







Mean field and full field modeling of dynamic and post-dynamic recrystallization: application to 304L steel

PhD defense of Ludovic Maire

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# **Supervised by:**

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  - Major improvements
  - Results b.
- II. Experimental testing on a 304L steel
  - Identification of model parameters for DRX
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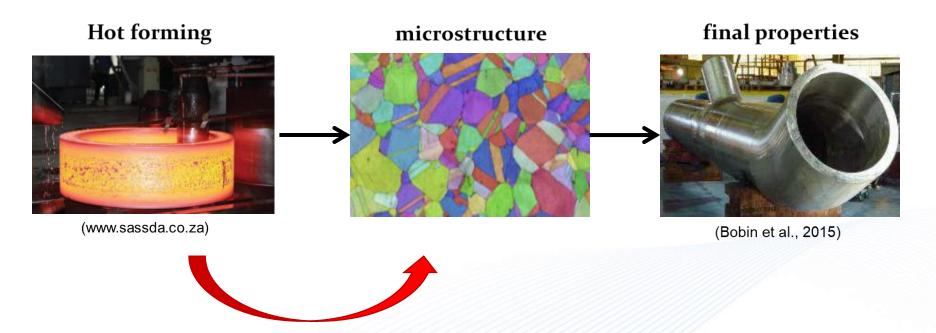






RESTRICTED Experimental LS-FE Conclusion New full field New mean Context **Formalism** model field model results **Prospects** 

# Context of the study



- During hot deformation:
- dynamic recrystallization (DRX) occurs
  - After hot deformation :
- post-dynamic recrystallization (PDRX) occurs













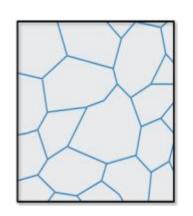




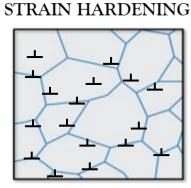




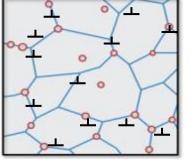
# Dynamic Recrystallization (DRX)







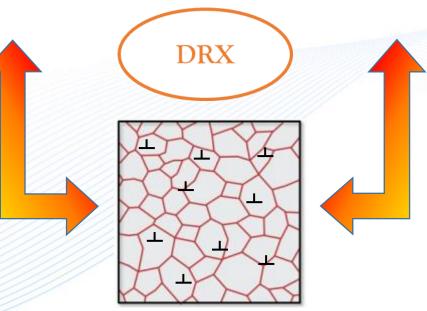




Initial microstructure

## DRX

- STRAIN HARDENING
- DYNAMIC RECOVERY
- NUCLEATION
- GRAIN BOUNDARY MIGRATION



GRAIN BOUNDARY MIGRATION





















New full field model

New mean field model Experimental results

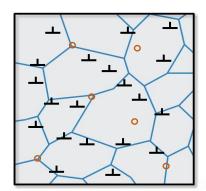
RESTRICTED Conclusion **Prospects** 

# Post-Dynamic Recrystallization (PDRX)

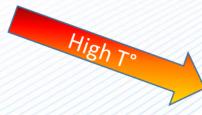
### GRAIN BOUNDARY MIGRATION

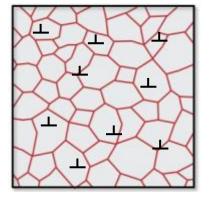
# Microstructure after hot deformation



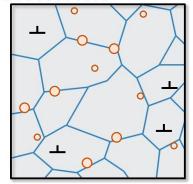








### STATIC RECOVERY + **NUCLEATION**



### **PDRX**

- STATIC RECOVERY
- **NUCLEATION**
- GRAIN BOUNDARY MIGRATION

















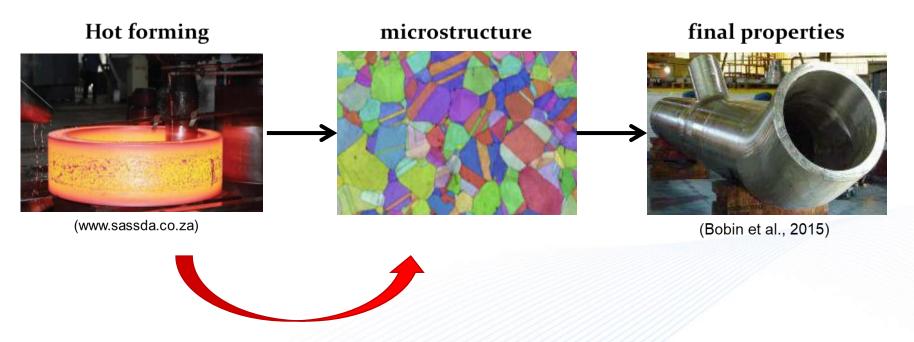






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# Context of the study



Importance to predict, control and optimize microstructural evolutions by DRX and PDRX







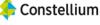






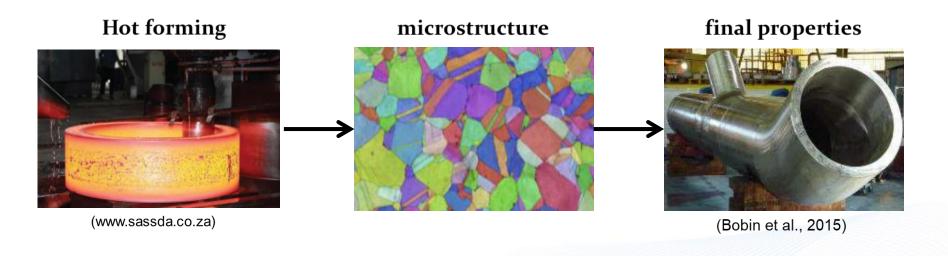






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# Context of the study



Importance to predict, control and optimize microstructural evolutions by DRX and PDRX Simulations













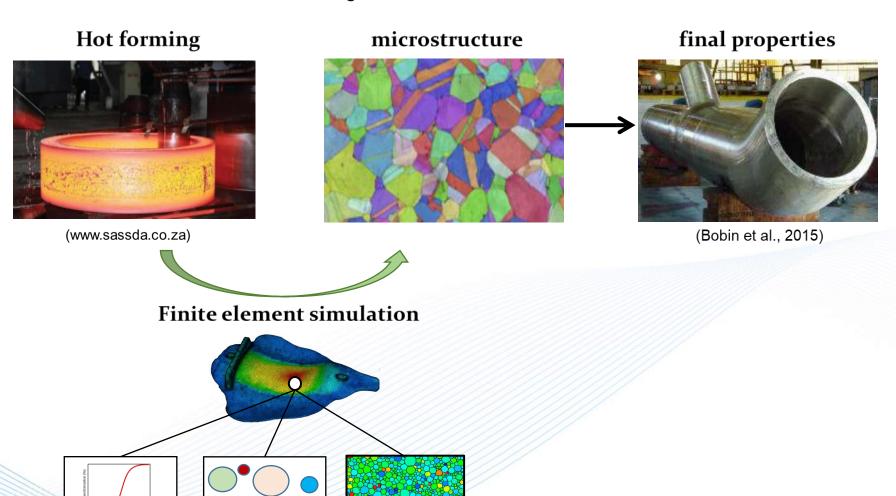








# Context of the study









Phenomenological





Mean field







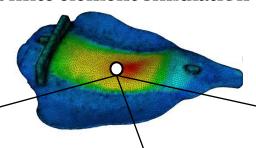
Full field



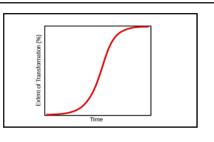


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### Finite element simulation

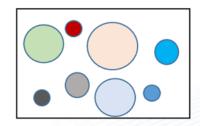


## Phenomenological models



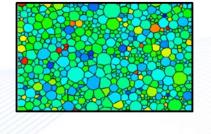
- Analytical laws (fast)
- **Averaged quantities**
- Recalibration for each particular condition (T°, έ) No description of the microstructure

### Mean field models



- Implicit description of the microstructure
- Versatile
- Analytical laws
- Prediction of grain size distributions
- Local mechanisms
- Homogenized microstructure

### **Full field models**



- Versatile
- Local mechanisms
- Explicit description of the microstructure
- **Numerical costs**









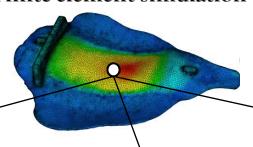




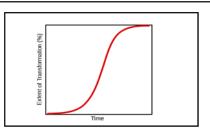




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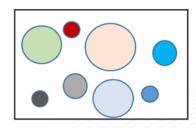


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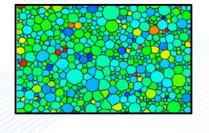
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# Full field modeling: The Level-Set method in a finite element framework

L. Maire, B. Scholtes, C. Moussa, N. Bozzolo, D. Pino Muñoz, A. Settefrati, M. Bernacki, Modeling of dynamic and postdynamic recrystallization by coupling a full field approach to phenomenological laws, Materials & Design 133 (2017) 498-519.





















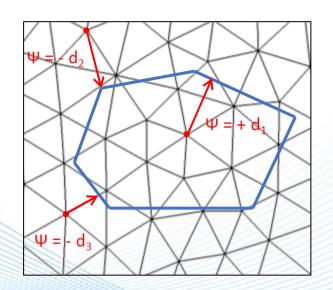
A Level-Set method in a finite element framework is considered in this work

# The Level-Set method

Level-Set functions:

$$\begin{cases} \psi(x) = d(x, \Gamma), x \in \Omega, \\ \Gamma = \{x \in \Omega, \psi(x) = 0\} \end{cases}$$

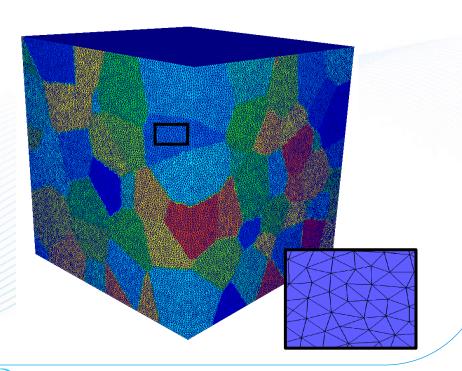
(Merriman et al., 1994, Bernacki et al., 2008) (Osher and Sethian, 1988)



# Generation of the initial microstructure

- Immersion of experimental micrographs
- Using a Voronoï tessellation
- Using a Laguerre-Voronoï tessellation

(Hitti et al., 2012, Fan et al., 2004)





















# ➤ The Level-Set method captures interfaces

# <u>Interfaces displacement</u>

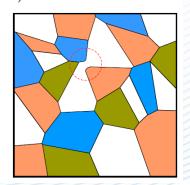
$$\begin{cases} \frac{\partial \psi_i(x,t)}{\partial t} + \vec{v}_i \cdot \vec{\nabla} \psi_i(x,t) = 0\\ \psi_i(t=0,x) = \psi_i^0(x) \end{cases}$$

# Reinitialization of the Level-Set functions

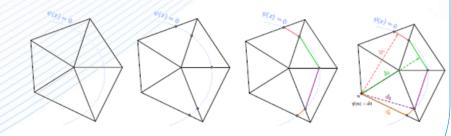


# Numerical tools to decrease computational costs

- Use of a recoloring schema with GLS functions (PhD Scholtes 2013-2016, Scholtes et al. CMS 2015; Scholtes et al. CMS 2016)



Use of a direct reinitialization algorithm (Shakoor & Scholtes, AMM 2015)





















# A new full field model for DRX and PDRX

L. Maire, B. Scholtes, C. Moussa, N. Bozzolo, D. Pino Muñoz, A. Settefrati, M. Bernacki, Modeling of dynamic and post-dynamic recrystallization by coupling a full field approach to phenomenological laws, Materials & Design 133 (2017)498-519.









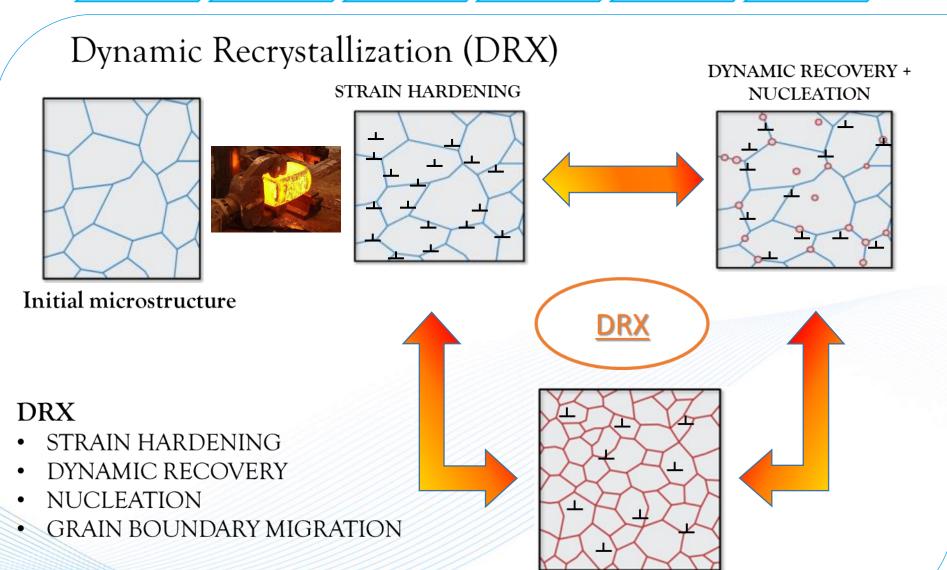






























GRAIN BOUNDARY MIGRATION

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# Mechanisms considered for **DRX**

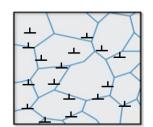
# Strain hardening/Recovery

(Yoshie et al., 1987)

$$\frac{\partial \rho_i}{\partial \varepsilon} = K_1 - K_2 \rho_i$$

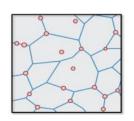


**Plastic** deformation



# Nucleation

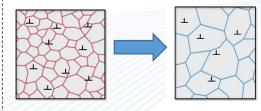
(Roberts et al., 1978) (Beltran et al., 2015) (Bailey & Hirsch, 1962)



# Which size?

$$r_{\rm cr} = \omega \frac{2\gamma_{\rm b}}{\rho_{\rm cr} \tau}$$

# Boundary migration



(Bernacki et al., 2011)

$$\dot{V} = K_{\rm g} \Phi \Delta t$$

$$\rho_{\rm cr} = \left(\frac{20K_1 \gamma_b \dot{\varepsilon}}{3M_b \delta \tau^2}\right)^{1/3}.$$

$$\rho_{\rm cr} = \left[\frac{-2\gamma_b \dot{\varepsilon} \frac{K_2}{M_b \delta \tau^2}}{\ln\left(1 - \frac{K_2}{K_1} \rho_{\rm cr}\right)}\right]^{1/2}$$

When/Where?

# How many?

$$\begin{cases} \frac{\partial \psi_i(x,t)}{\partial t} - M_b \gamma_b \Delta \psi_i + \overrightarrow{v_i^e} \cdot \nabla \psi_i = 0 \\ \psi_i(t=0,x) = \psi_i^0(x) \end{cases}$$
$$v_i^e = M_b[\delta \tau(\rho_j - \rho_i)]$$















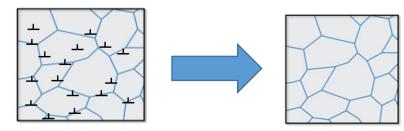




# Mechanisms considered for PDRX

# **Static Recovery**

$$\frac{\partial \rho_i}{\partial t} = -K_s \rho_i$$

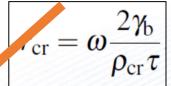


# **Nucleation**

(Roberts et al., 1978) (Beltran et al., 2015) (Bailey & Hirsch, 1962)

# **ASSUMPTION**

hich size?



### When/Where

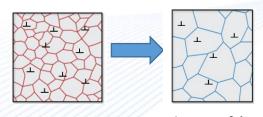
$$\rho_{\rm cr} = \left(\frac{20K_1\gamma_{\rm b}\dot{\varepsilon}}{3M_{\rm b}\delta\tau^2}\right)^{1/3}.$$

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How many?

$$\dot{V} = K_{\rm g} \Phi \Delta t$$

# Boundary migration



(Bernacki et al., 2011)

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$$v_i^e = M_b [\delta \tau(\rho_i - \rho_i)]$$













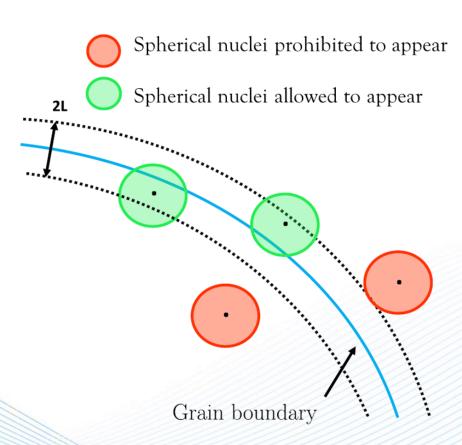


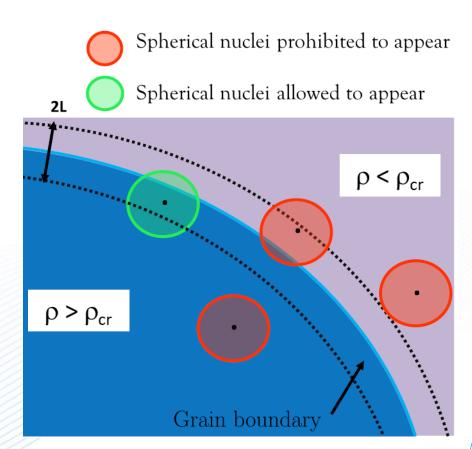






# Necklace nucleation in the considered full field framework













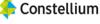




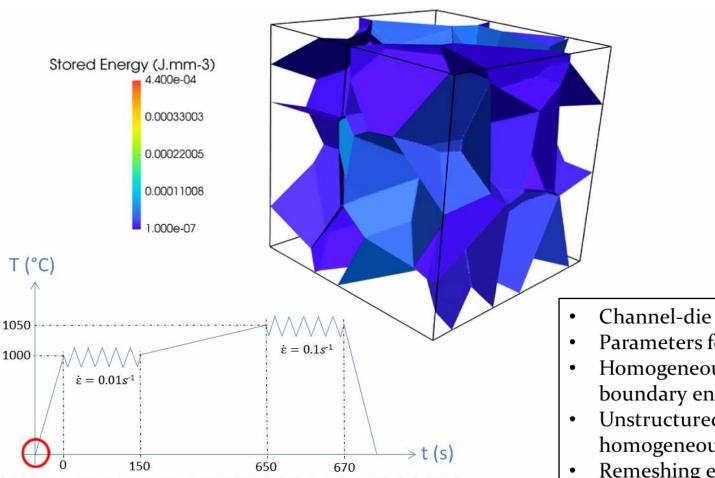


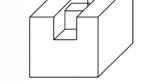






# A multi-pass process simulated with the full field model





Compression

- Channel-die compression
- Parameters for a 304L steel
- Homogeneous values of grain boundary energy and mobility
- Unstructured, isotropic and homogeneous mesh
- Remeshing every 0.2 of deformation (best compromise)
- An initial number of 64 grains



















# Sensitivity study for integration in the DIGIMU software package

# The sensitivity study identifies the ideal:

### DRX

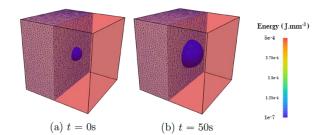
- initial number of grains
- safety factor for nuclei size
- deformation step
- mesh size

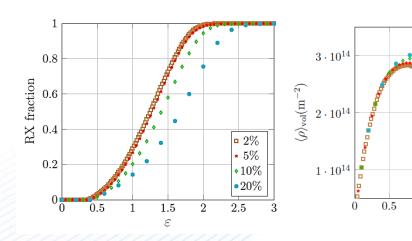
# To converge in terms of:

- RX fraction
- mean grain size
- mean dislocation density
- grain size distributions
- dislocation density distributions

# **PDRX**

time step





# Simulation of DRX at T = 1273K and $\dot{\epsilon}$ =0.01s<sup>-1</sup> during 200s

Before sensitivity study 10h on 3x24 procs



After sensitivity study 1h30 on 3x24 procs





















\* 5%

10%

• 20%

# A new topological approach for mean field modeling of DRX/PDRX

L. Maire, C. Moussa, N. Bozzolo, M. Bernacki, A new topological approach for the mean field modeling of dynamic recrystallization, Materials & Design 146 (2017) 194-207.







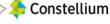




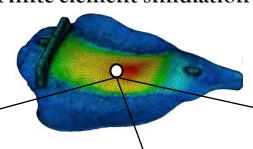




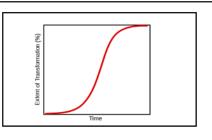




# Finite element simulation

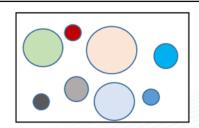


# Phenomenological models



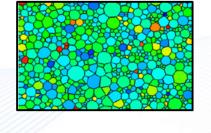
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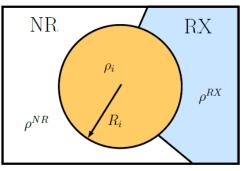




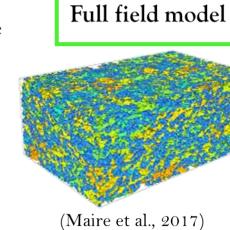


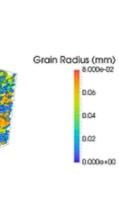


# Mean field model (CEMEF)

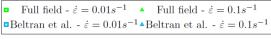


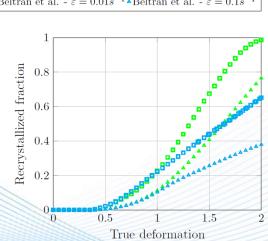
Comparisons using same metallurgical laws with same model parameters

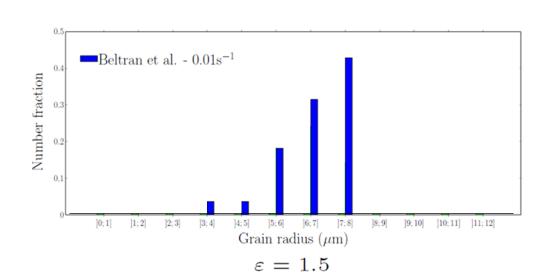




(Beltran et al., 2015)







Limitation already discussed in many papers (Beltran et al., 2015; Smagghe et al., 2016)



















The *NHM* is based on two main improvements in terms of DRX mean field modeling:

- The consideration of a particular neighborhood for each grain (topology)
- II. The modeling of grain shape evolution during the dynamic process



















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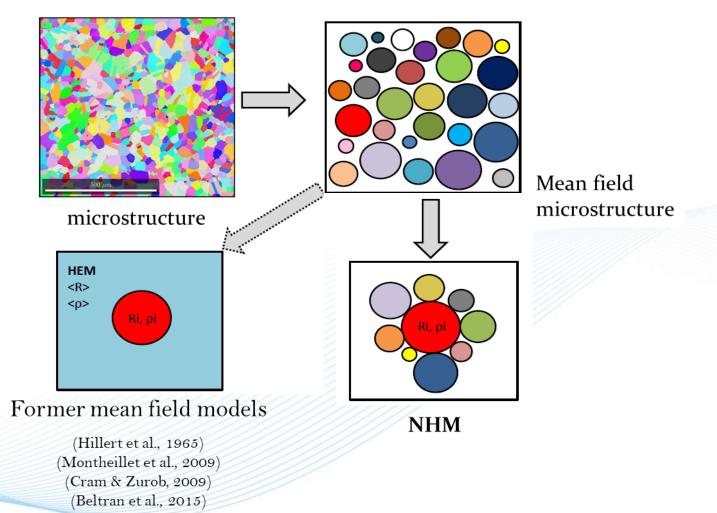








# The NHM vs Standard mean field models









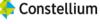




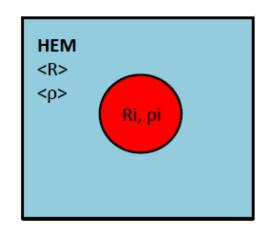








This new approach affects the grain boundary migration law



$$v_i = M_b \left[ \delta \tau (\overline{\rho} - \rho_i) + \beta \gamma_b (\frac{1}{\overline{R}} - \frac{1}{R_i}) \right]$$

$$\Delta V_i = v_i S_i \Delta t$$



$$v_{ij} = M_b[\delta \tau (\rho_j - \rho_i) + \gamma_b (\frac{1}{R_j} - \frac{1}{R_i})]$$

$$\Delta V_{ij} = v_{ij} S_i \psi_{ij} \Delta t$$

Surface fraction in contact between *i* and *j* 















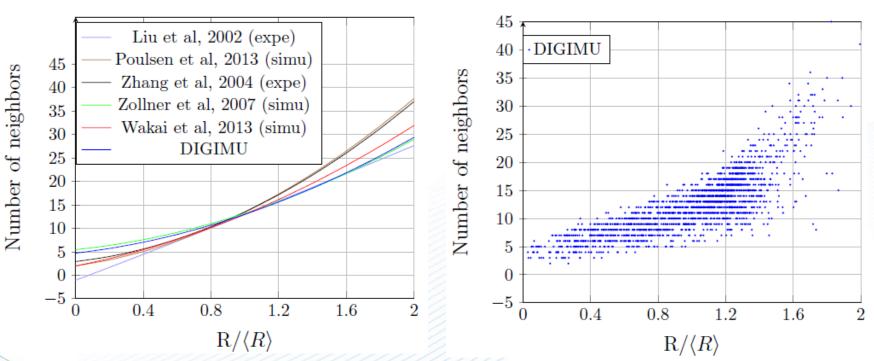




How to choose the number of neighbors for each grain?

Some laws from literature predict the number of neighbors of a grain depending on its size, within a steady-state or quasi steady-state regime

## Validation with DIGIMU



$$N_{\text{neigh}} = 4.06\omega^2 + 4.22 \omega + 4.71$$
  
with  $\omega = R/$ 









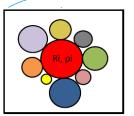








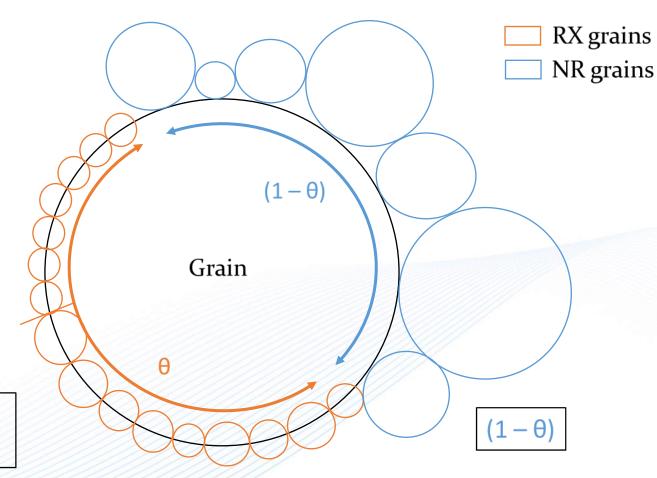




Number of neighbors occupying  $\theta$  is subdivided into two families



 $\theta_2$ : Number of other RX grains























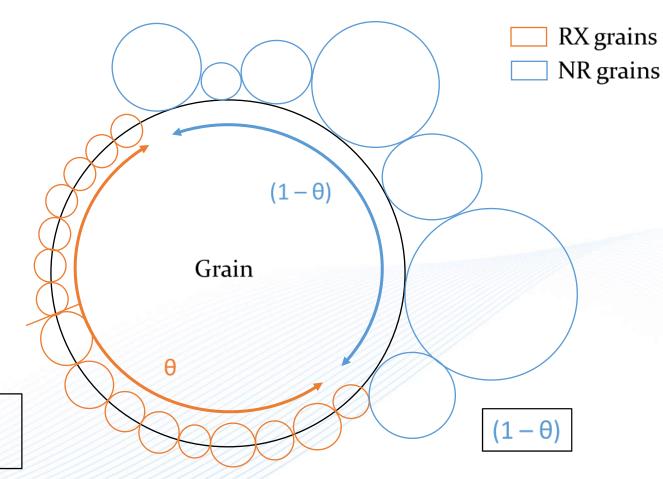
Number of neighbors occupying  $\theta$  is subdivided into two families



> Known at any time increment

 $\theta_2$ : Number of other RX grains

Known at any time increment













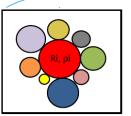












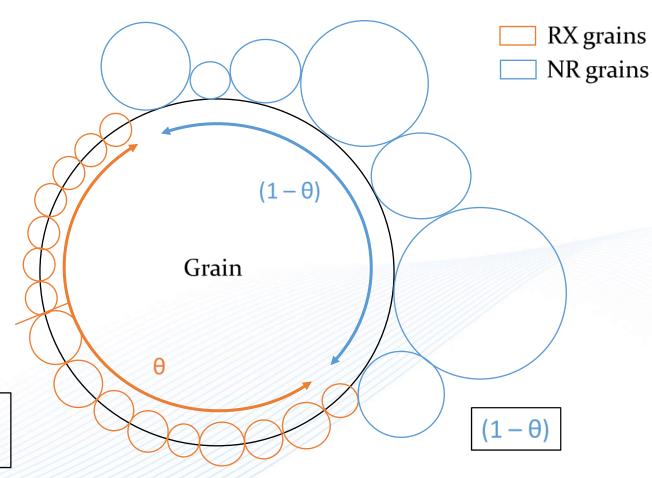
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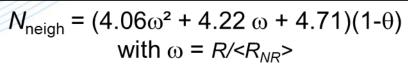


> Known at any time increment

 $\theta_2$ : Number of other RX grains

Known at any time increment

























The *NHM* is based on two main improvements in terms of mean field modeling:

The consideration of a particular neighborhood for each grain

II. The modeling of the grain shape evolution













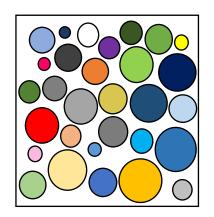


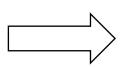


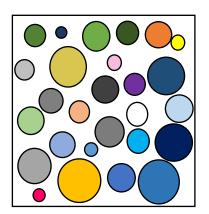


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### Standard Mean field models

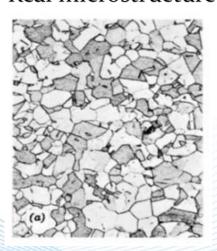




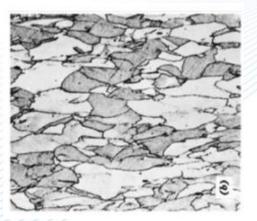


Grains remain spherical in MF models

### Real microstructure







Grain shape evolves in real microstructure

(Source: Bergström, 2015)













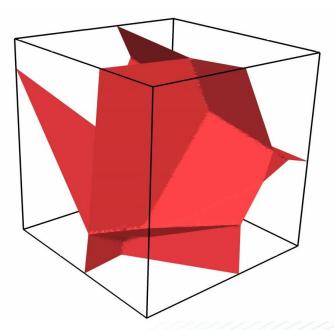




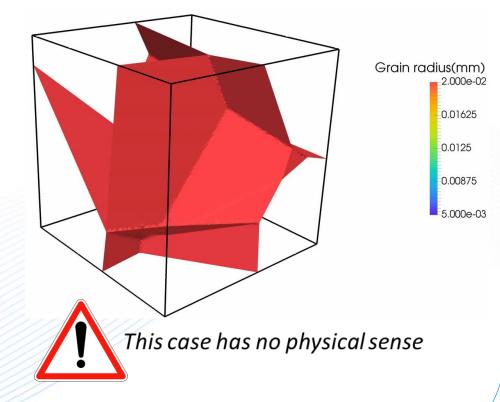


# Does the grain shape evolution influence results?

By considering deformation



Without considering deformation













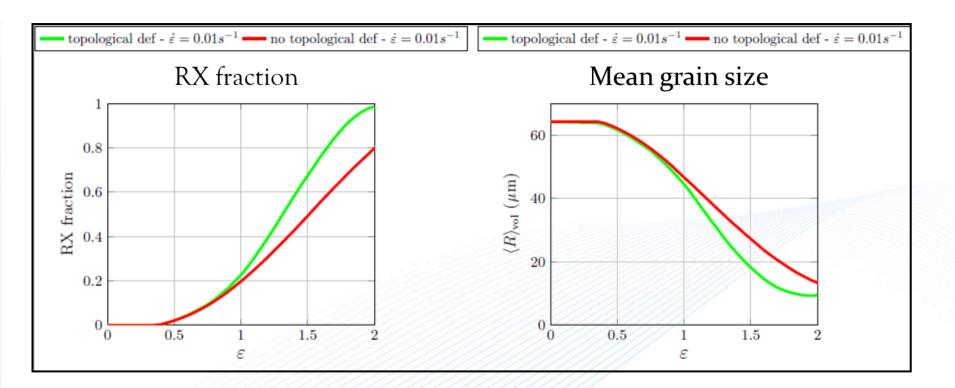








# Does the grain shape evolution influence results?



➤ Kinetics are faster in the physical case since grain boundary surface increases during deformation, increasing nucleation













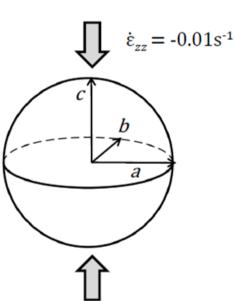






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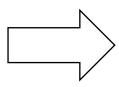




$$(\alpha_1, \alpha_2, \alpha_3) = (1, 1, 1)$$

$$\begin{cases} \alpha = \alpha_1 R = R \\ b = \alpha_2 R = R \\ c = \alpha_3 R = R \end{cases}$$

# Series of small time steps

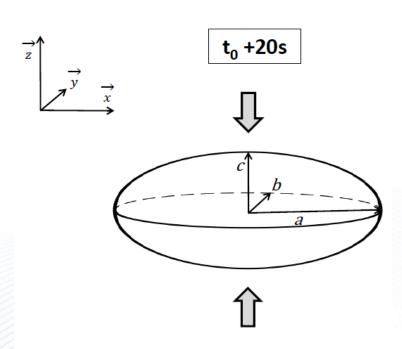


$$\alpha_1^{(t+\Delta t)} = \alpha_1^t + \dot{\varepsilon}_{xx} \Delta t,$$

$$\alpha_2^{(t+\Delta t)} = \alpha_2^t + \dot{\varepsilon}_{yy} \Delta t,$$

$$\alpha_3^{(t+\Delta t)} = \alpha_3^t + \dot{\varepsilon}_{zz} \Delta t,$$

$$M = \begin{bmatrix} \dot{\varepsilon}_{xx} & 0 & 0 \\ 0 & \dot{\varepsilon}_{yy} & 0 \\ 0 & 0 & \dot{\varepsilon}_{zz} \end{bmatrix}$$



$$(\alpha_1, \alpha_2, \alpha_3) = (1.105, 1.105, 0.82)$$

$$\begin{cases} a = 1.105R \\ b = 1.105R \\ c = 0.818R \end{cases}$$













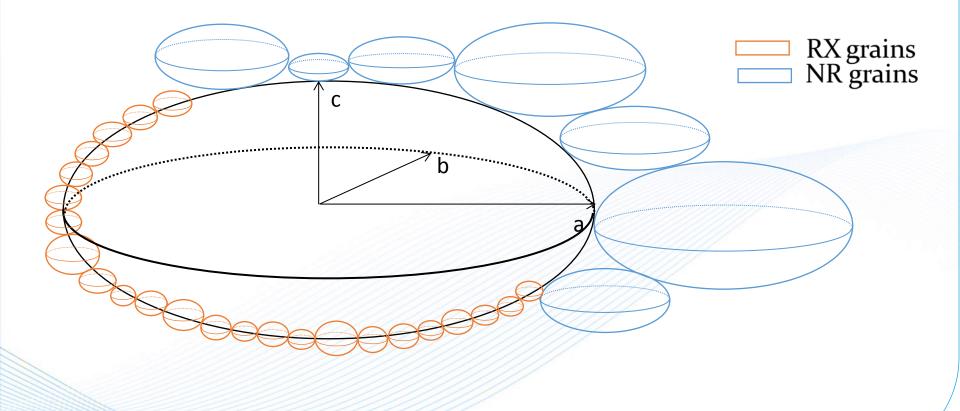








Final consideration of the neighborhood and the grain shape evolution:





















## RESULTS USING THE NHM In terms of:

RX Fraction and mean grain size Grain size distributions









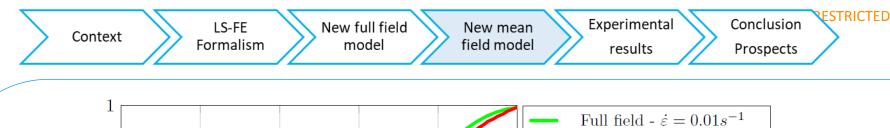


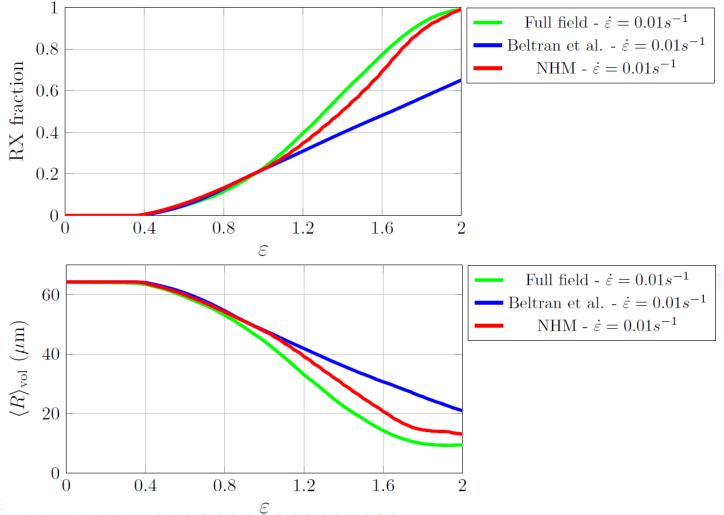


















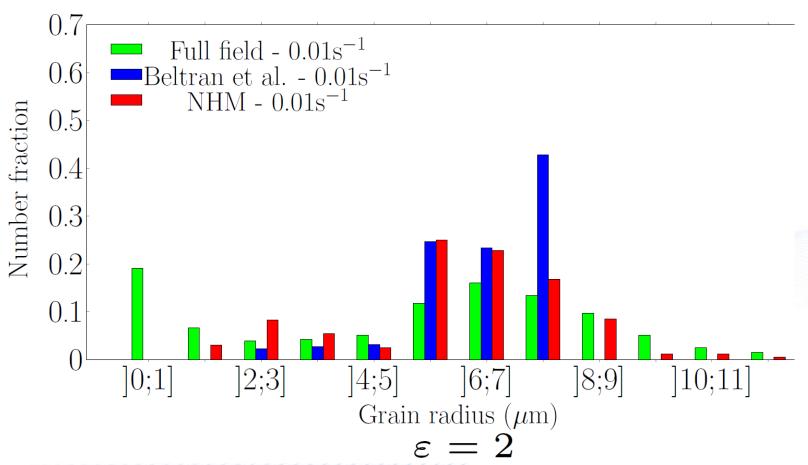
























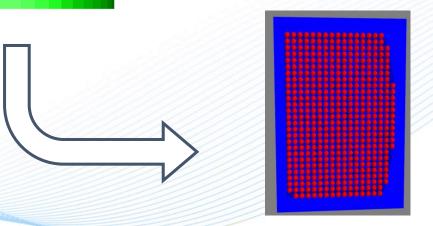






## First integration of NHM into a finite element software

#### (J. Barlier from Transvalor S.A.) Prediction of microstructural quantities Compression of a cylindrical sample 52.1 46.6 FORGE® 41.2 35.7 30.2 Sensors record the 24.7 thermomechanical paths 19.2





13.7



















Experimental Conclusion LS-FE New full field New mean Context field model Formalism model results **Prospects** 

# Experimental testings on 304L: Calibration and validation within the DRX regime











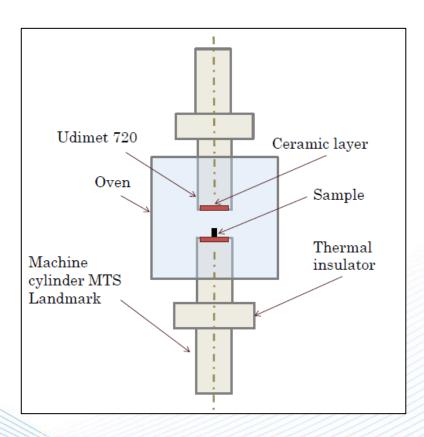




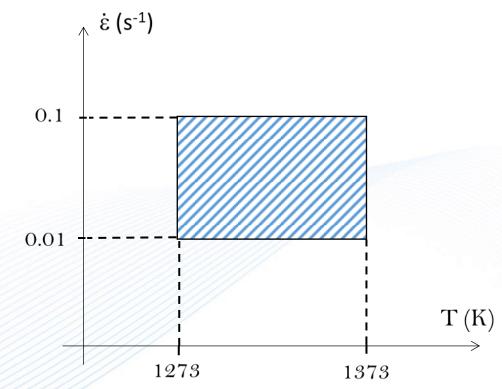




#### Compression test setup



#### Thermomechanical conditions





















New full field model

New mean field model Experimental results

**Nucleation** 

ESTRICTED Conclusion **Prospects** 

## 4 model parameters to be identified :

Hardening/Recovery

$$\frac{\partial \rho}{\partial \varepsilon} = K_1 - K_2 \rho$$

Identified on stress-strain curves before **DRX** initiates

Grain boundary migration

$$v_{ij} = M \left[ \delta \tau (\rho_j - \rho_i) + \gamma (\frac{1}{R_j} - \frac{1}{R_i}) \right]$$











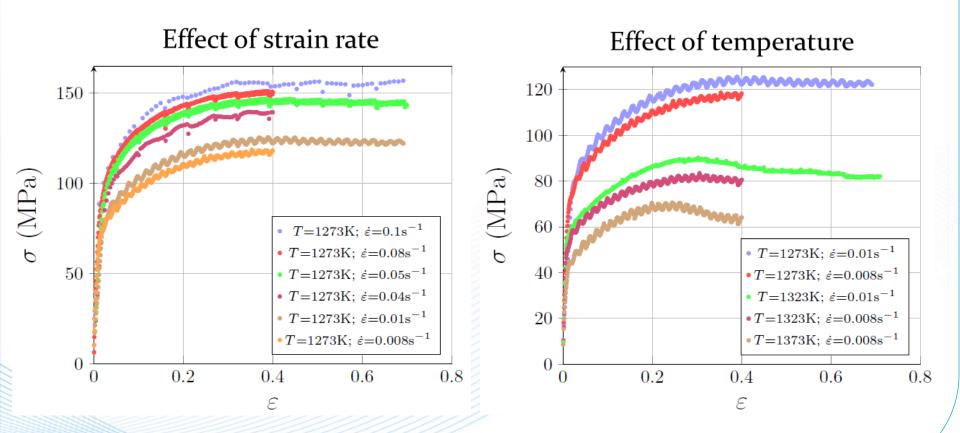








Stress-strain curves required to identify K1 and K2

















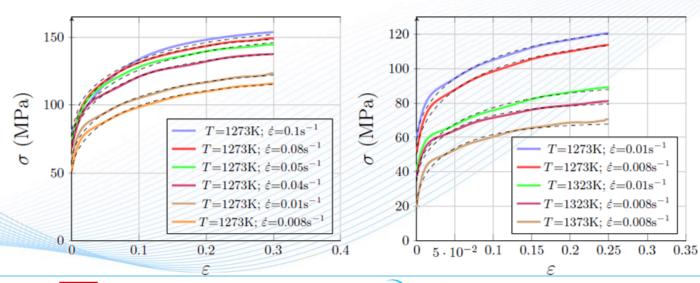




$$\frac{\partial \rho}{\partial \varepsilon} = K_1 - K_2 \rho$$

#### Identification of K1 and K2 based on stress-strain curves:

- 1. Method of Jonas et al. (2009) to get first approximations of  $K_1$  and  $K_2$
- 2. Inverse analysis on stress-strain curves using the Excel software. The portion of the curve considered is between yield stress and initiation of nucleation (about 80% of peak strain)











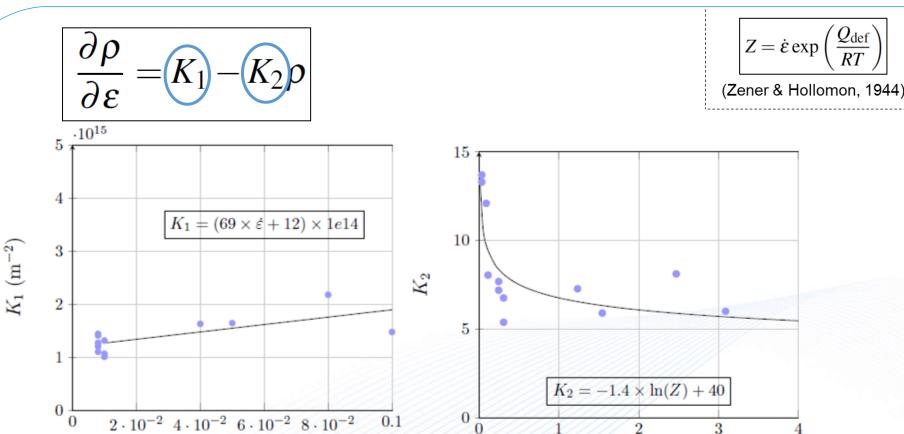












- Hardening is only dependent on strain rate and increases with it.
- Dynamic recovery decreases with strain rate and increases with temperature.
- Both parameter trends are in accordance with literature.











 $\dot{\varepsilon}(s^{-1})$ 









 $\cdot 10^{10}$ 

## 4 model parameters to be identified :

Hardening/Recovery

$$\frac{\partial \rho}{\partial \varepsilon} = K_1 - K_2 \rho$$

Identified on stress-strain curves before **DRX** initiates

**Nucleation** 

$$\dot{V} = K_g S_b \Delta t$$

Grain boundary migration

$$v_{ij} = M \left[ \delta \tau (\rho_j - \rho_i) + \gamma (\frac{1}{R_j} - \frac{1}{R_i}) \right]$$

Identified from microstructure investigations











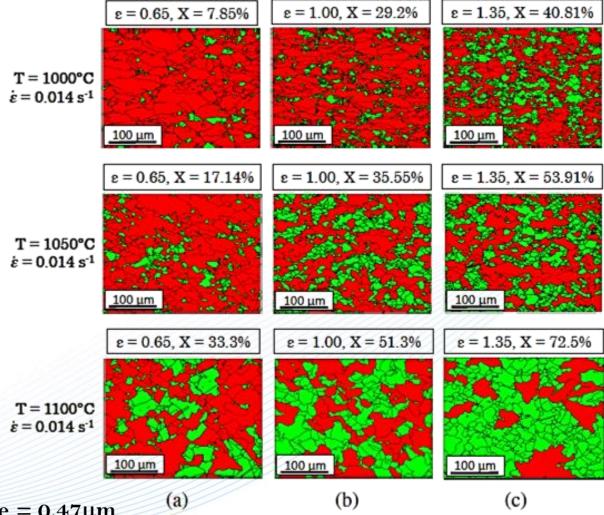








#### RX fractions obtained from different samples after compression



NR grains RX grains

Acquisition step size =  $0.47\mu m$ 

















#### The identification of $\delta$ and $K_g$ is made in two steps :

- 1. Use of the Saltykov method to transform 2D distributions into 3D ones (Saltykov 1958)
- Inverse analysis using BFGS inverse analysis algorithm from Python software

#### Experimental data 1.240 15 $T=1273K; \dot{\varepsilon}_{VM}=0.014s^{-1}$ T=1273K; $\dot{\epsilon}_{VM}=0.014s^{-1}$ T=1273K; $\dot{\epsilon}_{VM}=0.014s^{-1}$ $T=1273K; \dot{\varepsilon}_{VM}=0.07s^{-1}$ $T=1273K; \dot{\varepsilon}_{VM}=0.07s^{-1}$ $T=1273K; \dot{\varepsilon}_{VM}=0.07s^{-1}$ $3D \langle R_{RX} \rangle_{surf} (\mu m)$ T=1273K; $\dot{\varepsilon}_{VM}=0.14s^{-1}$ $T=1273K; \dot{\varepsilon}_{VM}=0.14s^{-1}$ $T=1273K; \dot{\varepsilon}_{VM}=0.14s^{-1}$ $\langle R \rangle_{\text{surf}} \ (\mu \text{m})$ 30 RX fraction 0.8 10 0.6 20 10 0.20 2.5 1.2 1.5 0.2 0.4 0.6 0.8 0.20.40.60.8 1.2 0.5 $\varepsilon_{\mathrm{VM}}$ $\varepsilon_{\text{VM}}$ $\varepsilon_{\mathrm{VM}}$

$$\dot{V} = K_g S_b \Delta t$$

$$v_{ij} = M * \left[\delta \tau(\rho_j - \rho_i) + \gamma(\frac{1}{R_j} - \frac{1}{R_i})\right]$$











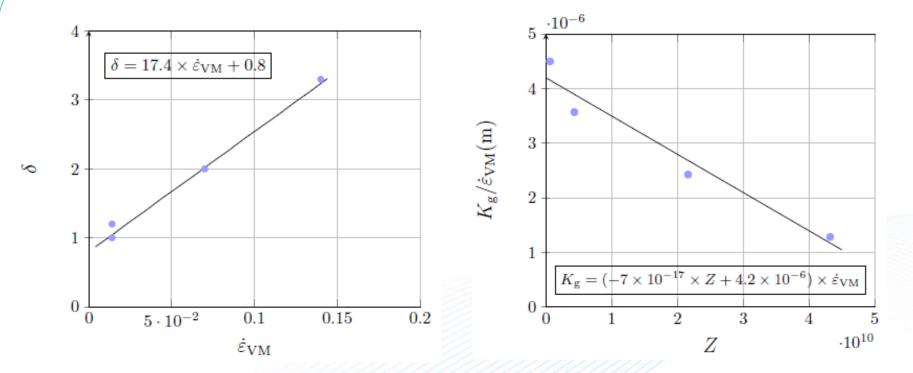








#### Inverse analysis directly from mean field simulations to identify $\delta$ and Kg



- The  $\delta$  parameter (accounting for the dependence of mobility on strain rate) increases with strain rate
- The Kg parameter acounting for nucleation increases with temperature and strain rate
- Both dependence are in accordance with literature















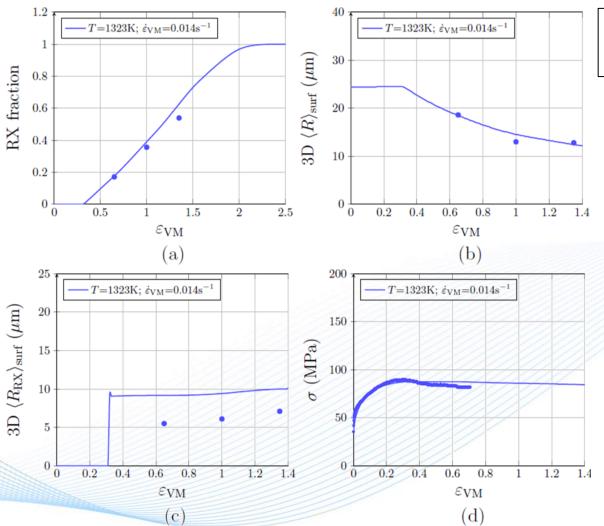






RESTRICTED Experimental Conclusion LS-FE New full field New mean Context Formalism model field model results **Prospects** 

#### Validation of the NHM:





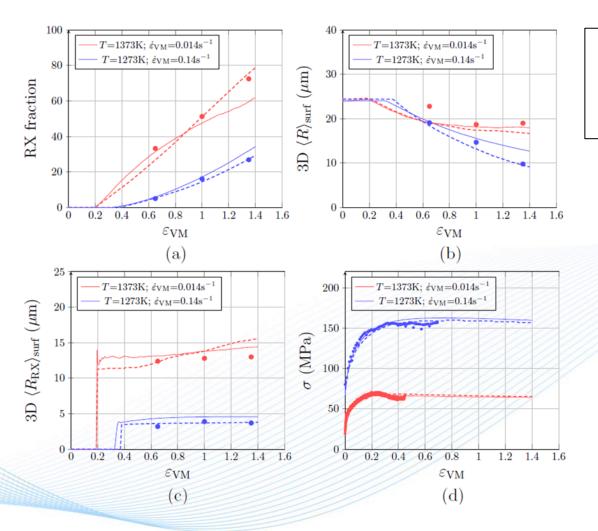


Experimental data

NHM

RESTRICTED Conclusion Experimental New full field LS-FE New mean Context Formalism model field model results **Prospects** 

#### Comparisons of the three models:



- Experimental data
- NHM
- Full field









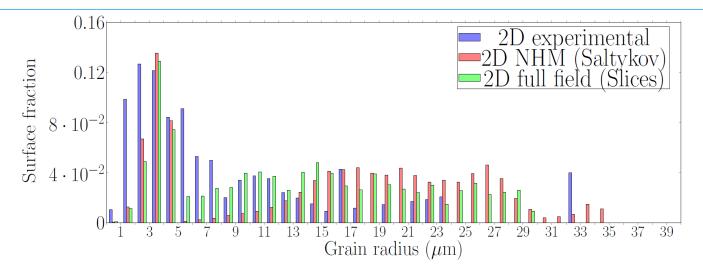




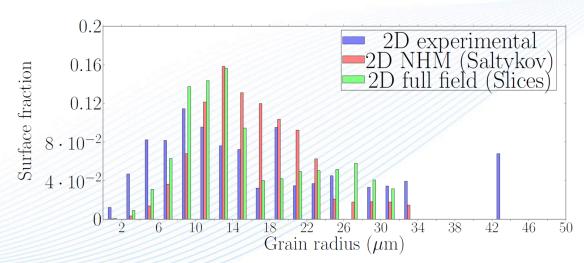








T=1273K,  $\dot{\varepsilon}_{\text{VM}}=0.14$ s<sup>-1</sup>,  $\varepsilon_{\text{VM}}=1.35$ ,  $X_{\text{expe}}=26.9\%$ 



T=1373K,  $\dot{\varepsilon}_{\text{VM}}=0.014$ s<sup>-1</sup>,  $\varepsilon_{\text{VM}}=1.35$ ,  $X_{\text{expe}}=72.5\%$ 











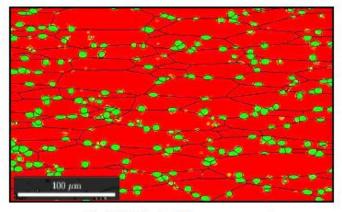




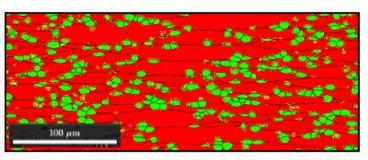




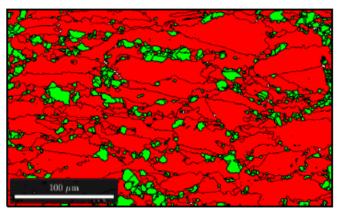
Comparaisons of experimental EBSD maps and 2D slices from 3D full field simulations  $(T = 1273K, \dot{\epsilon} = 0.014s^{-1})$ 



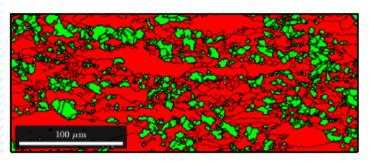
Full field,  $\varepsilon_{\rm VM} = 1$ 



Full field,  $\varepsilon_{\rm VM} = 1.35$ 



Experimental,  $\varepsilon_{\rm VM} = 1$ 



Experimental,  $\varepsilon_{\mathrm{VM}} = 1.35$ 

















#### Final conclusions

- A new full field model aiming to model DRX and PDRX in 3D, for large deformation and with low computational cost was proposed. This model is already integrated into the DIGIMU software package.
- With the help of full field simulations, a new mean field approach for modeling of DRX and PDRX was also proposed. This new approach tackles limitations of former mean field models, in particular concerning grain size distributions.
- An identification procedure applied on the 304L steel was proposed for these two models. This calibration method is based on stress-strain curves and microstructure quantities. After calibration, the predictions of these two models were validated for a new set of thermomechanical conditions.















#### Prospects related to this PhD work

- The full field model will be coupled with a crystal plasticity algorithm (PhD of David Ruiz) in order to tackle the assumptions made in analytical laws for strain hardening and recovery.
- Additional experimental investigations out of the considered range of thermomechanical conditions (1273-1373K and 0.01 and 0.1s<sup>-1</sup>) need to be performed to check the consistency of the two models.
- An identification procedure must be proposed during the PDRX regime to identify the static recovery parameters K<sub>s</sub> and check if static nucleation occurs.
- The identification procedure must be tested on other metals alloys (current works with partners of the DIGIMU consortium)



















### Prospects related to the DIGIMU software

- Consideration of anisotropic grain boundary energies. [ PhD, Julien Fausty (2016-2019) ]
- Consideration of solid-solid phase transformations. [ PhD, Chau-Thuy Pham (2017-2020) ]
- Improvement of the numerical framework. PhD, Sebastian Florez (2017-2020)
- Modeling of second-phase particles and their growth/shrinkage. [ PhDs, Karen Alvarado and Romane Quere (2017-2021) ]
- More explicit description of grain boundary mobility considered during simulations.

[PhD, Brayan Murgas (2018-2021)]









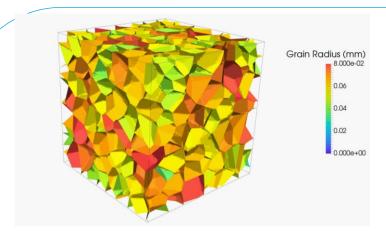




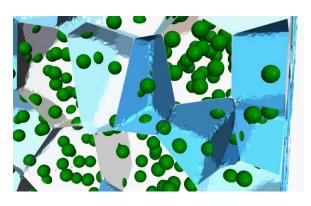






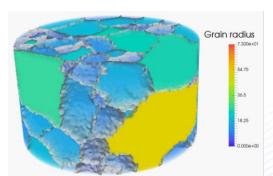


PhD Ludovic Maire



PhD Benjamin Scholtes

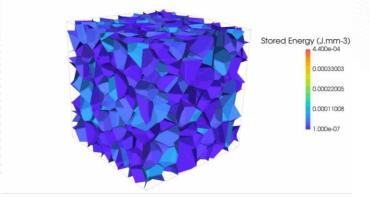
## Many thanks for your attention



PhDs Benjamin Scholtes and Julien Fausty Collaboration with C. Krill and M. Wang



Marc Bernacki



PhD Ludovic Maire

















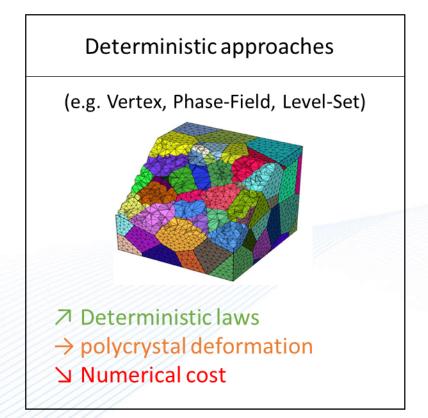
#### Two kinds of full field models

#### Stochastic approaches

(e.g. Cellular Automata, Monte Carlo)

2	2	2	2	7	7	7	7	7	7	7	7
2	2	2	2	7	7	7	7	7	7	7	7
8	8	1	1	1	1	1	7	7	7	7	7
8	8	8	1	1	1	1	1	9	9	9	9
8	8	8	1	1	1	1	1	9	9	9	9
8	8	8	8	1	1	1	9	9	9	9	9
8	8	8	8	8	1	1	9	9	9	9	9
8	8	8	8	8	5	5	5	5	5	9	9

- parallelization
- → Implementation
- → polycrystal deformation
- ✓ Stochastic aspect



A Level-Set method in a finite element framework is considered in this work



















#### Ideal ratio between nucleus size and mesh size

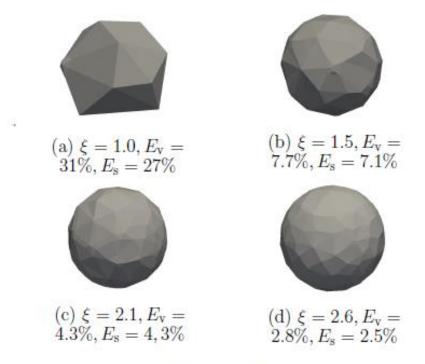


Fig. 3.5. Four nuclei generated according to different mesh sizes.  $\xi$  corresponds to the ratio between the nucleus radius  $r_{cr}$  and the mesh size.  $E_v$  (resp.  $E_s$ ) corresponds to the  $L^1$  error between the volume (resp. surface) of the generated nucleus and the volume (resp. surface) of a sphere of same radius.





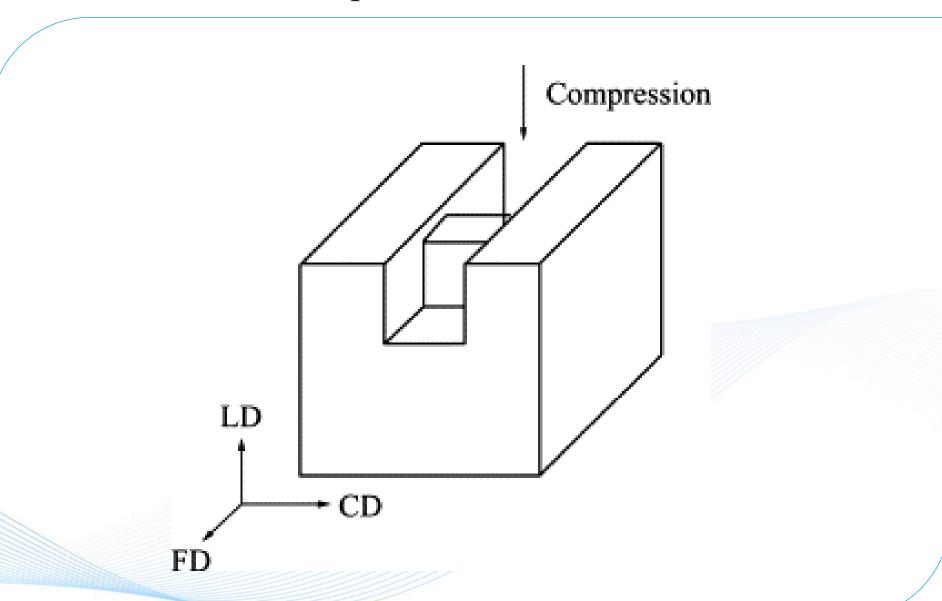








## Channel-Die compression test









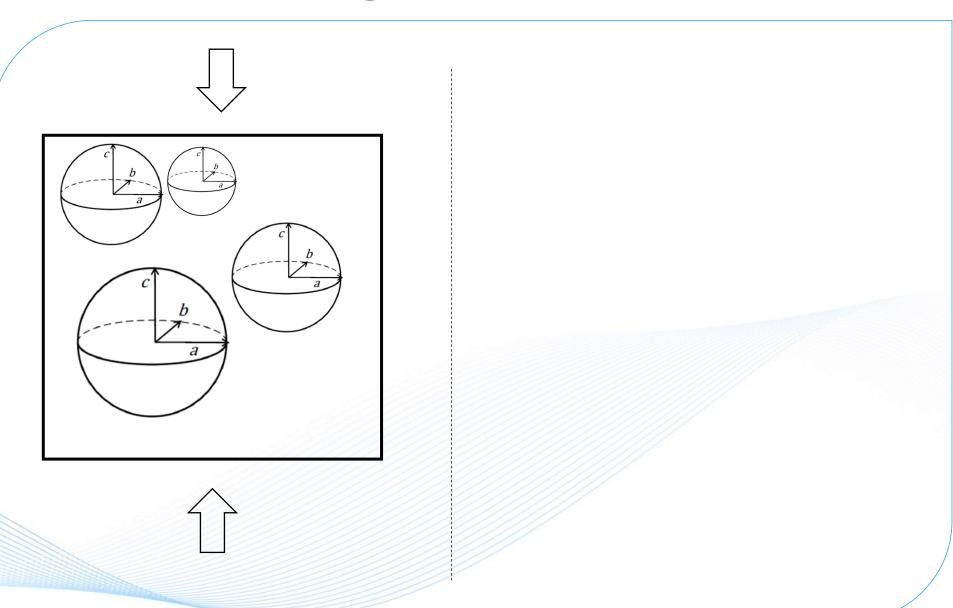


















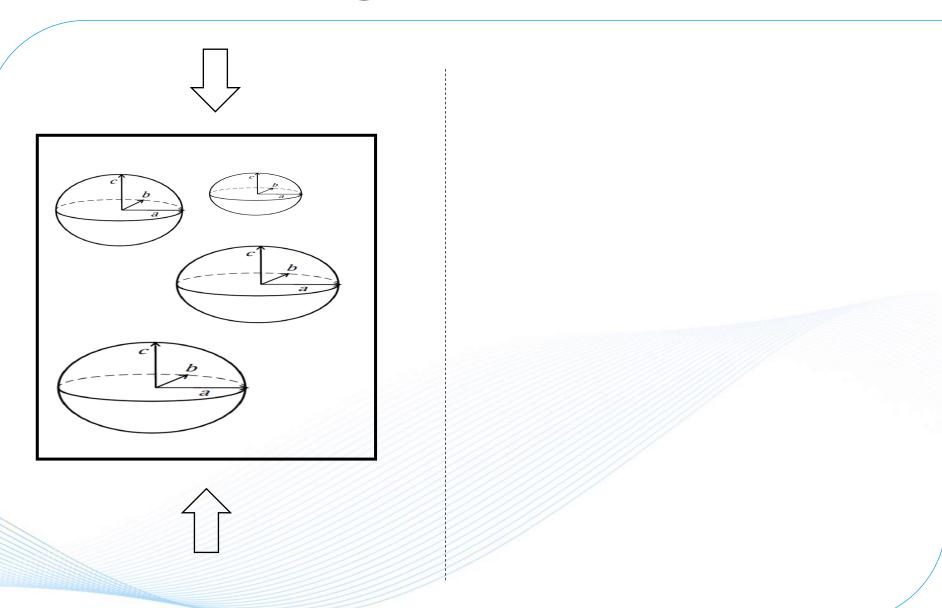




















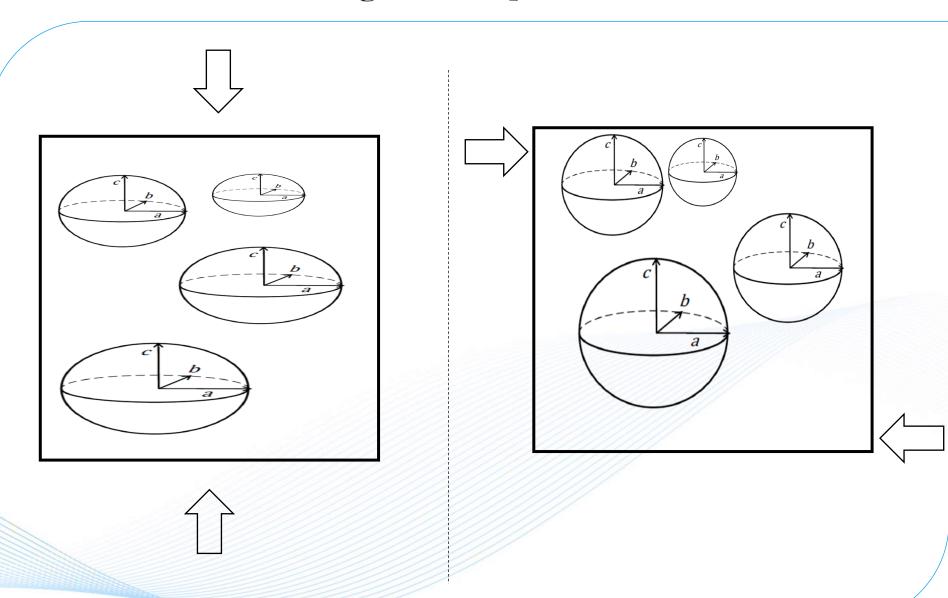




















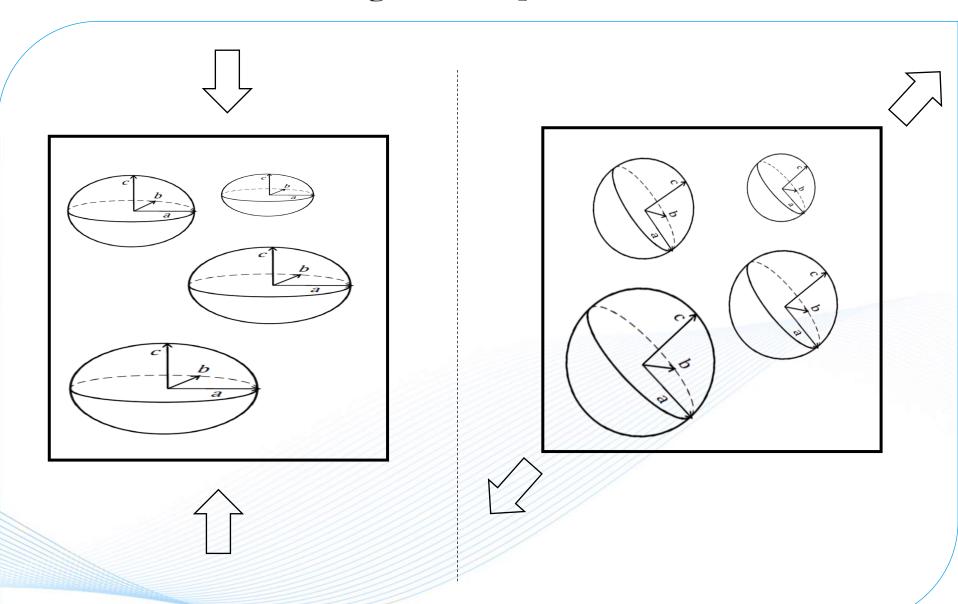




















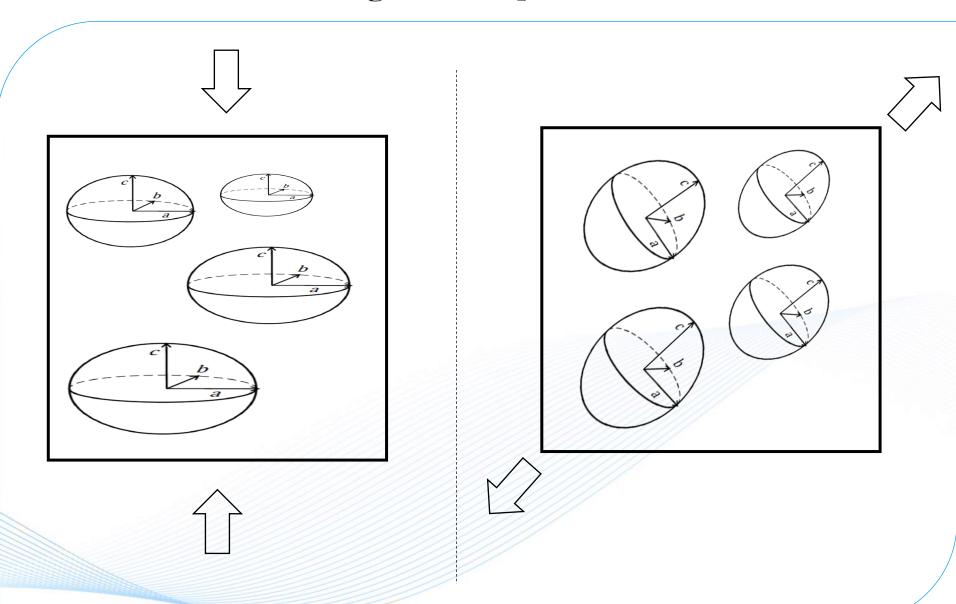




















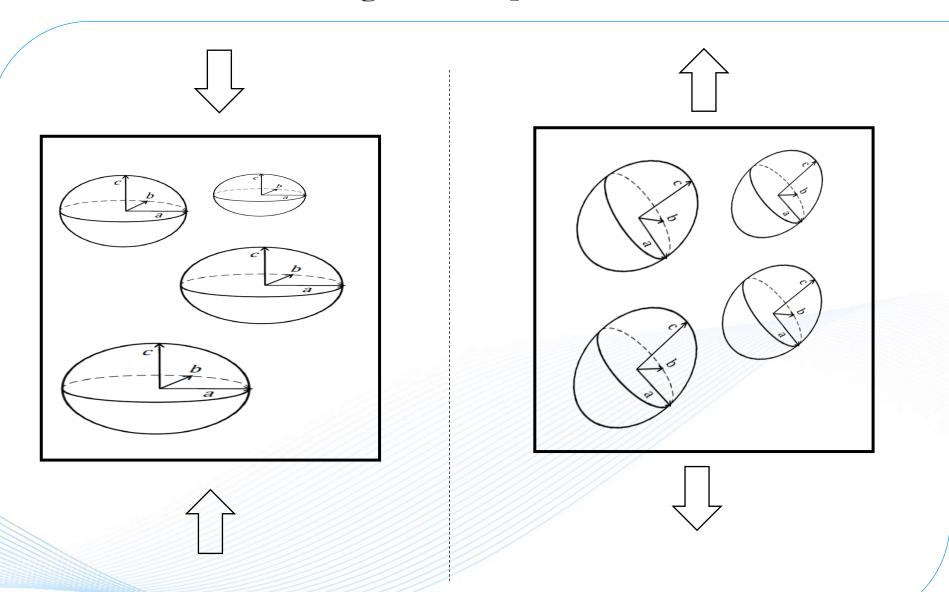




















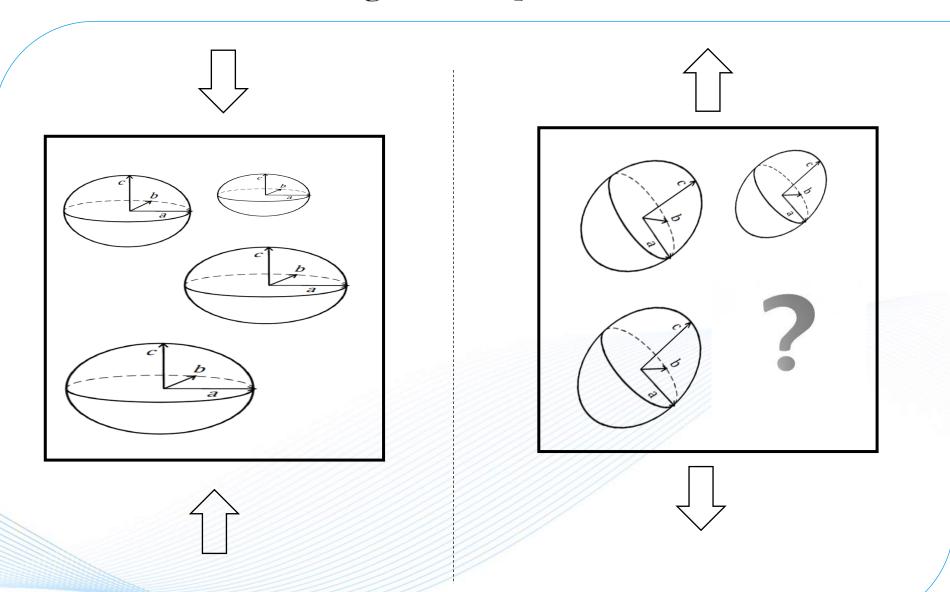




















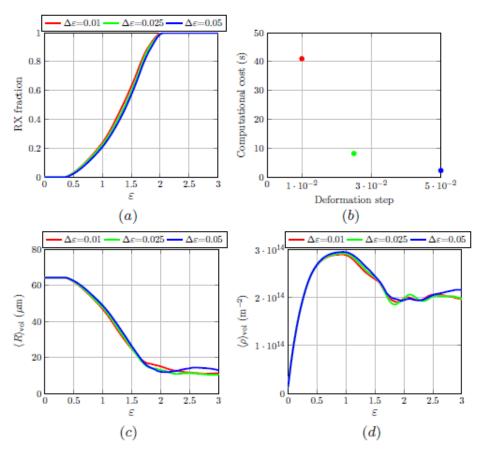








### Idealized deformation step in the NHM



Considered in all NHM simulations

$$\Delta \varepsilon = 0.025$$

$$\Delta t = \Delta \epsilon / \dot{\epsilon} = 0.025 / \dot{\epsilon}$$

To avoid prohibitive time steps due to low strain rates:

$$\Delta t = \max (\Delta t; 5s)$$

Fig. 4.12. Sensitivity study of the deformation step on results obtained with the NHM: (a) recrystallized fraction (b) computational cost (c) mean grain radius (weighted by grain volume) (d) mean dislocation density (weighted by grain volume). Simulations were performed at a strain rate of  $0.01s^{-1}$  and a temperature of 1273K.









