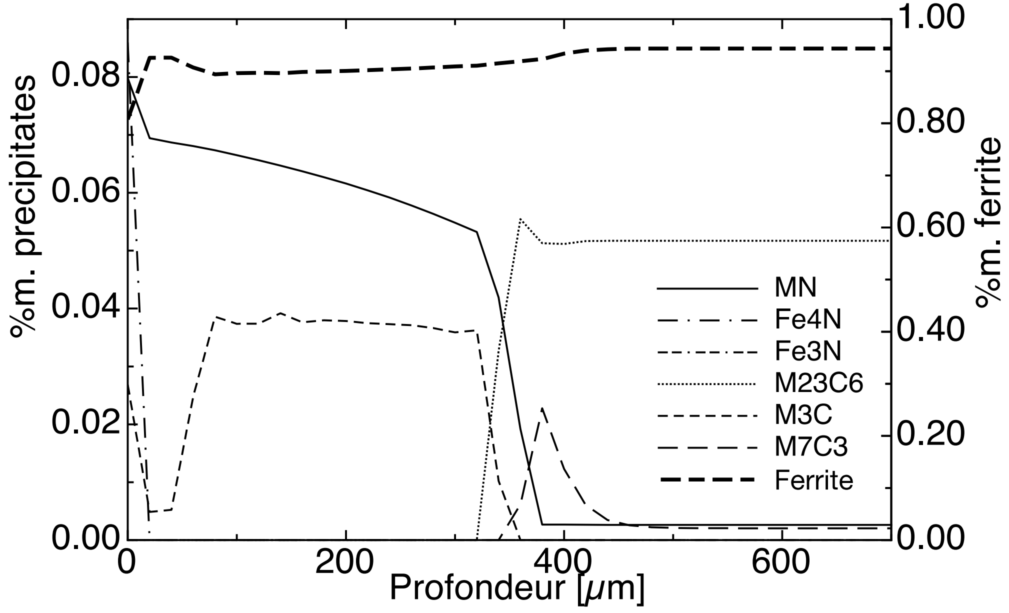
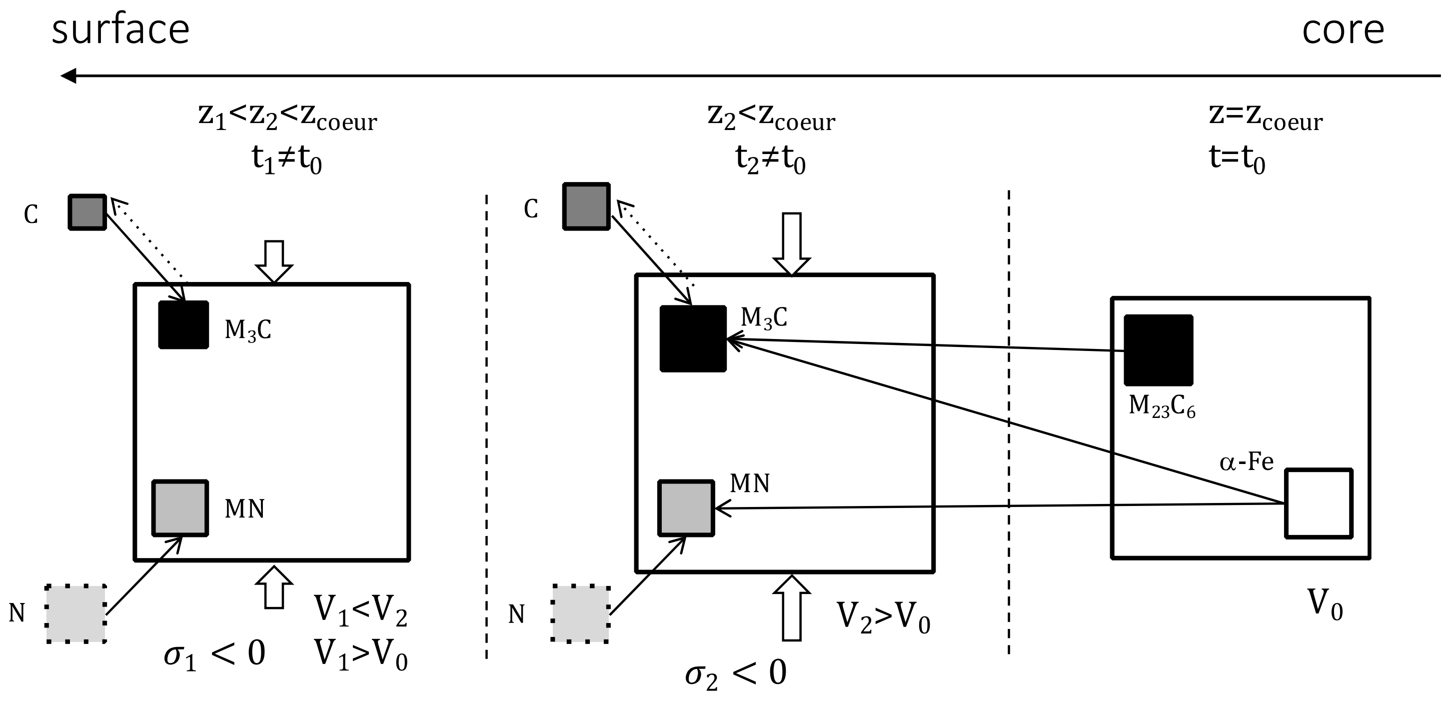


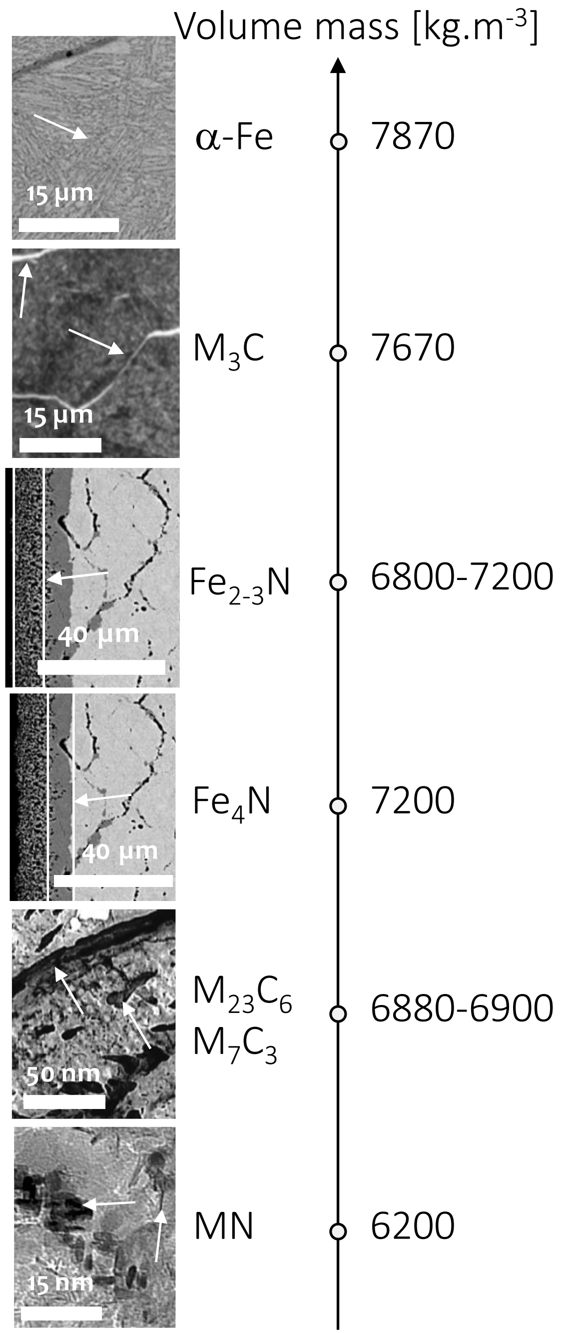




32CrMoV13, T=520°C, t=50 h, $K_N$=4,3 atm$^{-1/2}$

[Data Thèse B.Guillot 2016]

# Nitriding simulation
## Mechanics

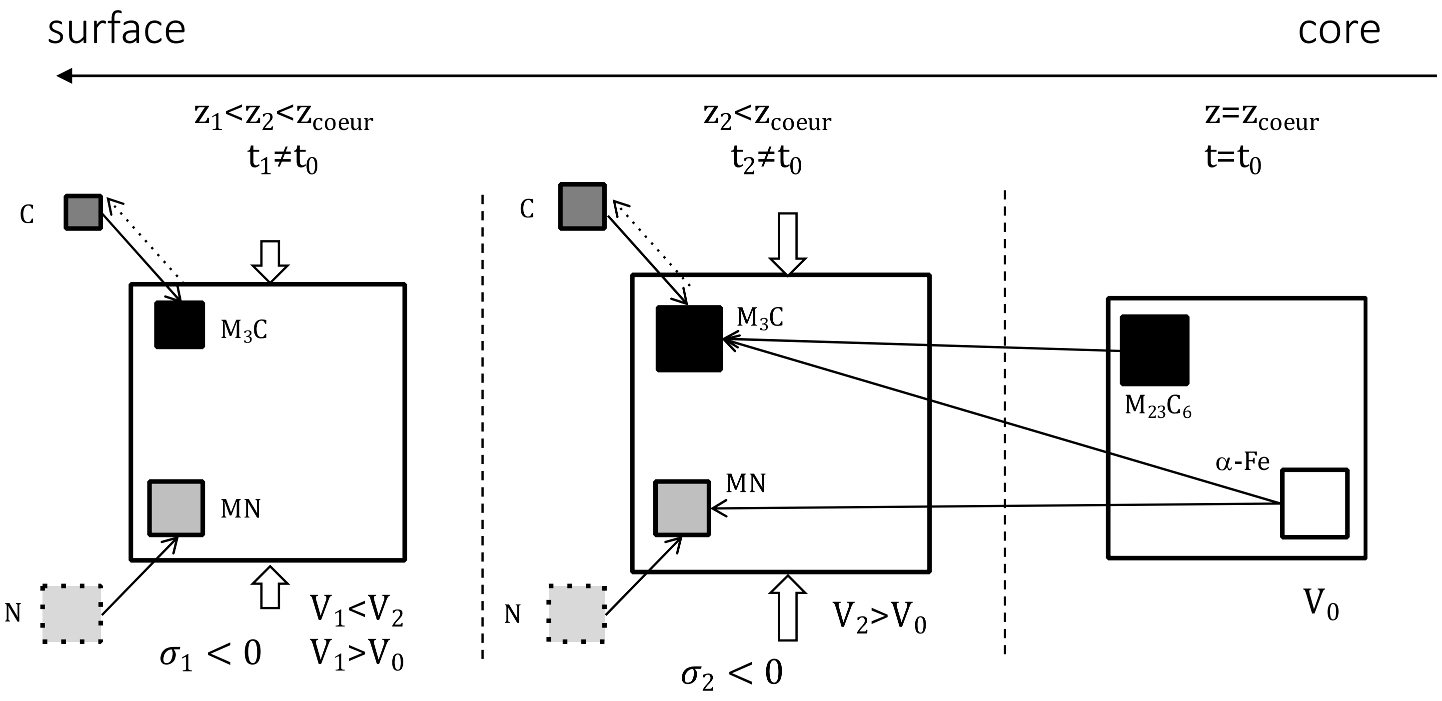


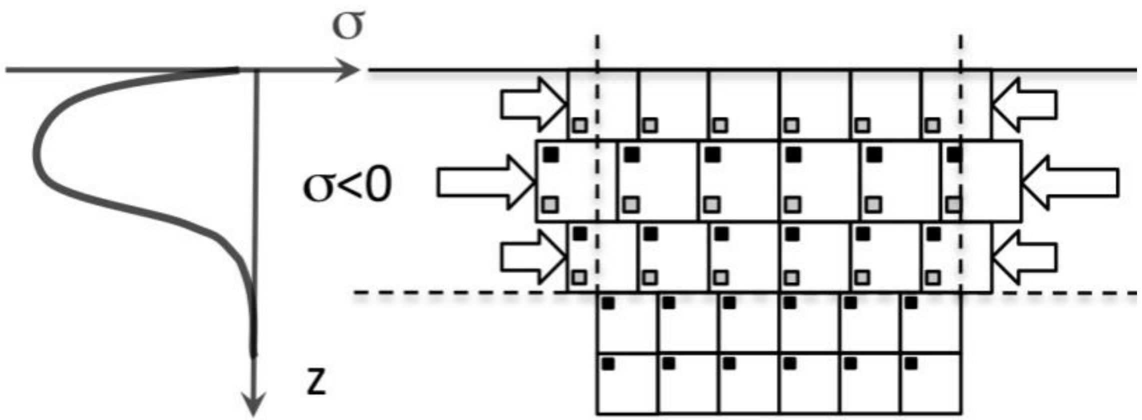



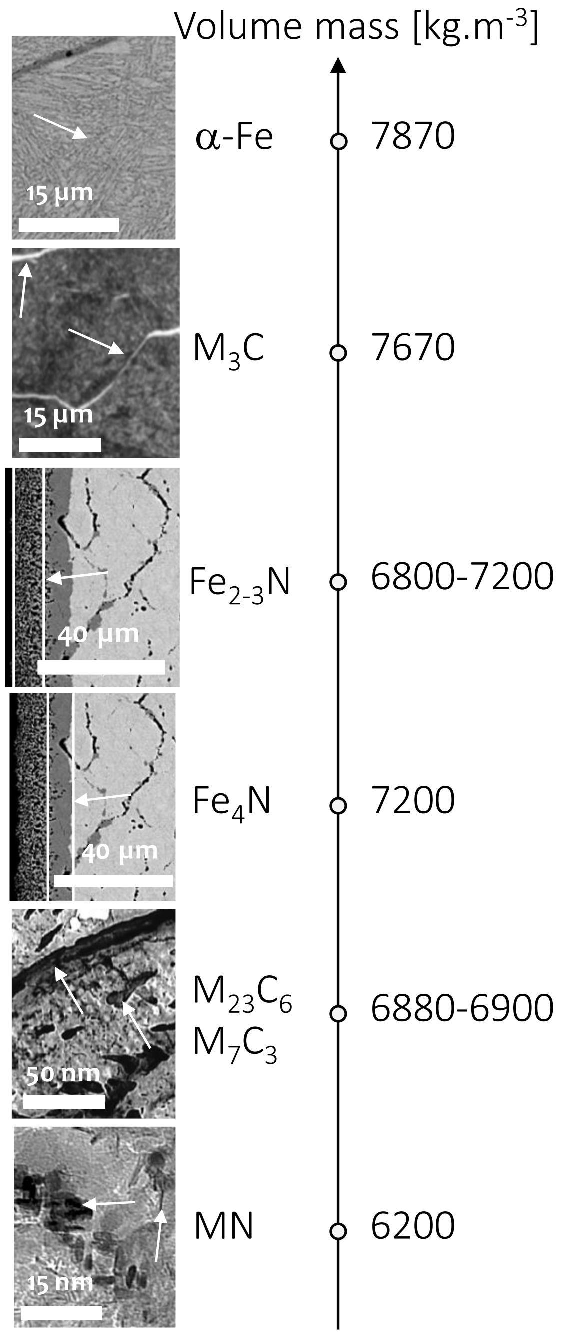

- Multiphase material
- Volume loading :
  - Specific volume
  - Thermal expansion
  - Lattice parameter
- Chemical and microstructure gradients

- Multiscale modeling (self-consistant approach)
- High effect of $Fe_3C$

# Nitriding simulation
## Mechanics



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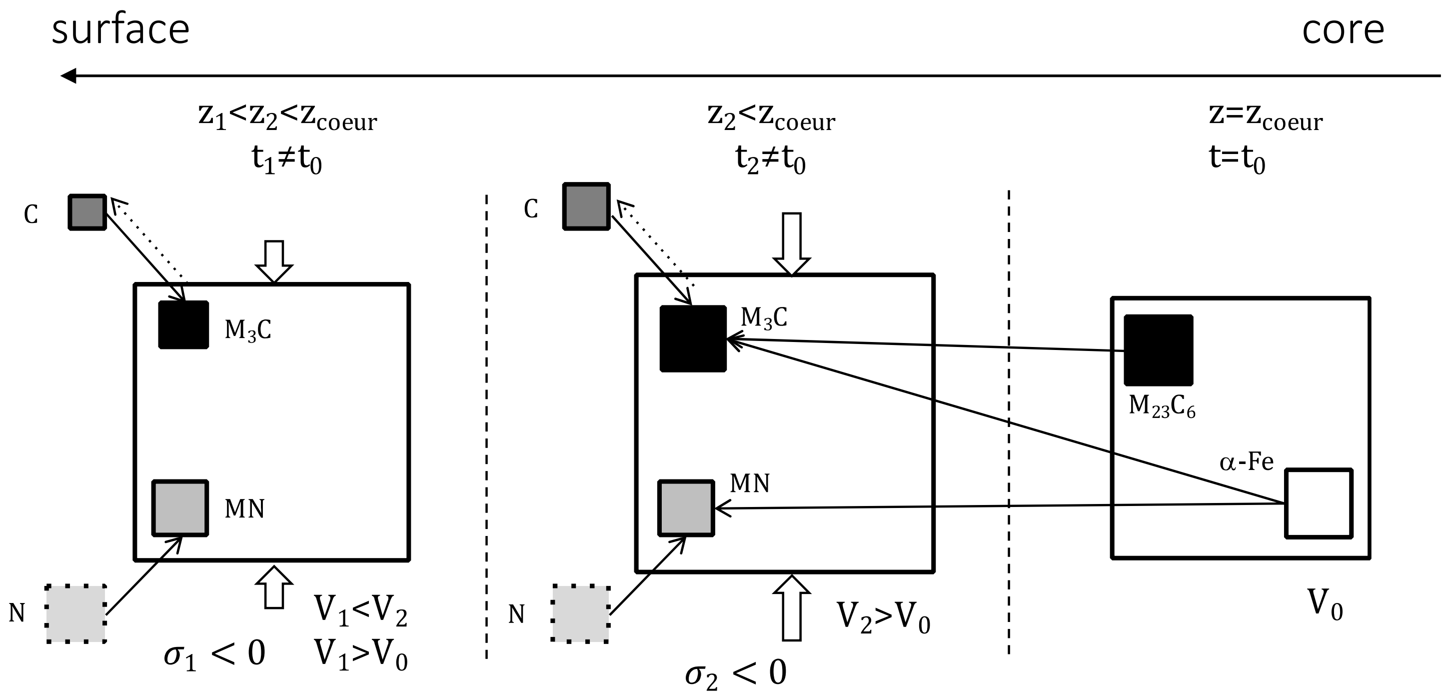
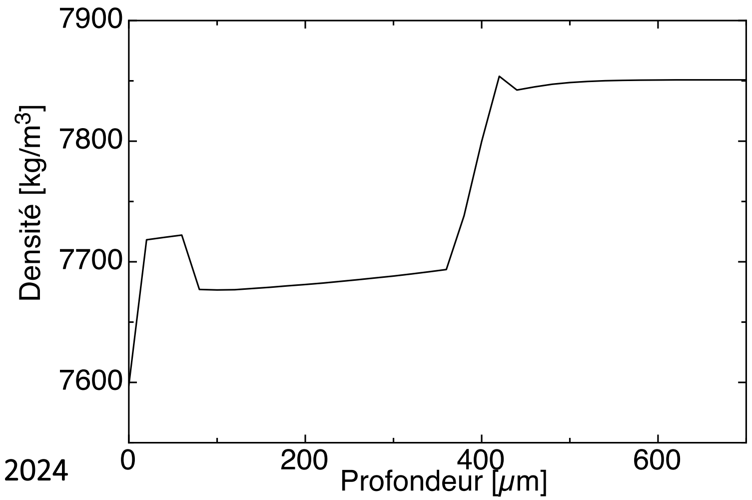
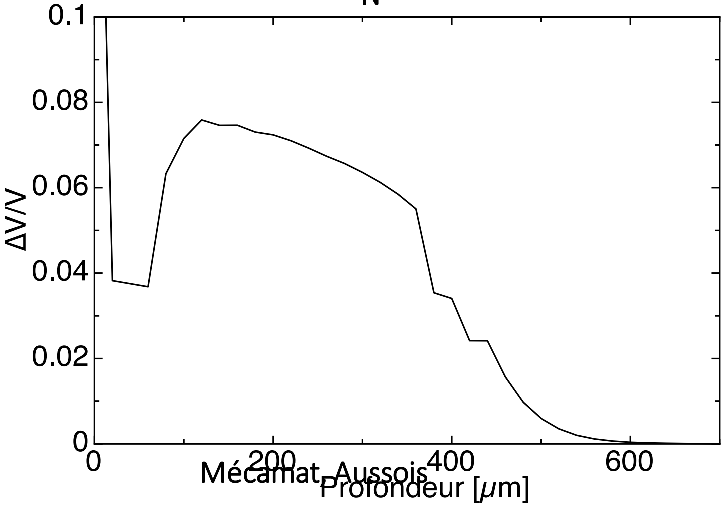
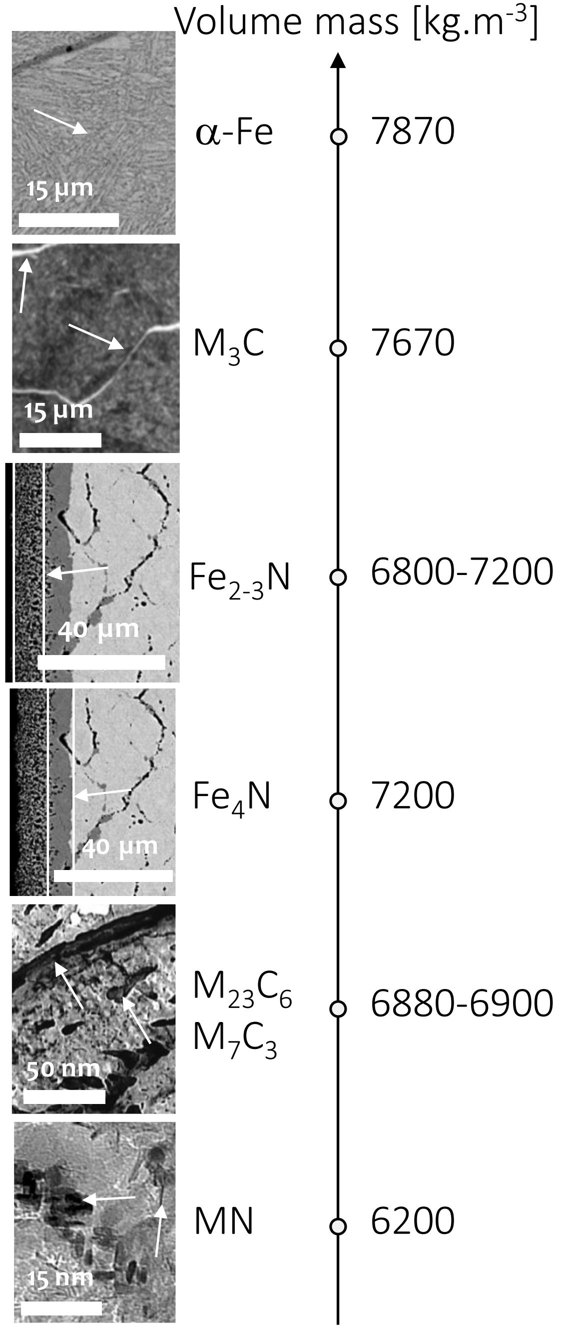
## Mechanics




32CrMoV13, T=520°C, t=50 h, $K_N$=4,3 atm$^{-1/2}$



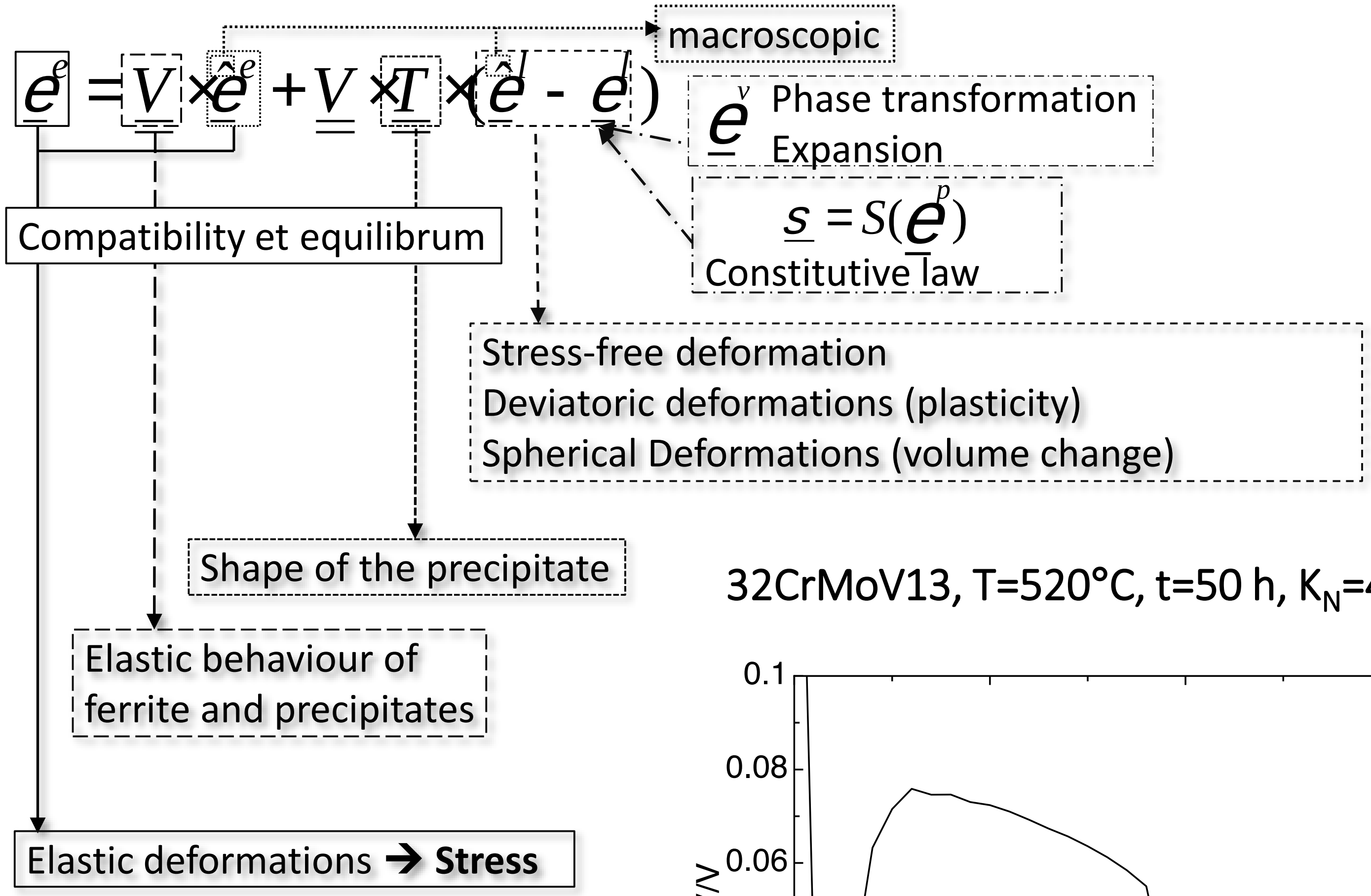



# Nitriding simulation
## Multiscale approach

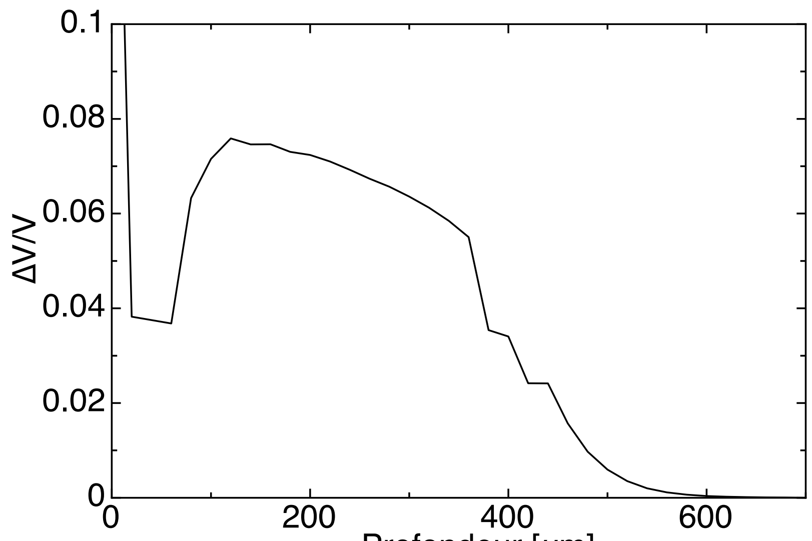


- Kröner-Eshleby approach
- Ferrite and precipitates

- Simulation of Micro and macro stresses




32CrMoV13, T=520°C, t=50 h, $K_N$=4,3 atm$^{-1/2}$



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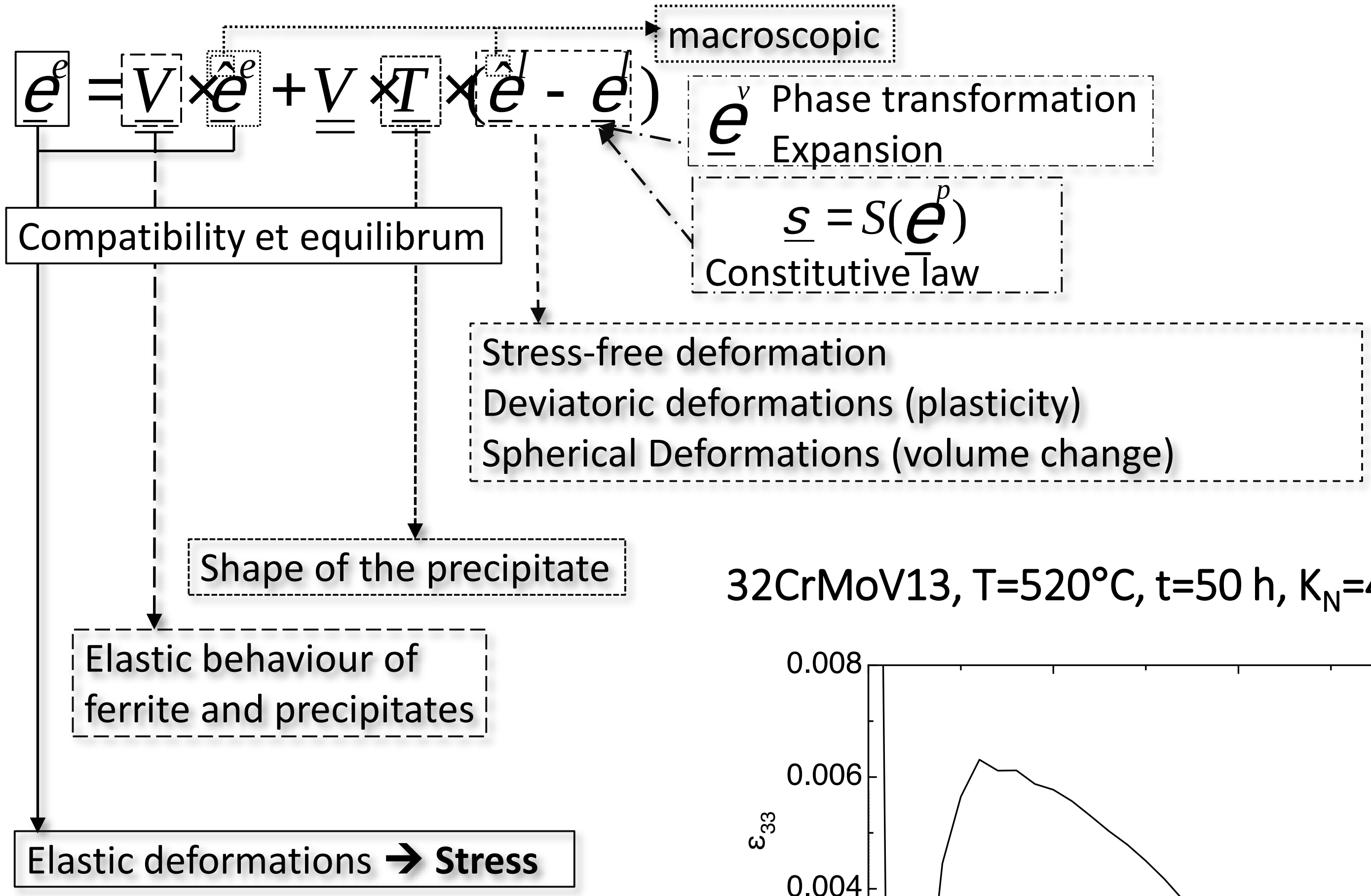


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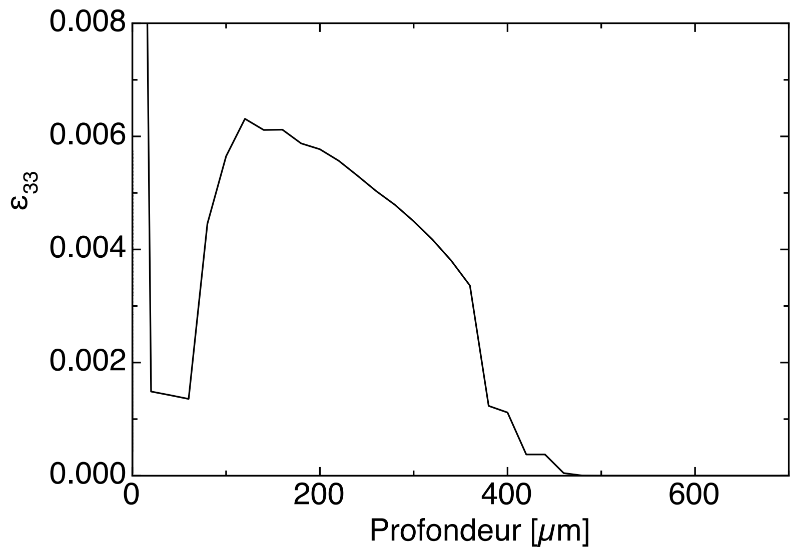

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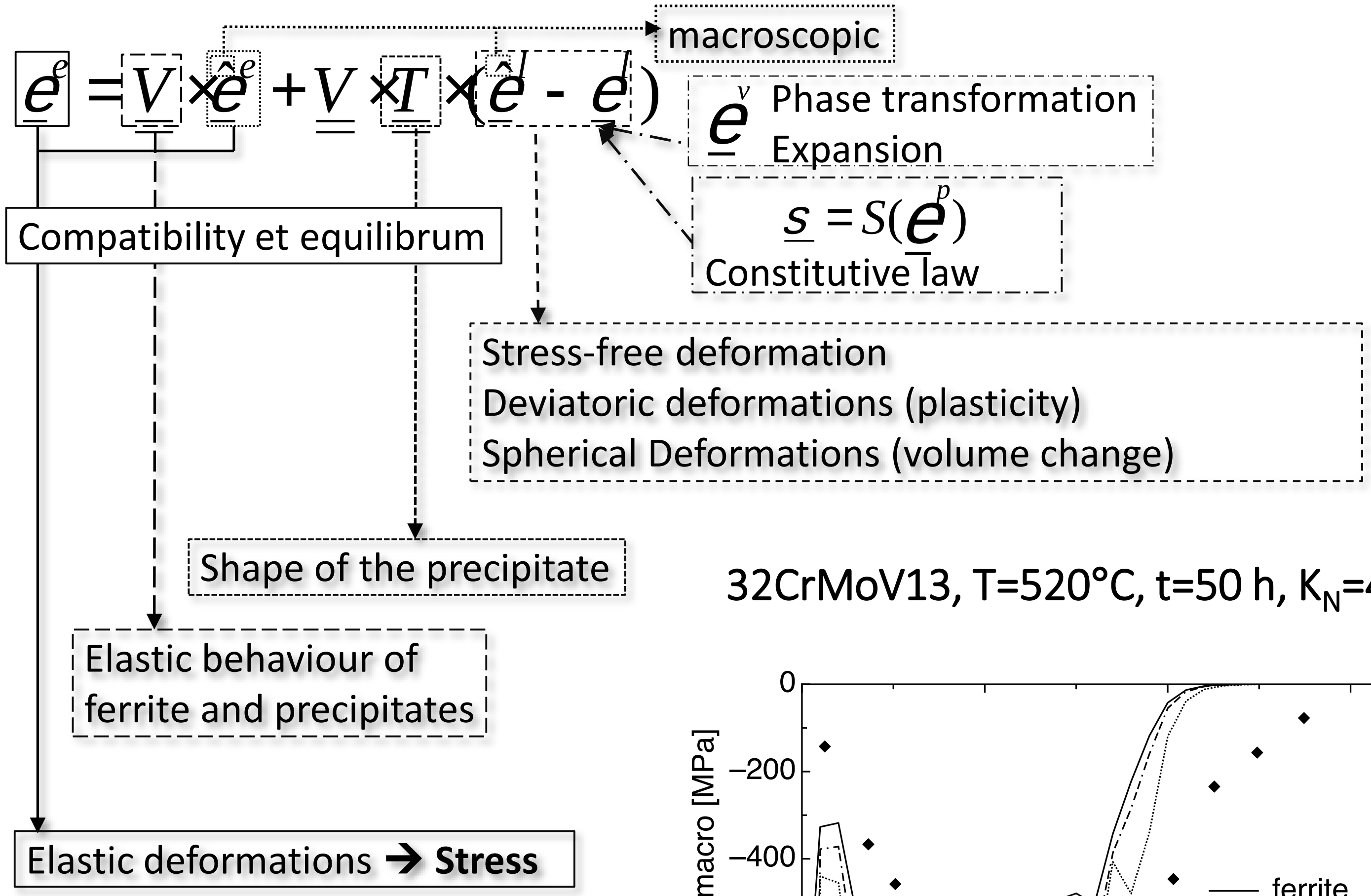
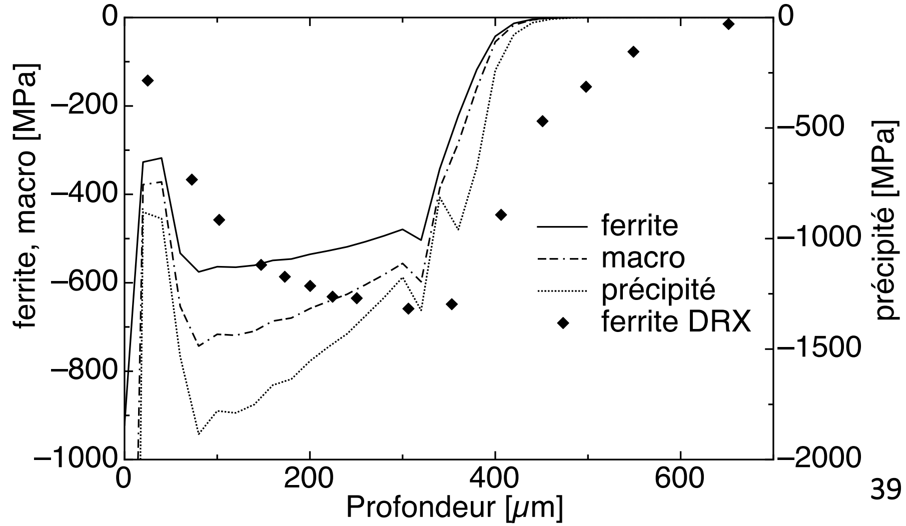


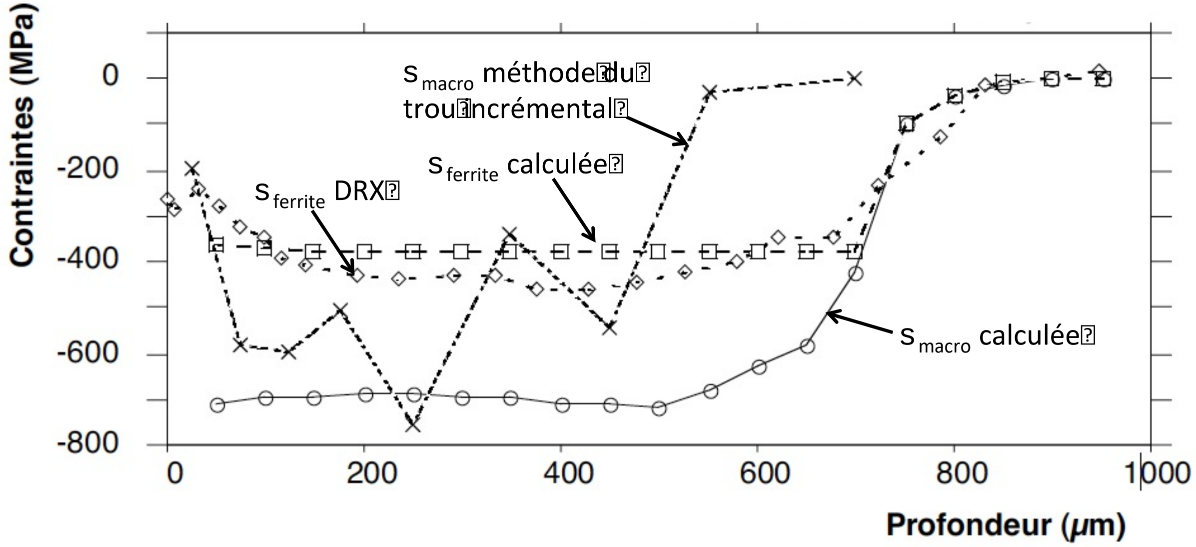

32CrMoV13, T=520°C, t=50 h, $K_N$=4,3 atm$^{-1/2}$



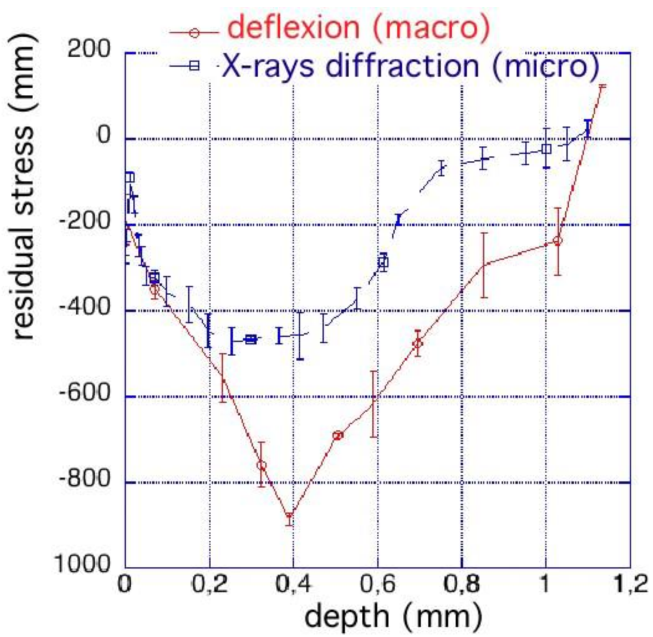
# Macro and pseudo-macro stresses



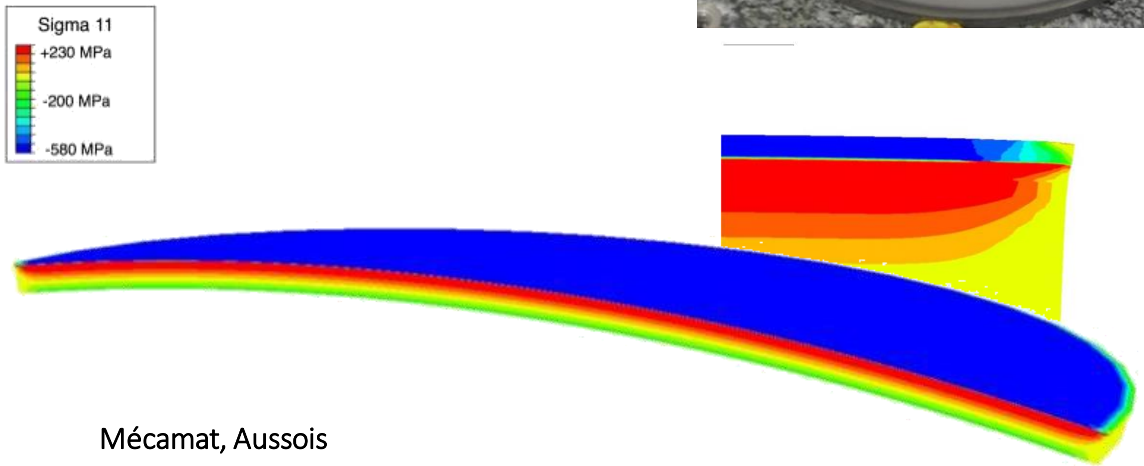
32CrMoV13, T=560°C, t=96 h




[Thèse L.Barrallier 1992]

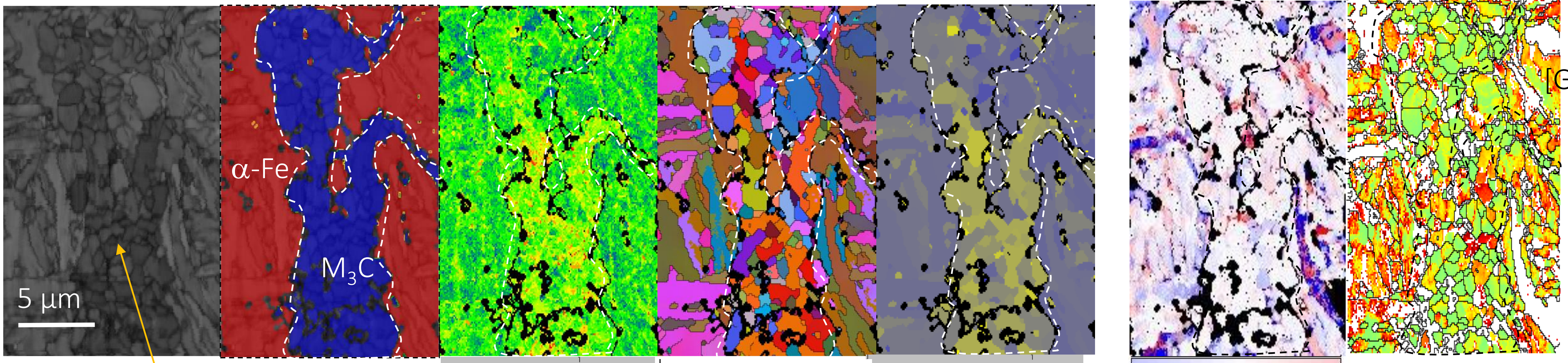


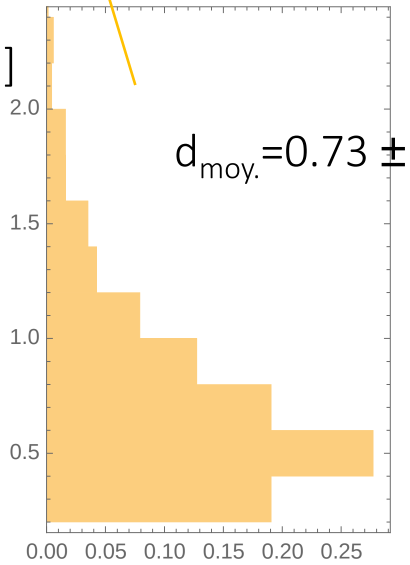

[Thèse de V.Goret 2006]



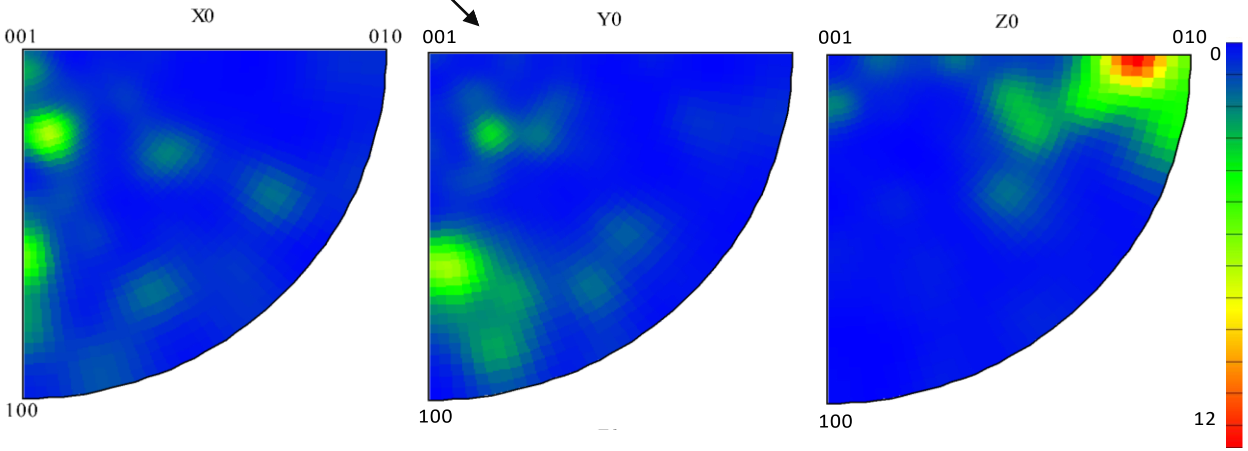
# Macro and pseudo-macro stresses

32CrMoV13, T=520°C, t=30 h, $K_N$=4,3 atm$^{-1/2}$



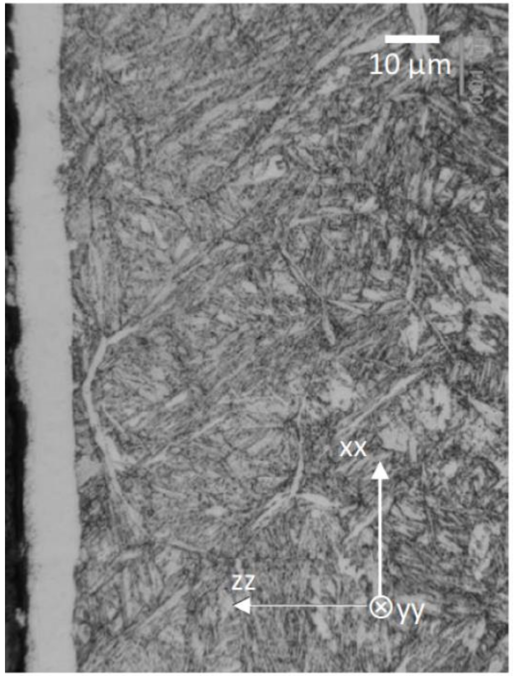

$d_{moy.}$=0.73 ± 0.4 µm

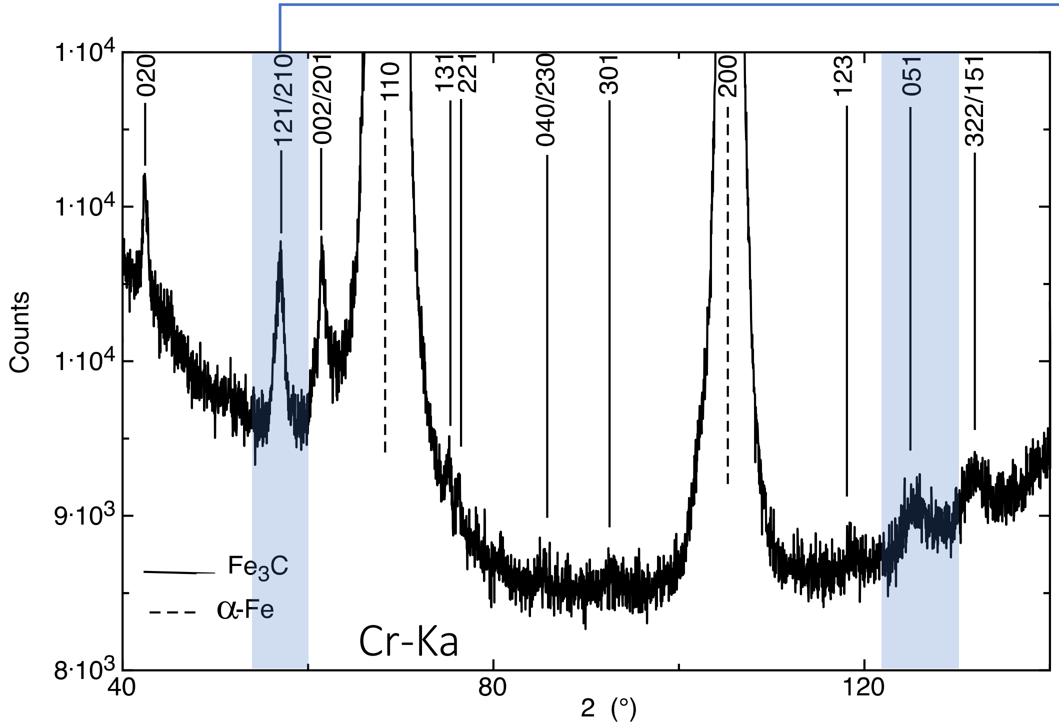


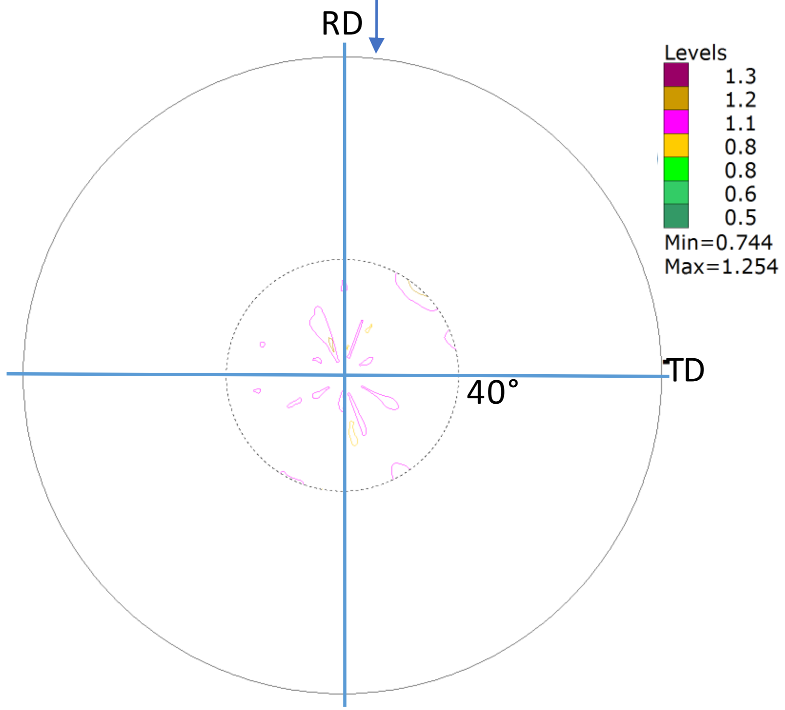

Texture @ joints de grains [010] $M_3C$ // zz

[Barrallier et al. ICRS10 2016]

# In lab. X-ray diffraction analysis (@z=50µm)




- 33CrMoV13-9

950 C°, 30 min, oil quenched
Annealed @ 590 °C, 2.5 h
Setaram SETSYS Evo thermobalance
520 °C / 30 h / 4.3 atm$^{-1/2}$
$NH_3$-$N_2$-$H_2$ gas mixture (200 mL/min)

| Texture | Stress | Phase |
|---|---|---|
| α 0-40° Δa 10° | {211} α-Fe 300s/peak, 13 ψ | Rietveld |
| β 0-360° Δb 10° | {051} $M_3C$ 7200s/peak, 9 ψ | 2000s/step 40-140° 2θ |

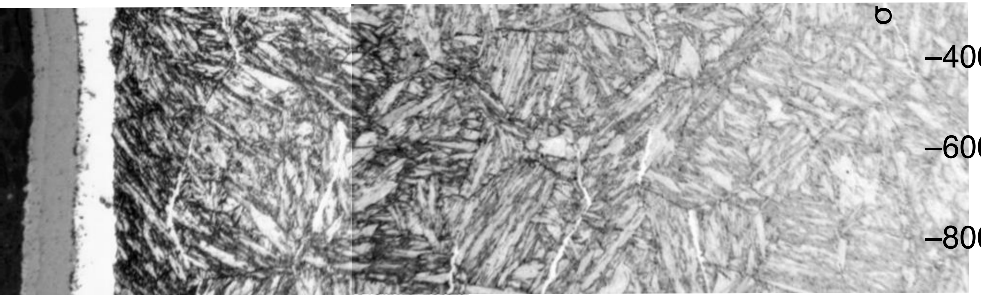
- Isotropic material ($Fe_3C$ a-Fe)
- Long time acquisition
- Biaxial stress $\sigma_{11}=\sigma_{22}$ no shear stresses

⇒ $y(M_3C)=4.6\pm0.7$ %  $\sigma_{11}-\sigma_{33}(M_3C)=-619\pm92$ MPa  $\sigma_{11}-\sigma_{33}(\alpha\text{-Fe})=-1325\pm1$ MPa

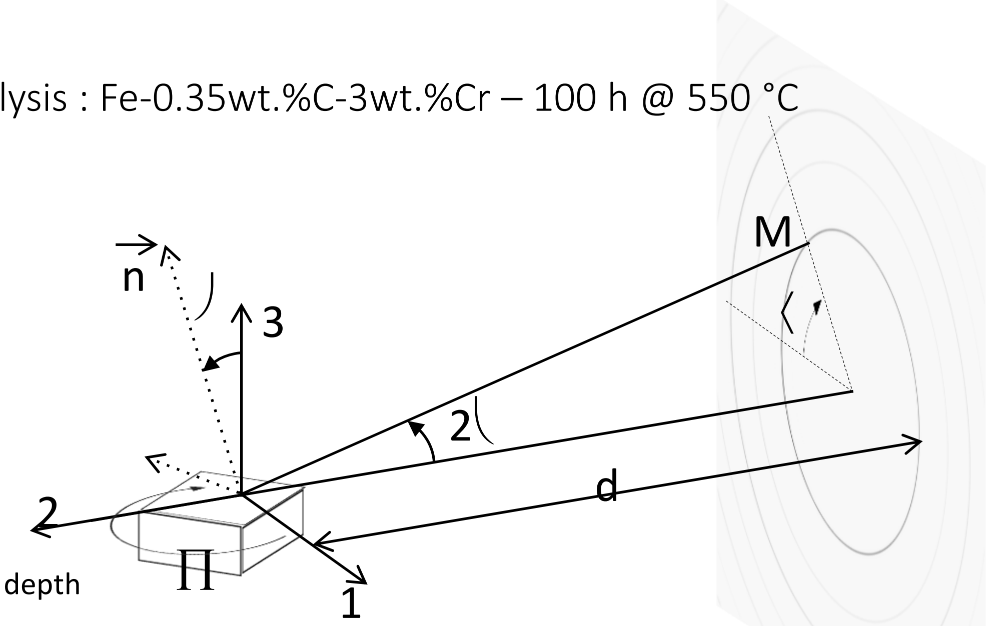
[Barrallier et al. ICRS10 2016]

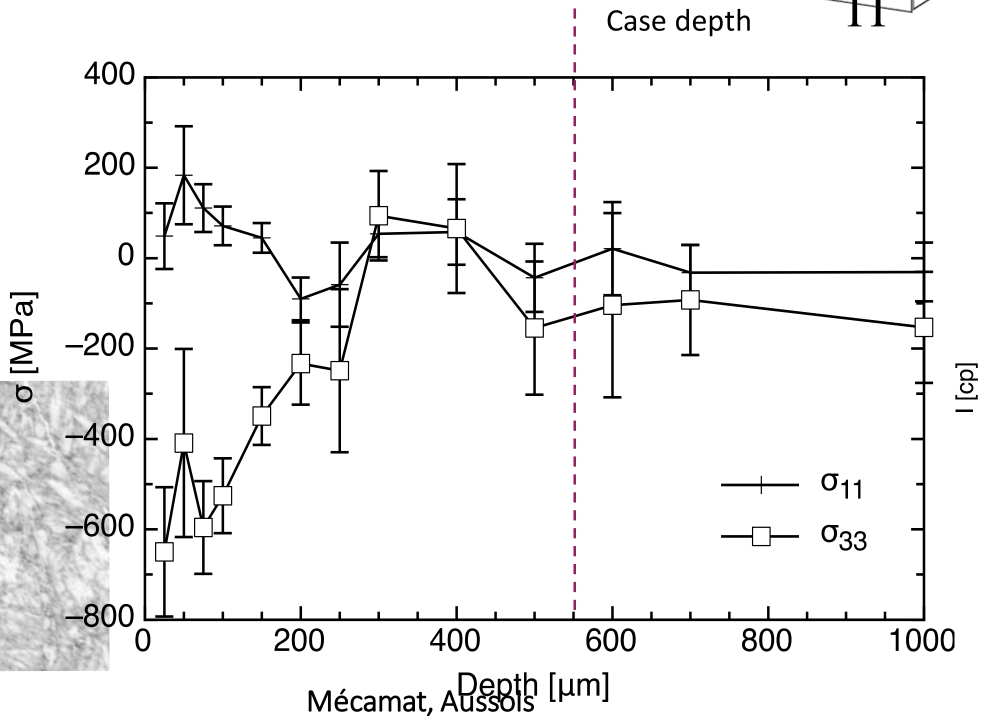
# Stress triaxiality ($\sigma_{33}$ in ferrite)

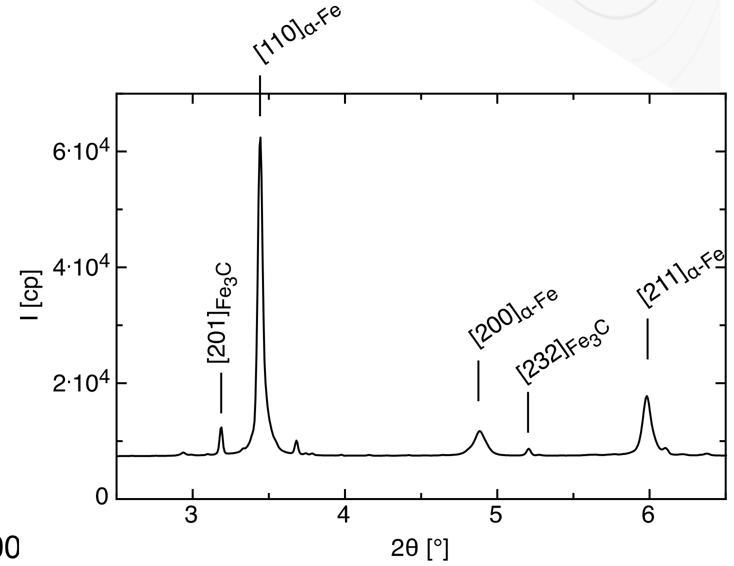
- P07-PIII @ Hasylab/Desy, Hamburg, Germany
- Primary beam : width : 1mm, height : 25 µm
- Energy : 100 keV
- Measuring time :
  - 24 images / step
  - 5 s / image
- Depth profiling : 25 µm step
- Flat panel detector :
  - CsI-scintillator
  - 2048x2048 pixels - 400x400 mm
- Sample to detector lenght : 1700 mm
- DEC calculated using Eshelby/Kröner model from α–Fe and $Fe_3C$ single crystal constants



α-Fe Residual stress analysis : Fe-0.35wt.%C-3wt.%Cr – 100 h @ 550 °C



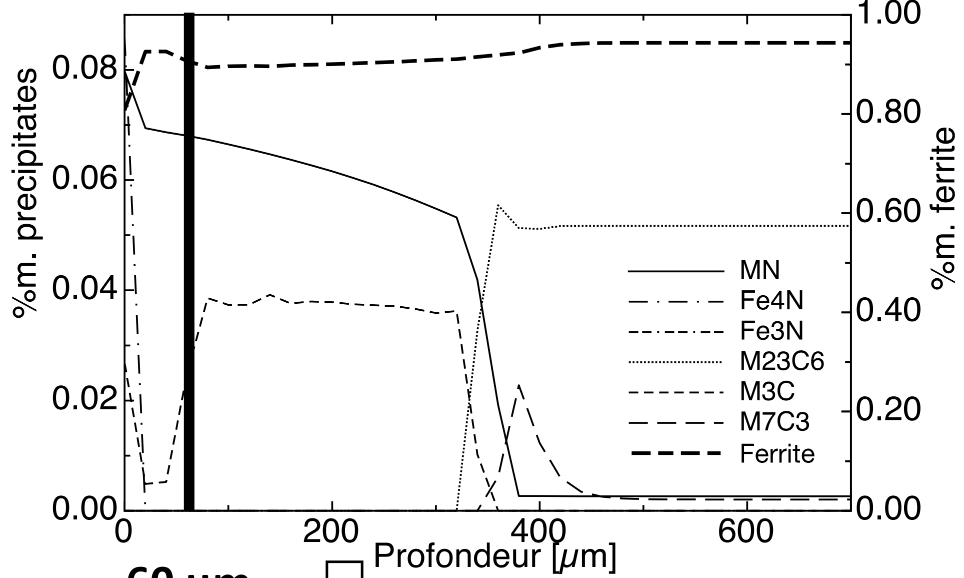



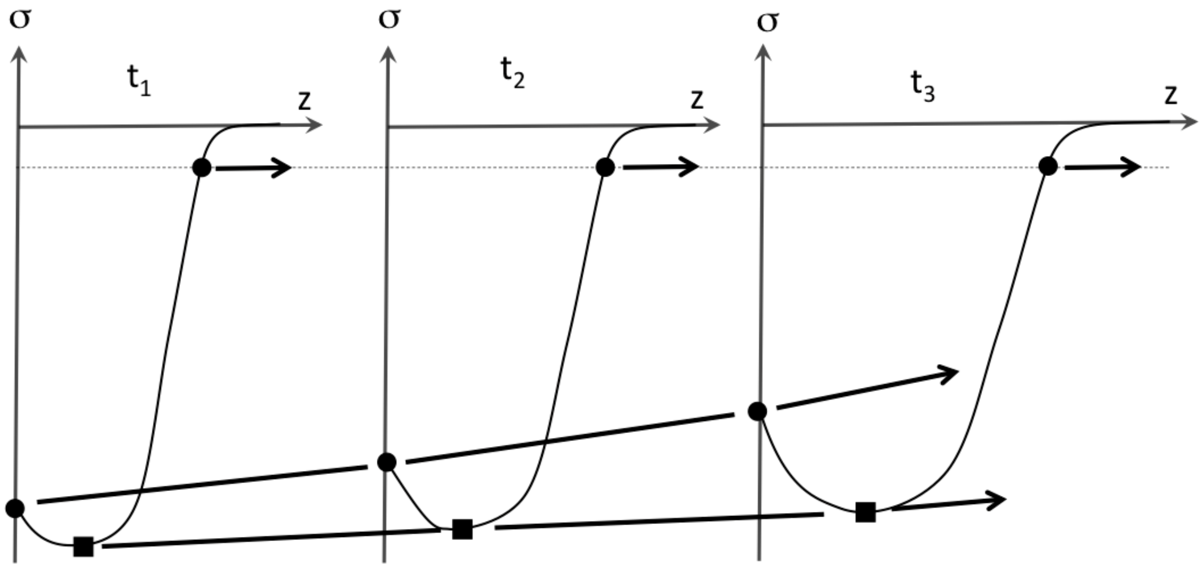

[Jegou et al. ICRS9 2012]

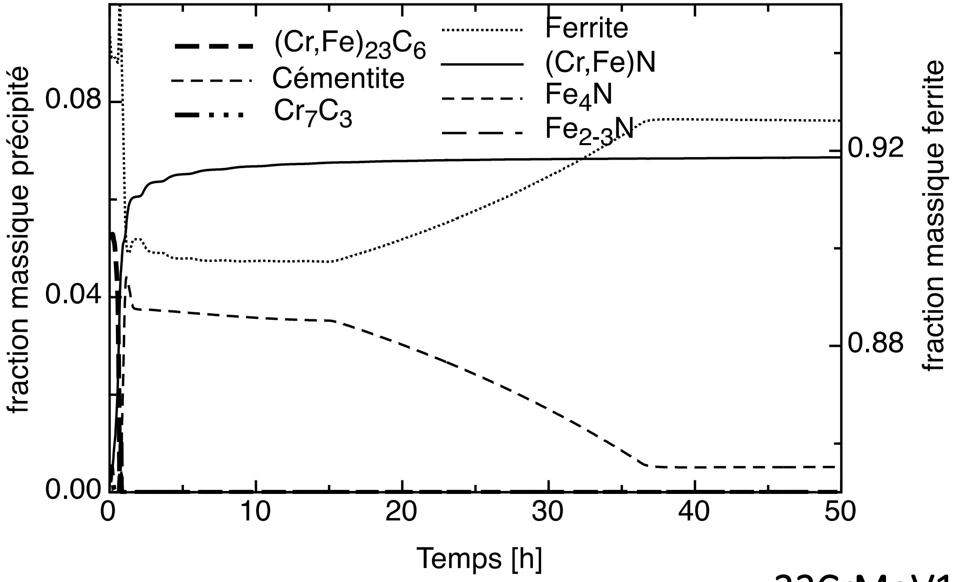
# Nitriding simulation

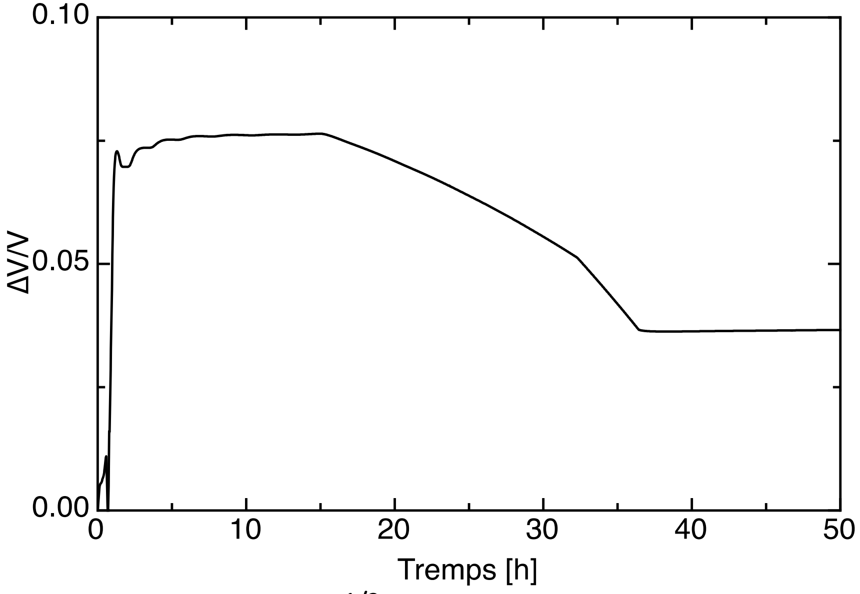
## Kinetic




**60 µm**



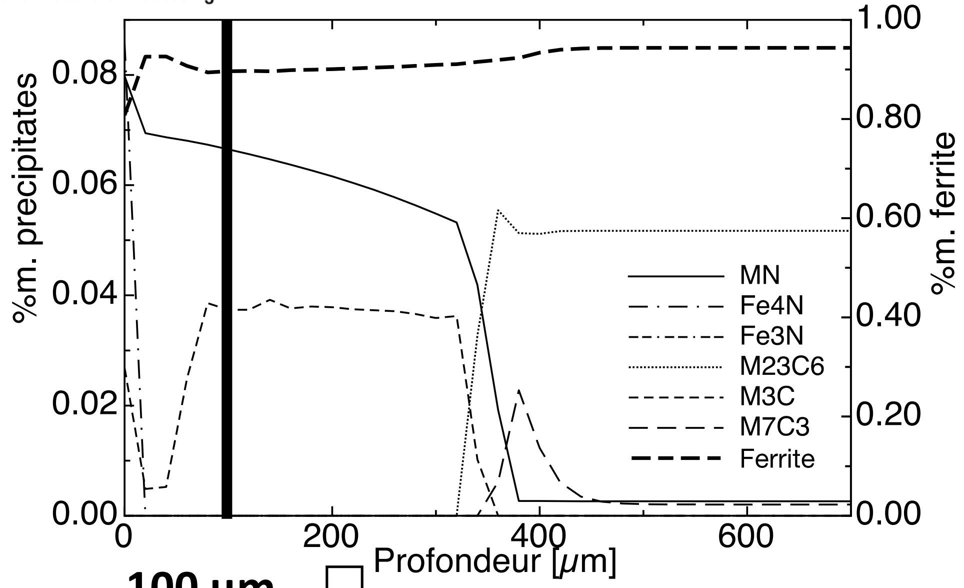

**Coupling diffusion/ precipitation/ mechanical with the time**

**Effect on the residual stress near the surface**

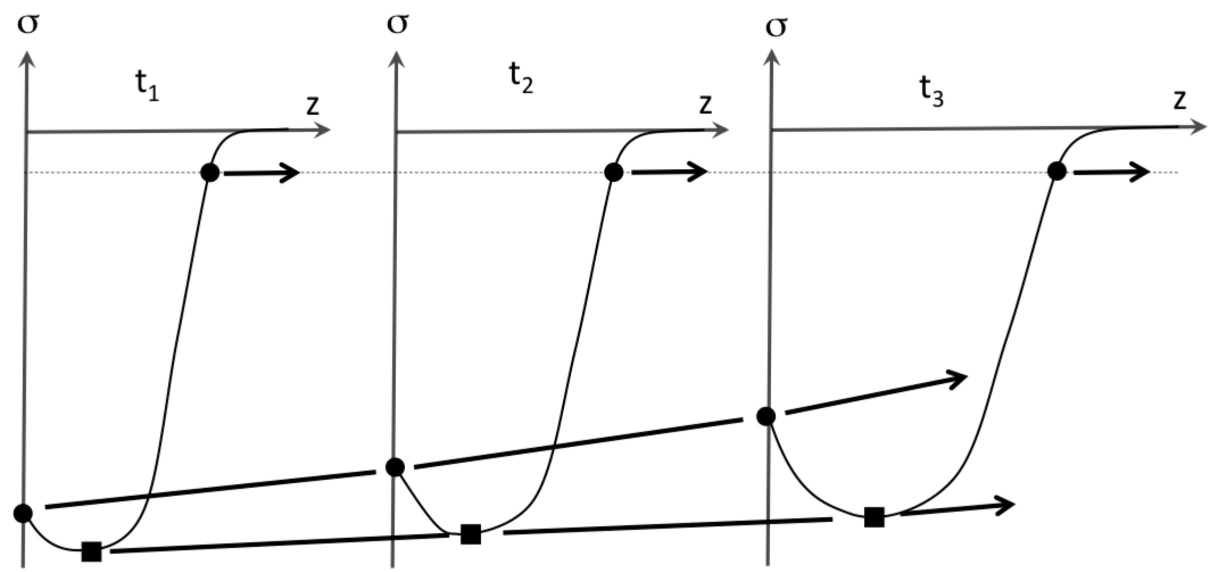
32CrMoV13, T=520°C, t=50 h, $K_N$=4,3 $atm^{-1/2}$

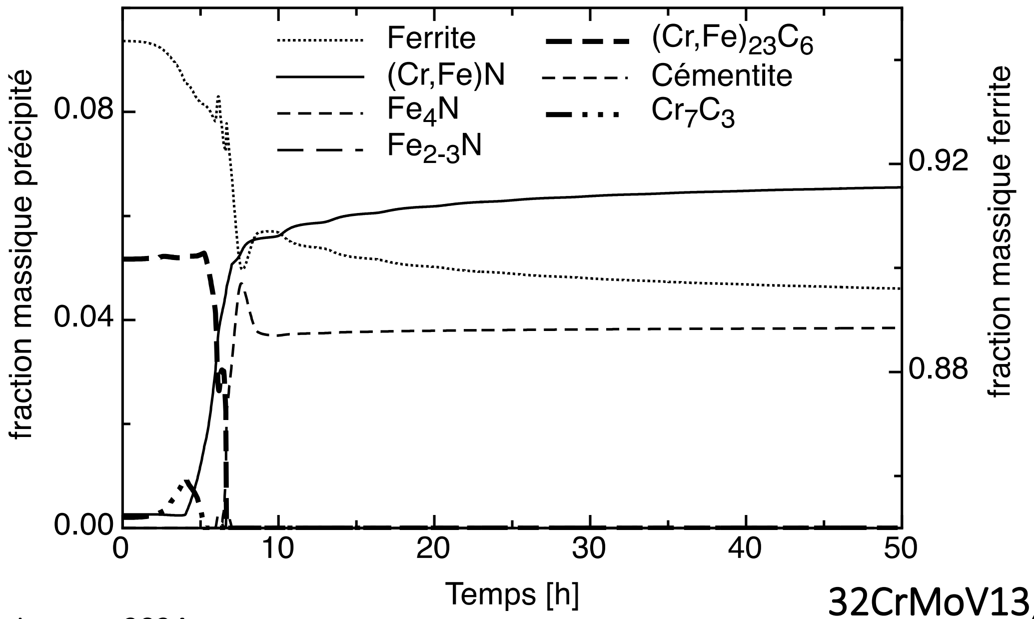
# Nitriding simulation

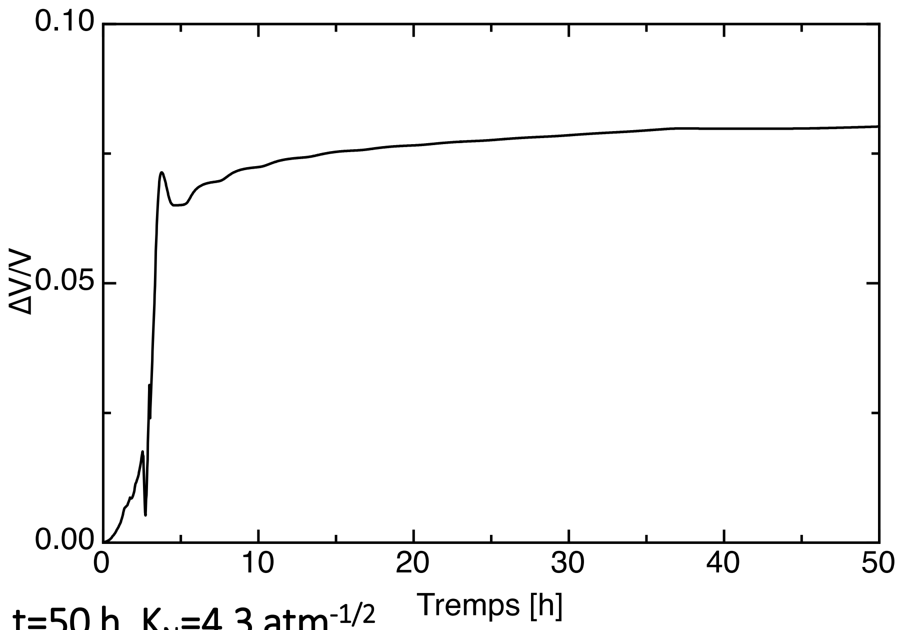
## Kinetic




**100 µm**




**Coupling diffusion/ précipitation/ mechanical with the time**

**Effect on the residual stress near the surface**

32CrMoV13, T=520°C, t=50 h, $K_N$=4,3 atm$^{-1/2}$

# Stress relaxation

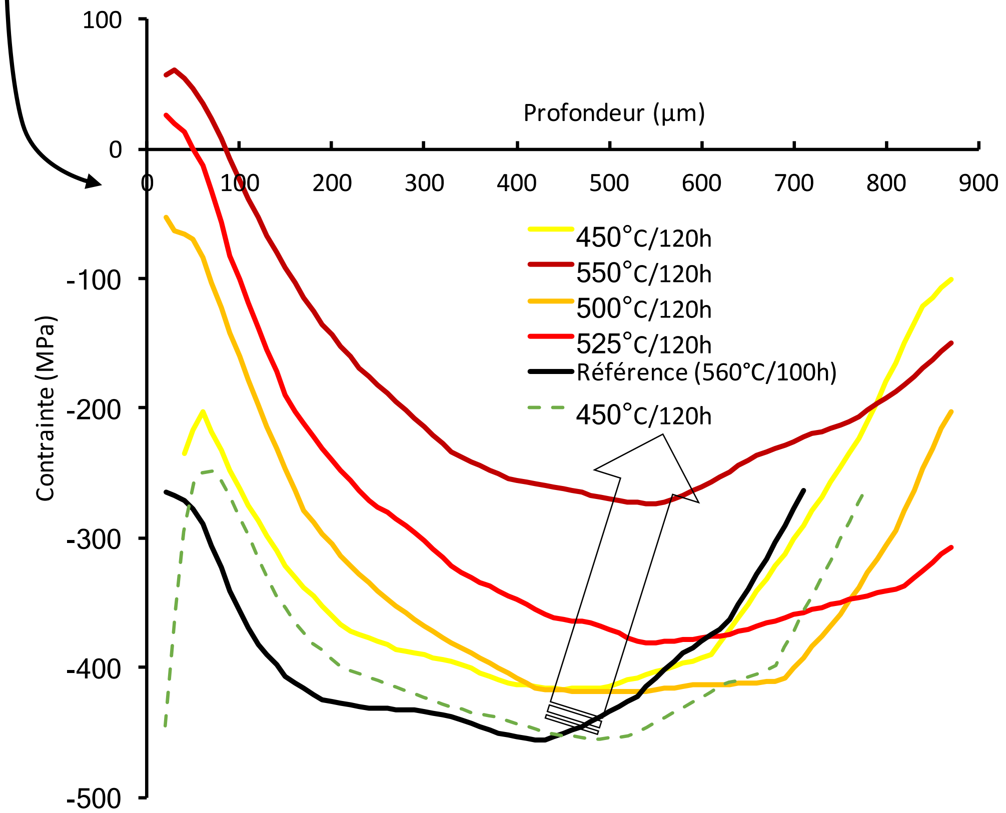
Thermal relaxation

- Quite stable up to the temperatures close to the nitriding temperature
- Time and temperature effect, nitriding is continuing

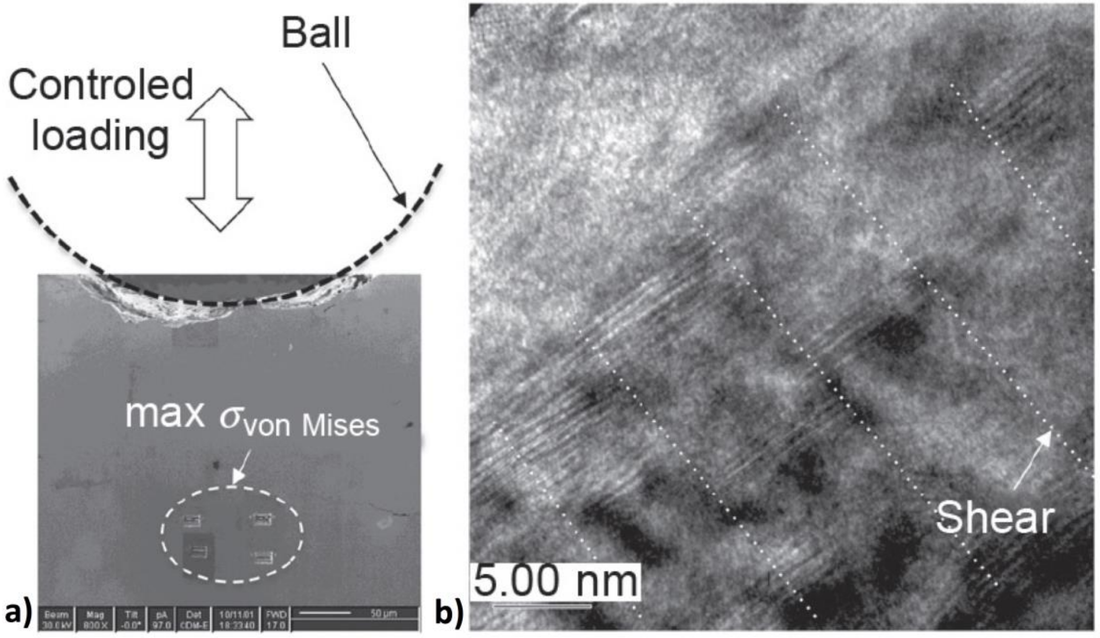
Mechanical relaxation

- Not really important
- Shearing of semi-coherent precipitates, hardness modification

Good stability of the nitriding residual stress




32CrMoV13



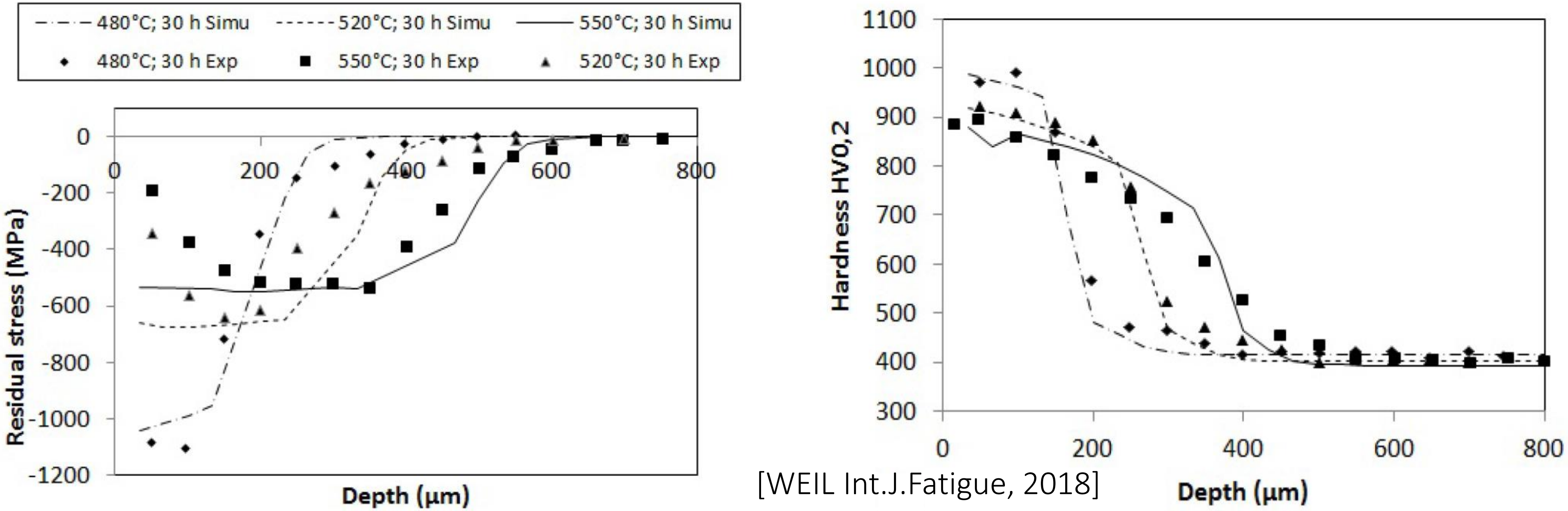

[Data Thèse L.Barrallier 1992]

# – Hardness modeling

- based on Orowan mechanism

$$HV(z) = HV_0 + (HV_s - HV_0)\sqrt{\frac{t_{\text{eff}}}{t_{\text{eff}}} \cdot (\text{Norm}(y_{\text{prec}}^{\text{semi-cohrent}}(z)) \cdot (1-I) + \text{Norm}(y_{\text{prec}}^{\text{globulaire}}(z)) \cdot I)}$$

- $HV_0$ dureté du matériau de base
- $HV_S$ dureté à 50 µm de la surface
- $\text{Norm}(y_{\text{prec}}^{\text{semi-cohrent}}(z))$ fraction volumique normalisée des précipités semi-cohérents
- $\text{Norm}(y_{\text{prec}}^{\text{globulaire}}(z))$ fraction volumique normalisée des précipités globulaires
- fraction volumique à partir du calcul thermodynamique
- I partition entre précipités globulaires et semi-cohérents, I=A.exp(ΔH/RT).$t^n$



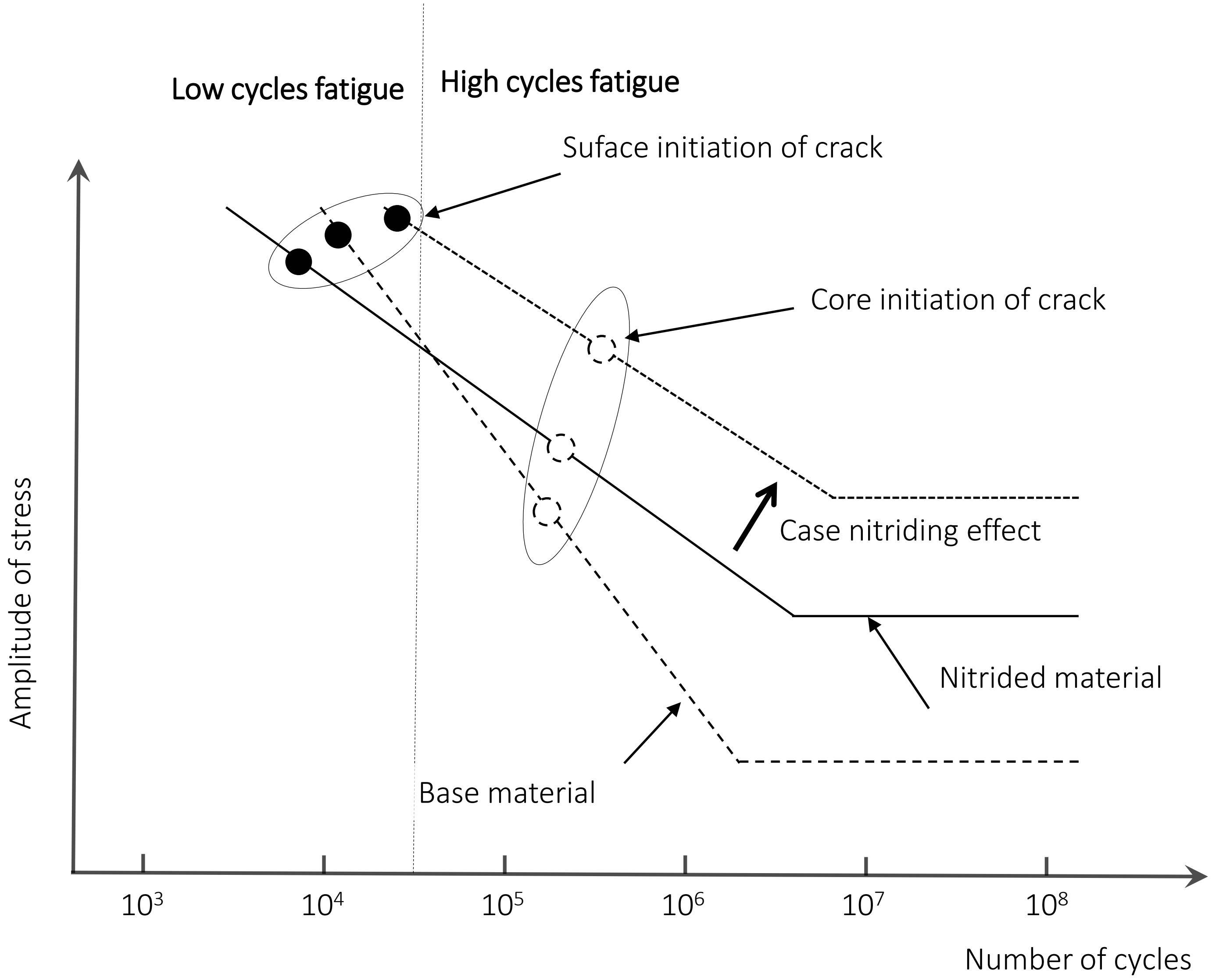

[WEIL Int.J.Fatigue, 2018]

# Fatigue life of nitriding case

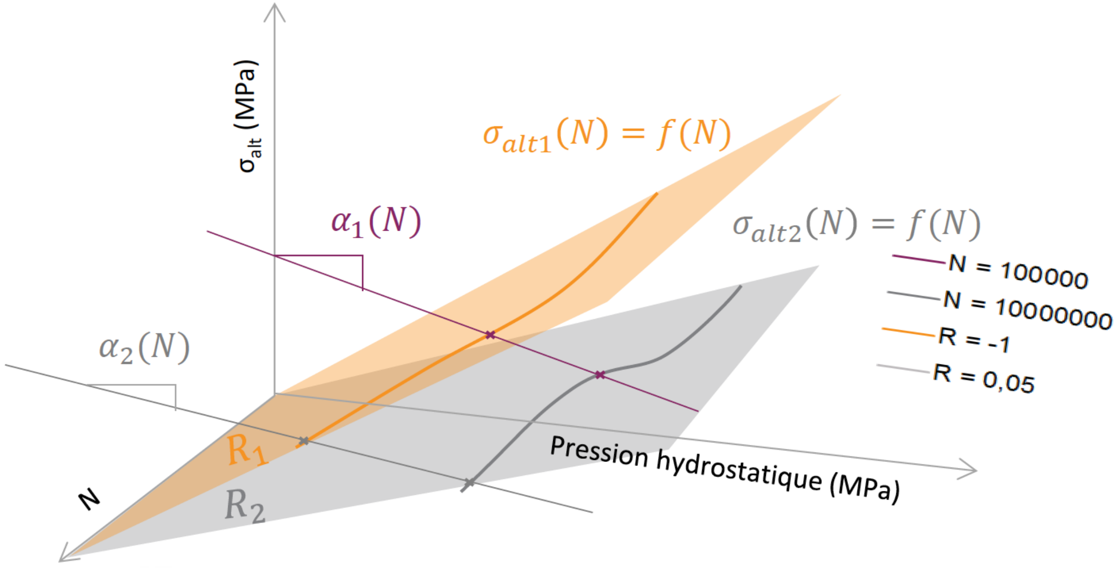


## Stress and hardness effect on fatigue life

Improvement of fatigue life (>30%)
No temperature effect ($T<T_{nituration}$)



# Fatigue design for mechanical contacts (gears and roll bearings)

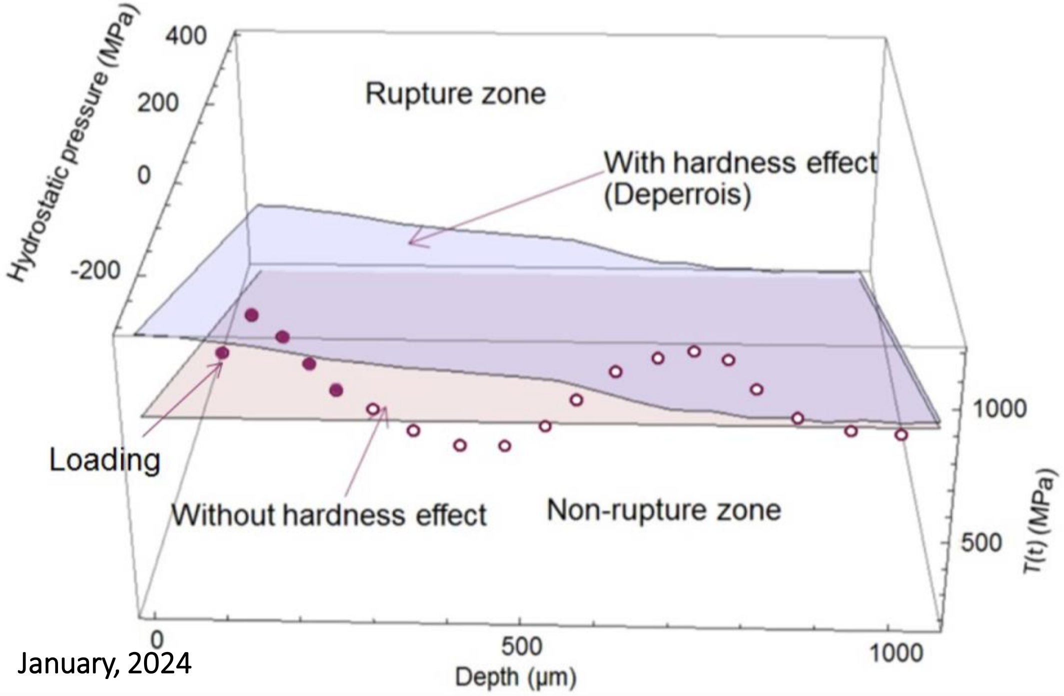


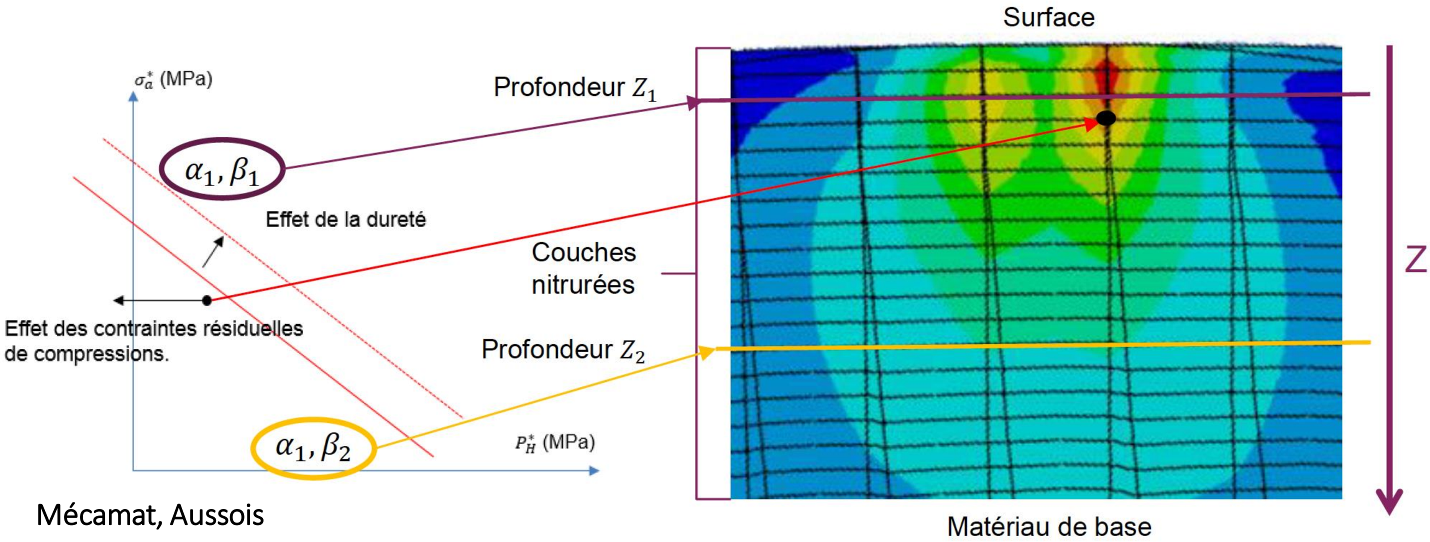

- Microstructure gradients
- Induced residual stress gradients
- non proportional mechanical loadings
- Low-High cycle Fatigue
- Local criterion such as Fatamie-Socie approach (localized plasticity)
- Critical plane criterion such as Dang Van approach

$$\text{Max}\left[\frac{1}{2}\left|\sigma_I^{alt}(t,z) - \sigma_{II}^{alt}(t,z)\right| + \alpha(z).\text{pH}(t,z)\right] - \beta(z) = 0$$

$$\alpha(z) = \alpha(\text{surface}) = \alpha(\text{base material})$$

$$\beta(z) = \beta_0 \left(\frac{HV(z)}{HV_0}\right)^n$$ [DEPEROIS 1991]

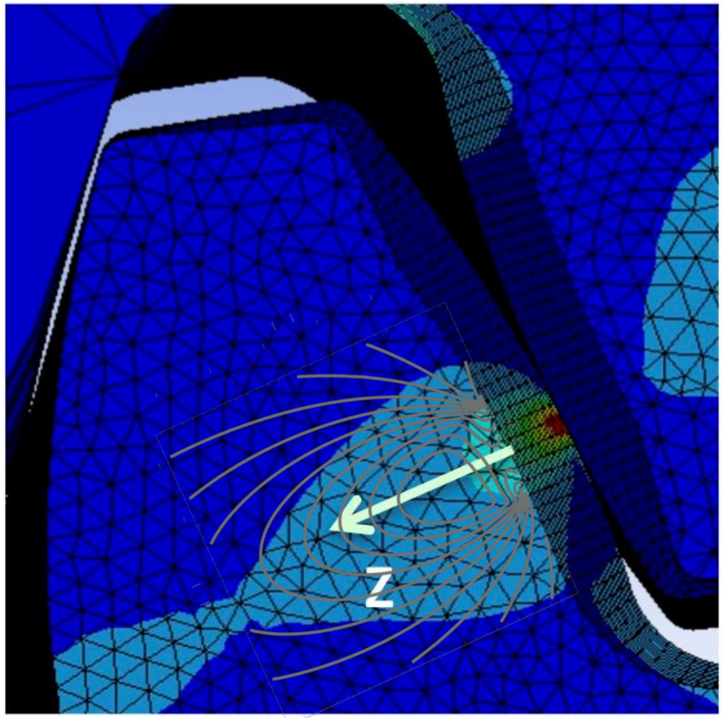


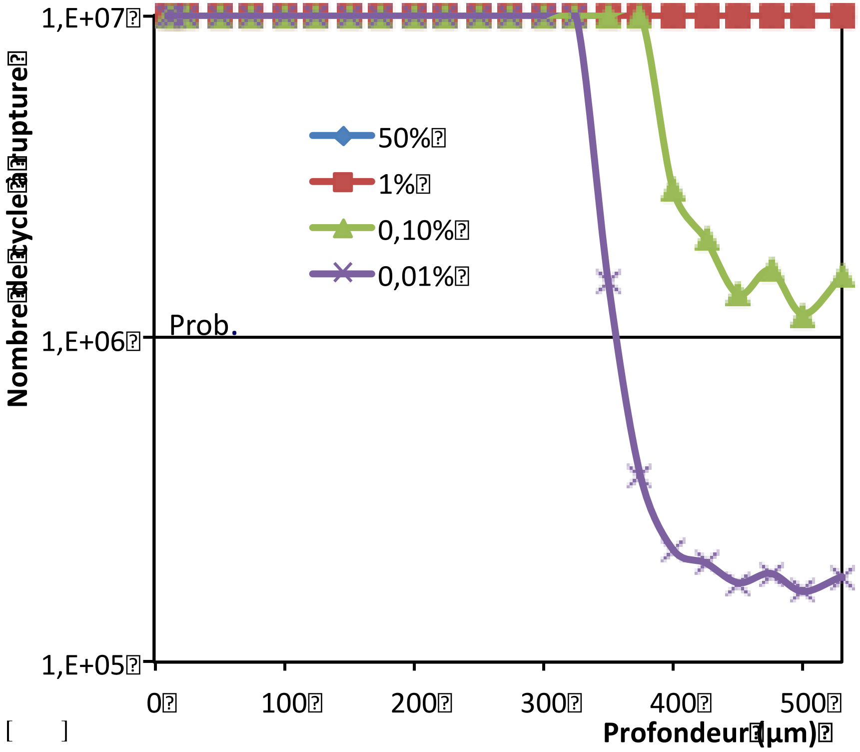
# Simulation exemple : surface fatigue of gear tooths

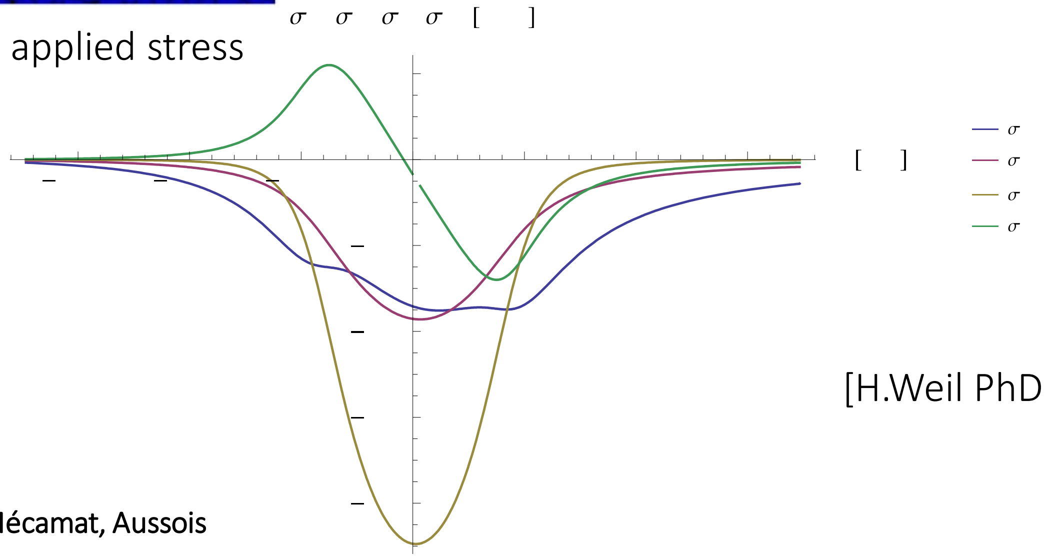
Real mechanical loading and nitriding

Complete modeling from the technogical parameters (T, t, $K_n$) to the fatigue life



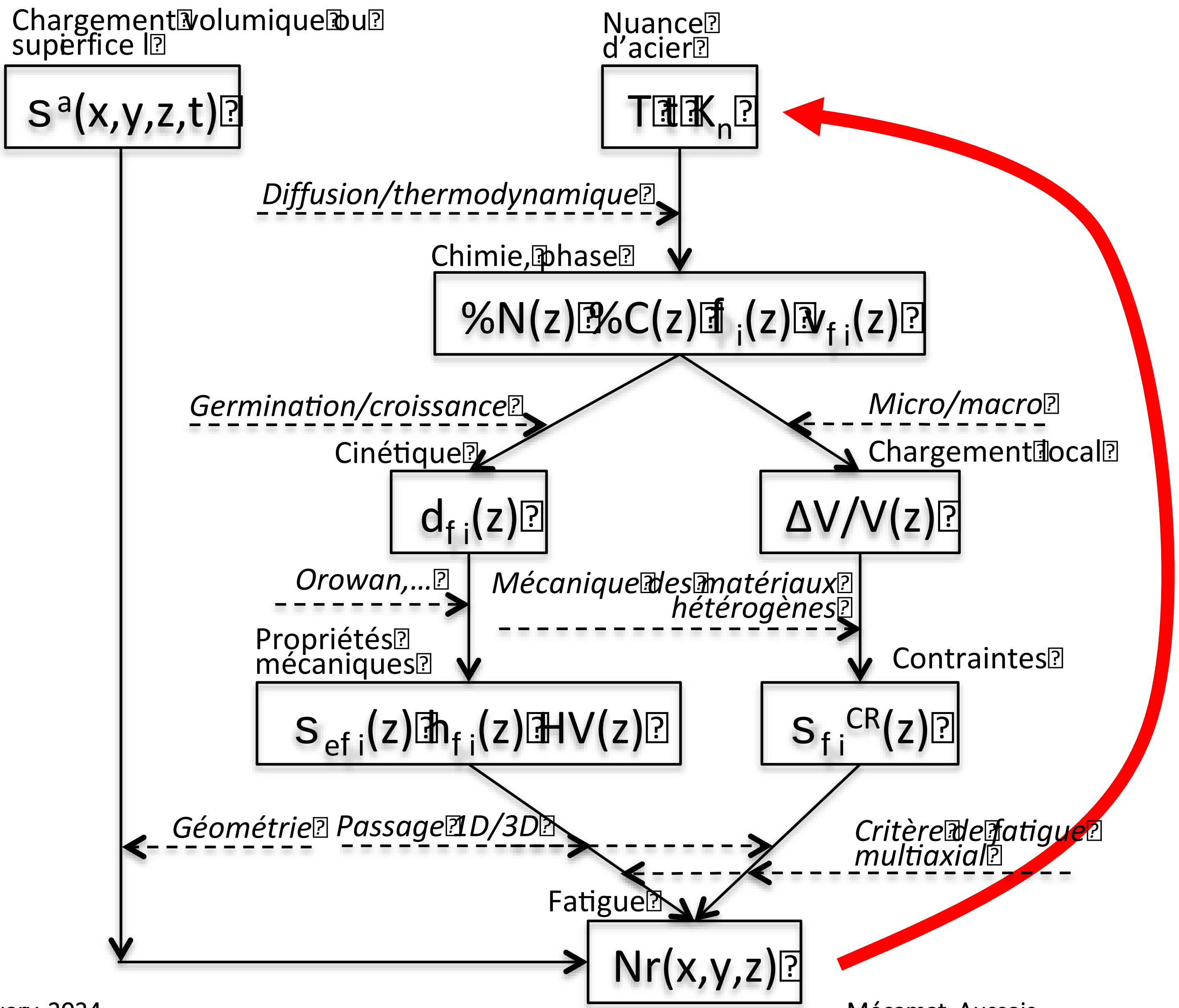

3D loading with dephased applied stress components



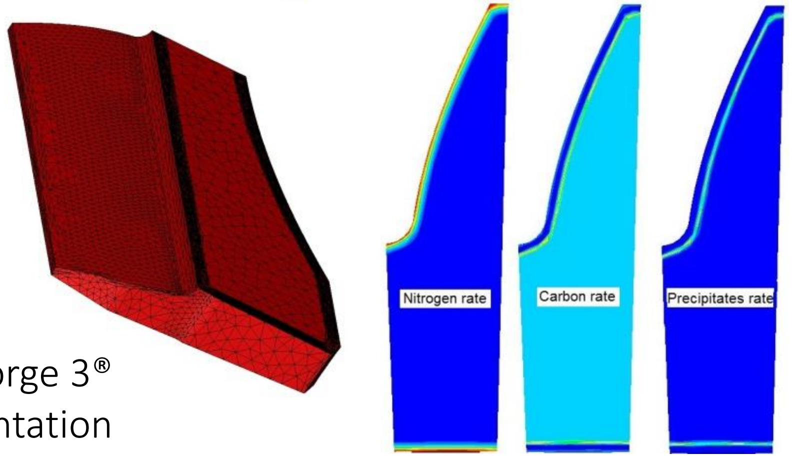



[H.Weil PhD 2017]

# Reverse engineering



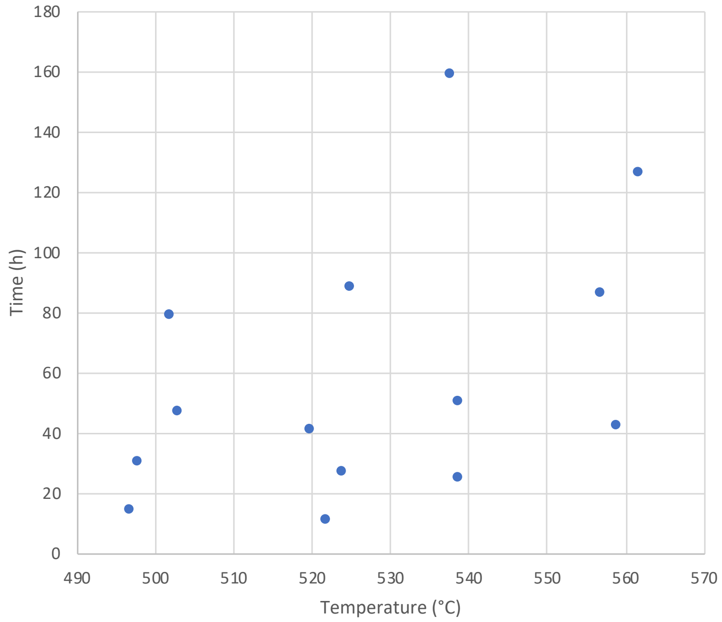

- From the nitriding parameters (T,t,Kn)
- Complete simulation of the physico-chemical and mechanical processes
  - diffusion
  - precipitation
  - hardness
  - **residual stress**
- Nitriding kinetic is very important for the final residual stress field
- Fatigue life (number of cycles, crack localization)




3D -> Forge 3®
implementation

## Gradient Boosting / XG Boost (usually used for few data set)

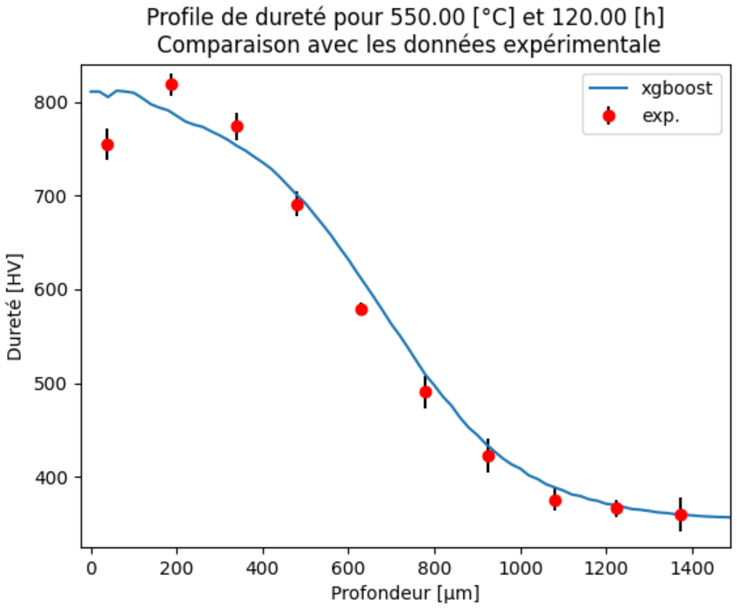
HV and Stress profiles from experiments
14 (T, t)
Unstructured data in z

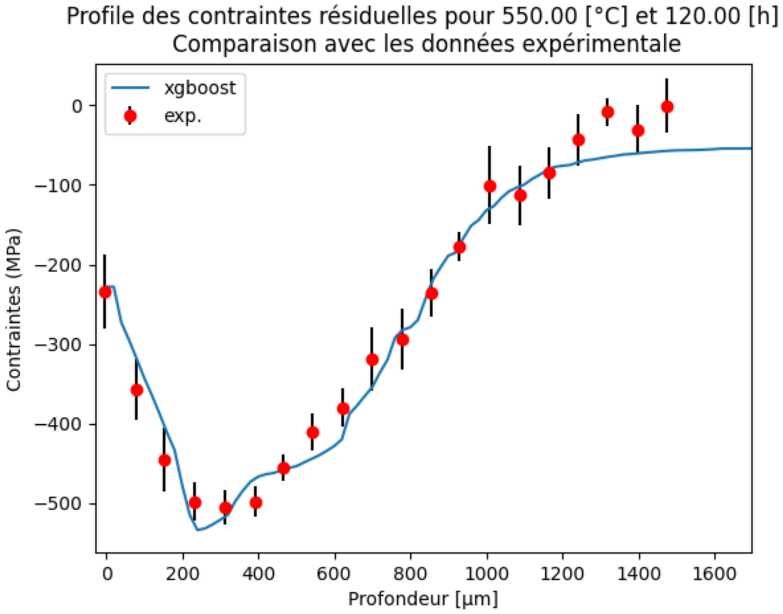



- AI
  - Easy to use (if you don't understand it, it can do it)
  - Good accuracy (seems to be)
  - Improvement with new data

- Extension
  - Nitrogen potential $K_N$
  - Multistages treatment ($T_1$, $t_1$, $KN_1$, $T_2$, $t_2$, $KN_1$, ...) -> a few physics is necessary

**But for one steel composition and heat treatment**



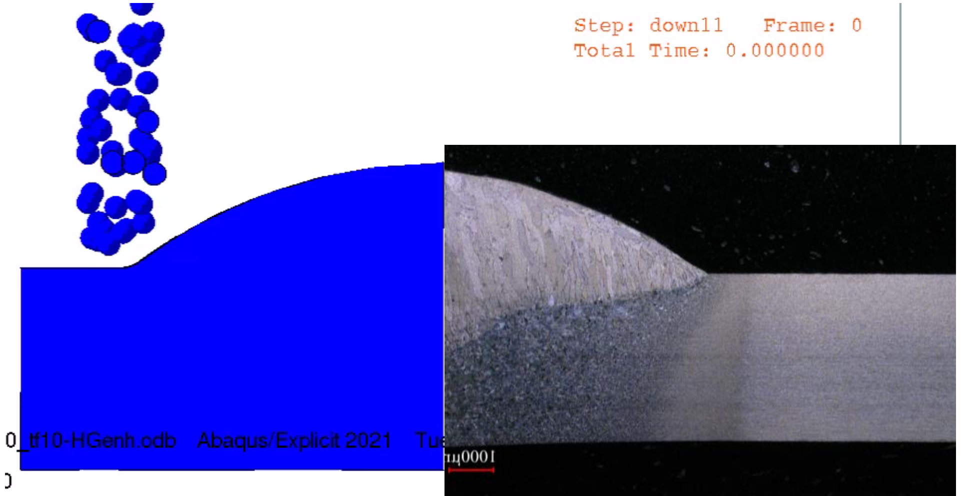



# Conclusions et perspectives

- Simulation des  déformations similaire à la modélisation des contraintes résiduelles
- Il faut connaitre la déformation libre de contraintes ou le profil de contraintes résiduelles

- Modification, évolution (relaxation) des contraintes résiduelles si modification des incompatibilités ou modification de la géométrie
- Réaliser le lien avec les changements microstructuraux

- Numérique: développer un Elément (EF) Traitements de Surface
-  Adaptation à des géométries complexes et chainage de procédés/ sollicitations
- Une « nouvelle ère » s’ouvre avec l’IA !!??



# Merci pour votre attention
# Vous avez des questions?

Arts et Métiers Sciences et Technologies

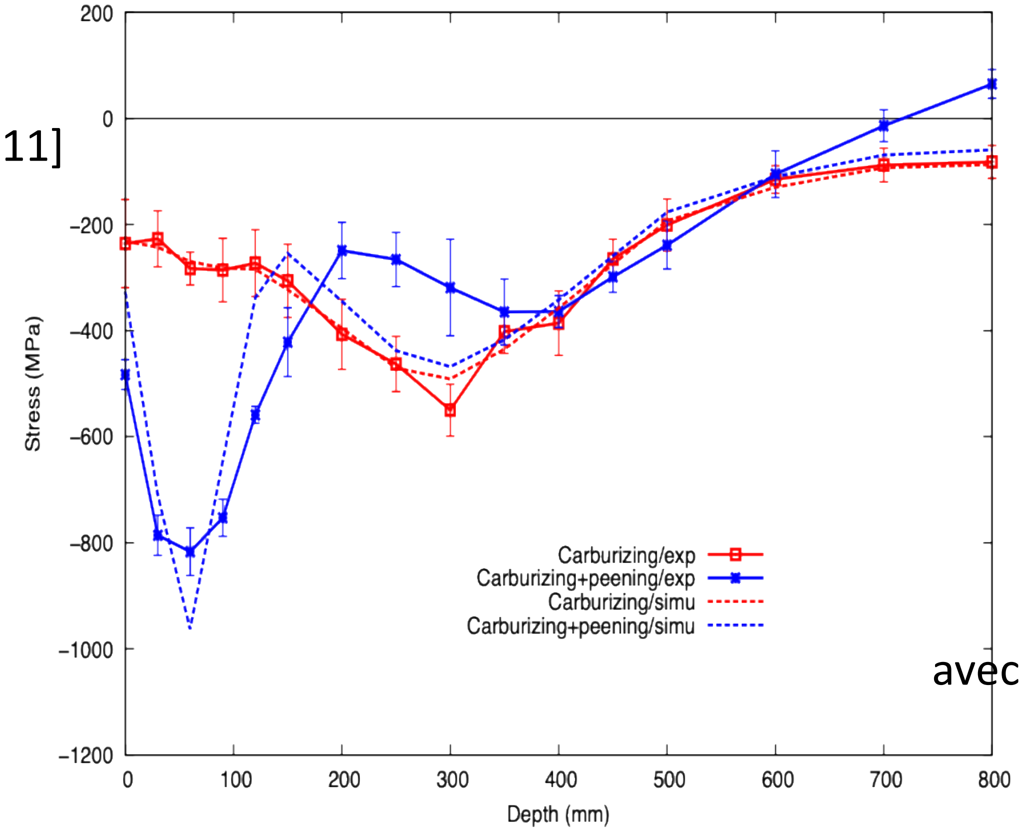
MSMP Mechanics, Surfaces and Materials Processing

# Méthode thermique fictive

Application à des traitements de surface combinés

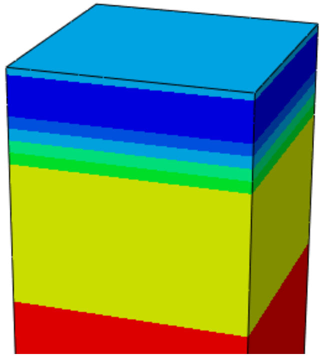
Cémentation puis chainage Grenaillage

[PhD Renaud 2011]



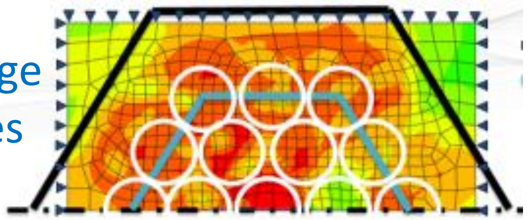

avec

Méthode thermique fictive



+

Grenaillage multibilles



$$\underset{\sim}{\alpha}^*(z) = -\frac{2\mu(z) + C + K(z)}{2\mu(z).\Delta\theta^*}.\underset{\sim}{\varepsilon}^p(z)$$

$$|K(z)| = \left|\frac{\sigma_y}{3.\varepsilon^p_{xx}(z)}\right|$$

Arts Sciences et Technologies et Métiers