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Modeling of dynamic recrystallization on 304L steel by coupling a full field approach to mean field laws

L. Maire, N. Bozzolo, C. Moussa, M. Bernacki

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MINES ParisTech

Summary

I- Mechanisms of dynamic (DRX) and post-dynamic recrystallization (PDRX)

II- Modeling scales for DRX and PDRX and state of art

III- Modeling of recrystallization by coupling a full field approach to mean field laws

- Modeling of microstructure
- Strain hardening and recovery
- Grain boundary migration
- Nucleation mechanism

IV- First results and confrontations to experimentations

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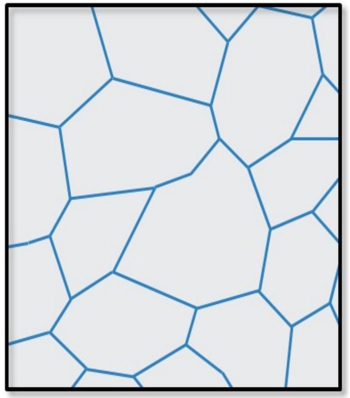
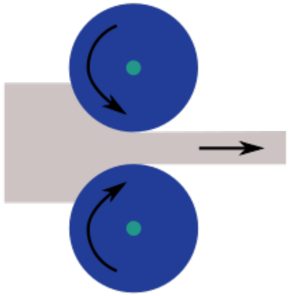
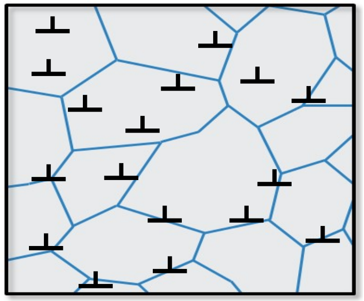
Dynamic recrystallization phenomenon

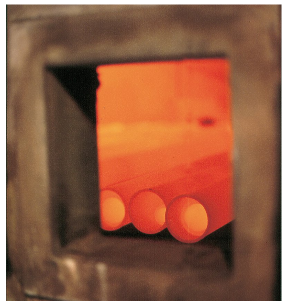


Initial microstructure

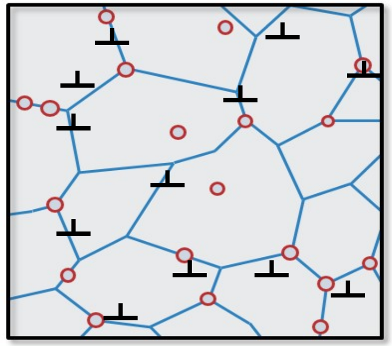


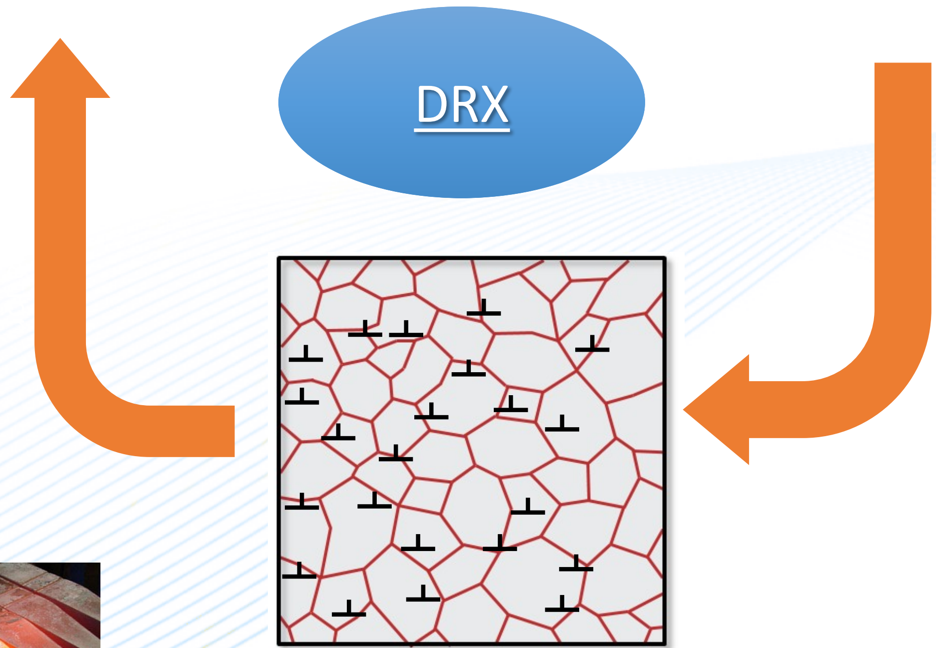
STRAIN HARDENING





RECOVERY + NUCLEATION





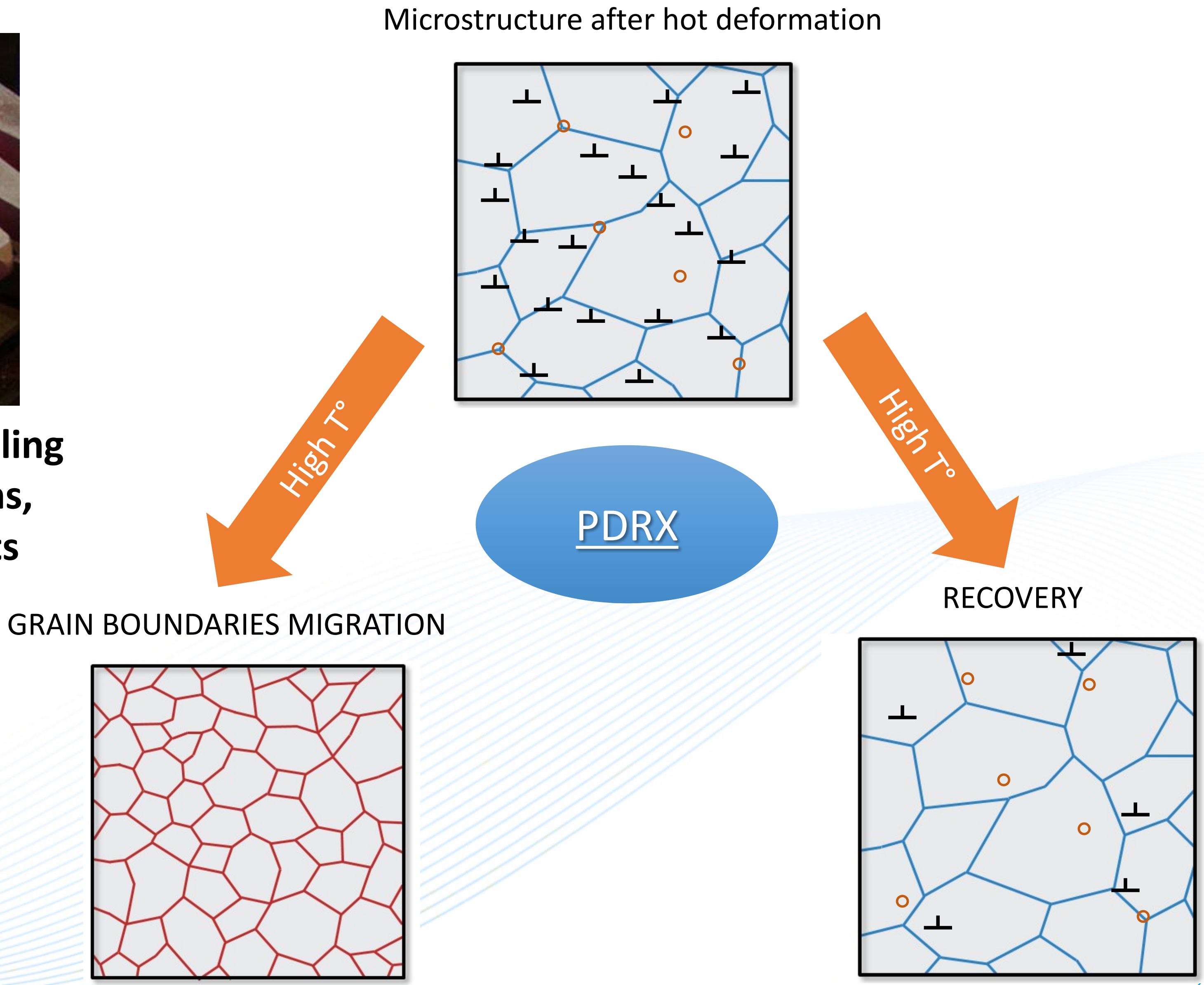
WHAT ABOUT AFTER DEFORMATION ??

GRAIN BOUNDARIES MIGRATION

Post-dynamic recrystallization phenomenon

Importance of controlling grain size, distributions, heterogeneities effects

MODELS



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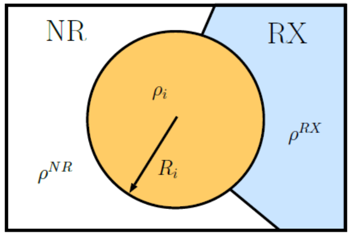
Source : www.hhallberg.com

Modeling scales

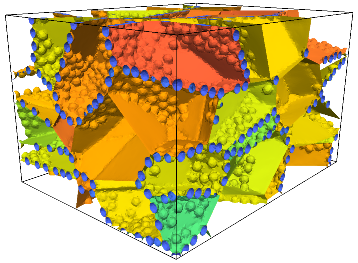
Macro (mean-field)



Bernard et al. (2011)

- ☼ Analytical laws (low costs)
- ☼ Large-scale simulations
- ✘ Homogenized results
- ✘ Implicit microstructure

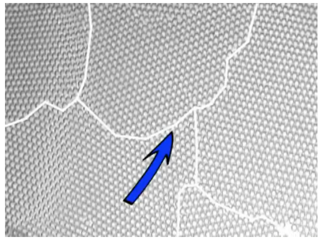
Meso (full-field)



B. Scholtes (2015)

- ☼ Explicit microstructure
- ☼ Local results
- ✘ High costs

Micro (atomistic simulation)



Loyola Bubblez

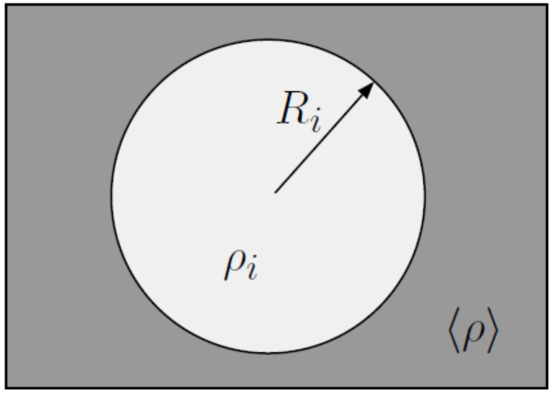
- ☼ High resolution
- ✘ Very high costs
- ✘ Computational requirements

Modeling of DDRX and PDRX is induced by a modeling of :

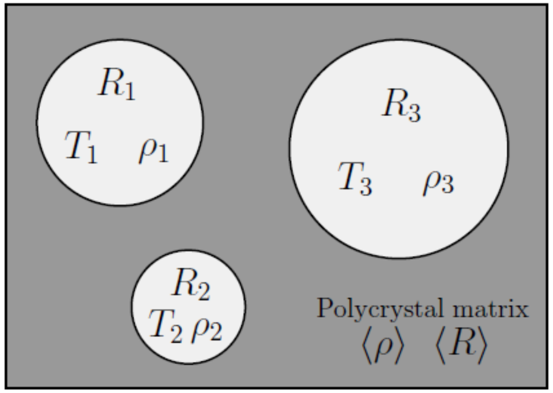
- Microstructure
- Strain-hardening and recovery mechanisms
- Grain boundaries migration
- Nucleation mechanism

Mean field models of DRX

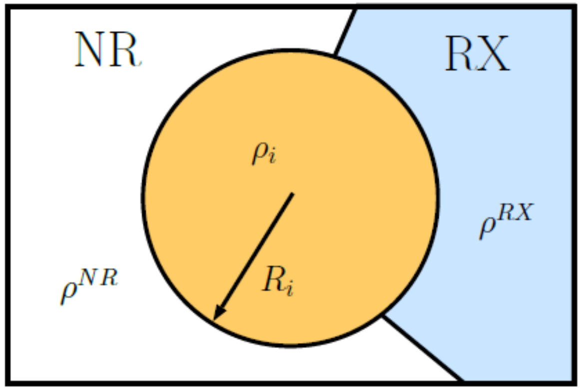
Montheillet et al. 2009



Cram et al. 2009



Bernard et al. 2011



Hardening & Recovery

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

Nucleation

$$r^* = \omega\frac{2\gamma_b}{\rho_{cr}\tau} \qquad \dot{N} = K_g S_c \Delta t$$

GB migration

$$v_i = M * [\tau(\overline{\rho} - \rho_i) + \gamma(\frac{1}{\overline{R}} - \frac{1}{R_i})]$$

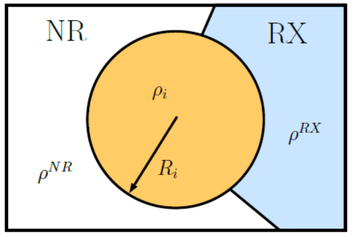
Good description of macroscopic results

(Mean grain size, stress, recrystallized fraction)

Bad description of grain size distributions & high sensitivity to heterogeneities

Modeling scales

Macro (mean-field)



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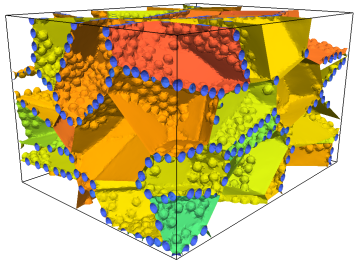

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- Explicit microstructure

- ✘ High costs

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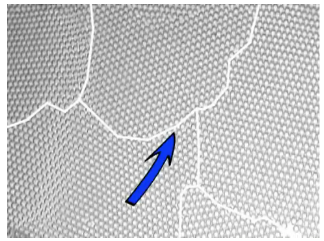

Loyola Bubblez

- High resolution

- ✘ Very high costs
- ✘ Computational requirements

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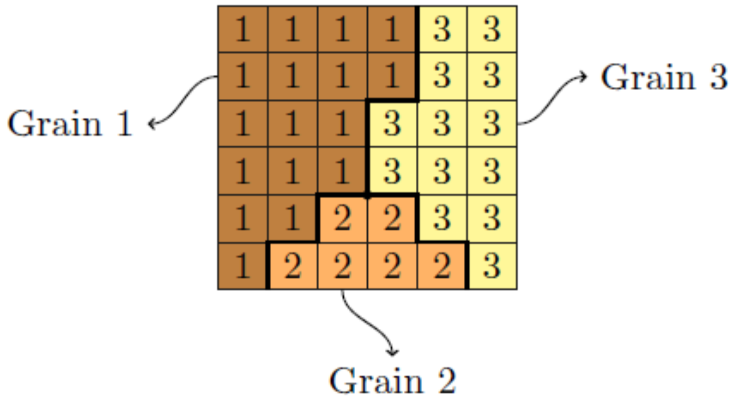
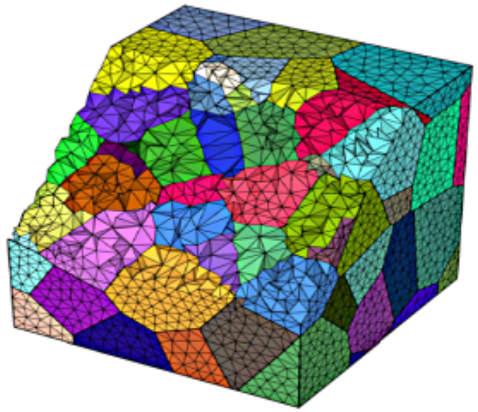
Full field models

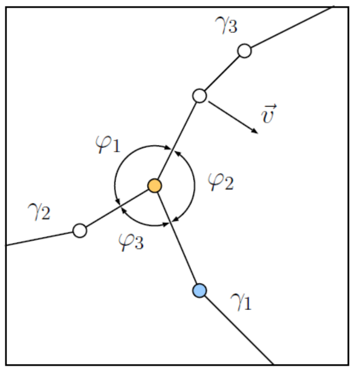
Stochastic approaches (MC, CA)



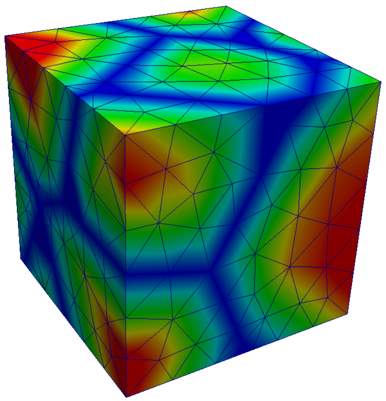
Deterministic approaches (Vertex, PF, LS)



Front tracking (Vertex)

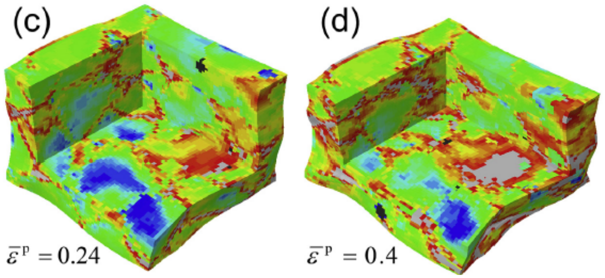


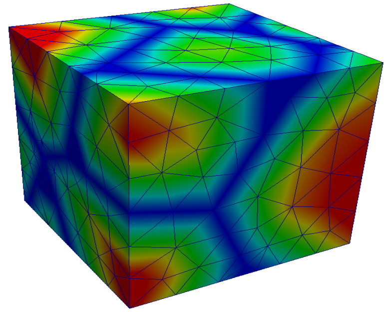
Front capturing (LS, PF)

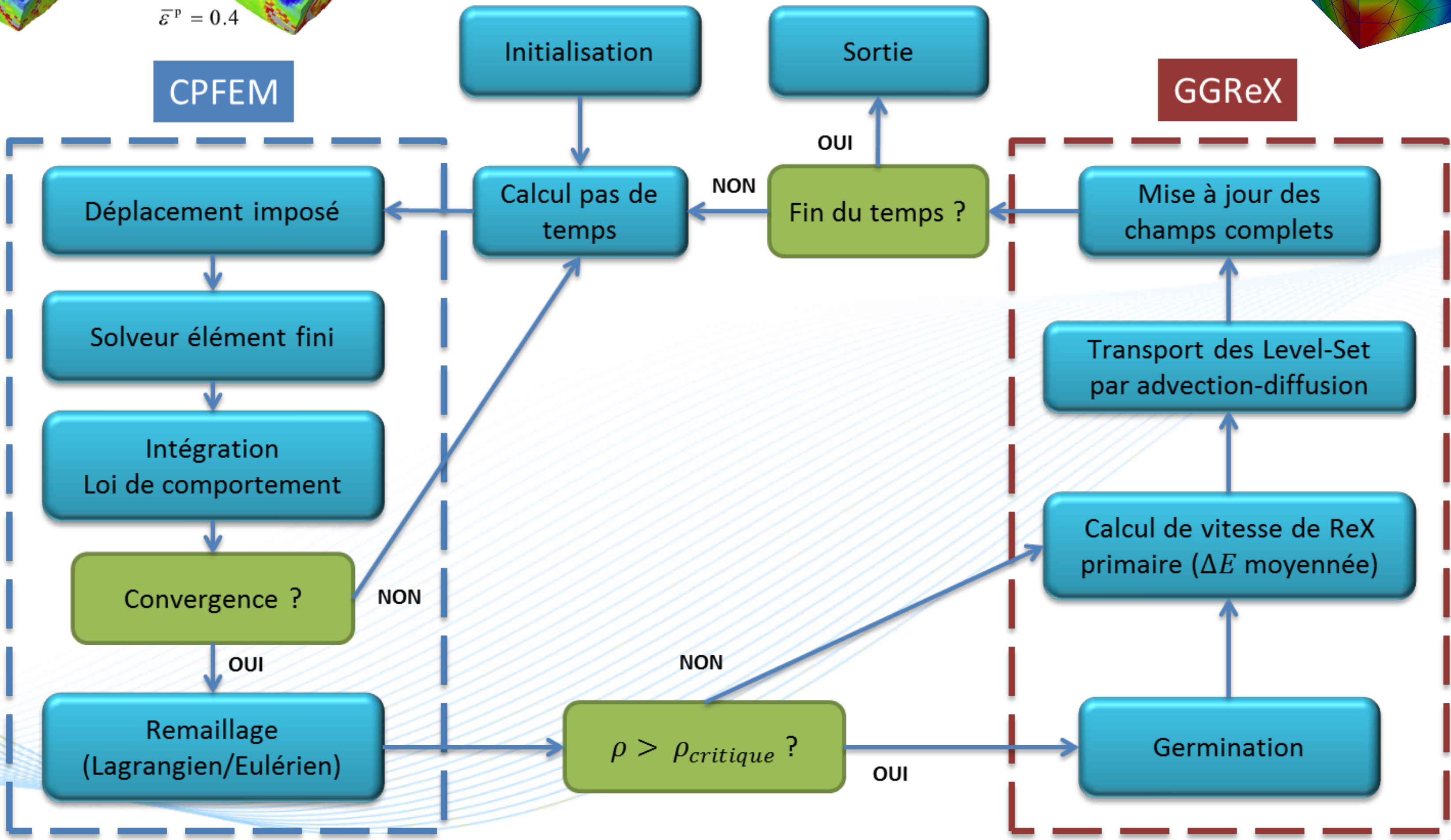


Full field models of DRX

Hongwei et al. 2016

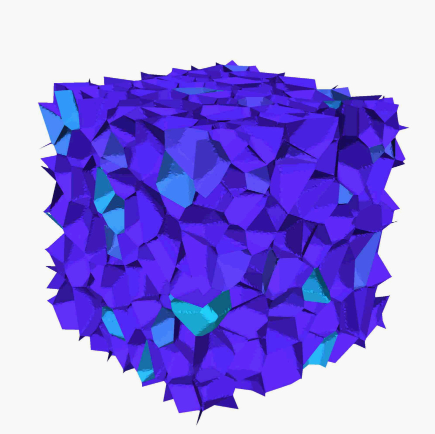




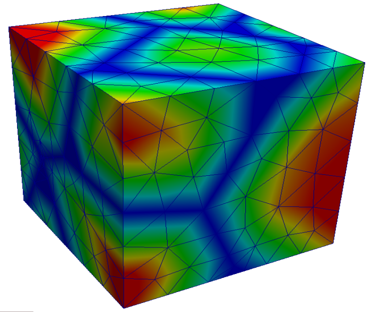


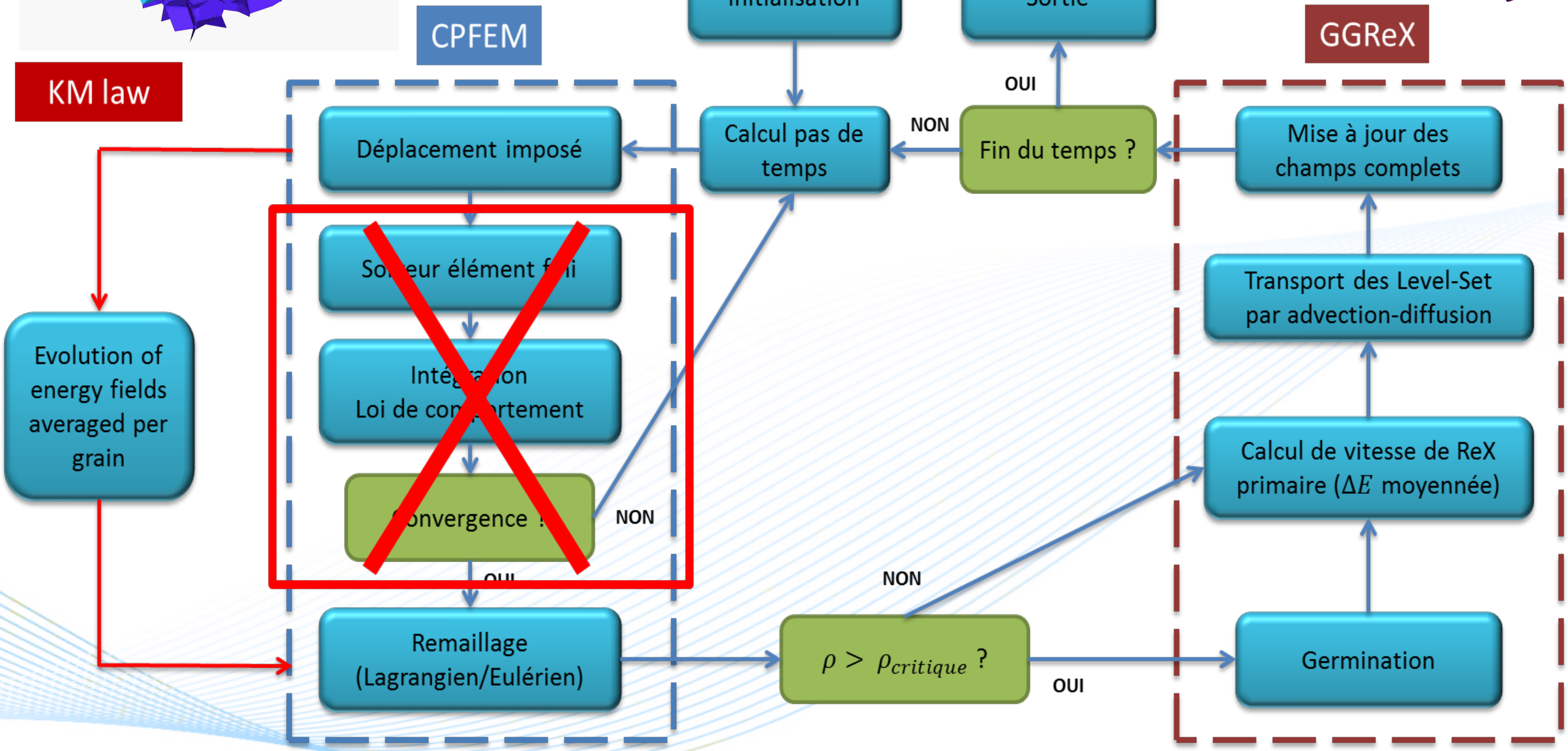
State of art for modeling DRX and PDRX

Full field models of DRX



Lagrangian deformation
Interfaces Eulerian description





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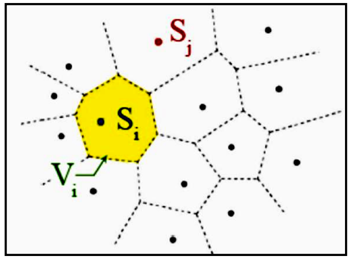
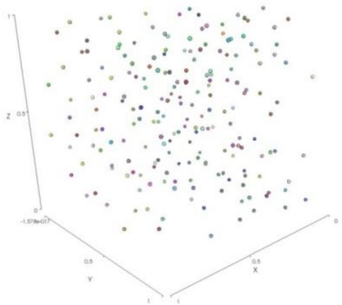
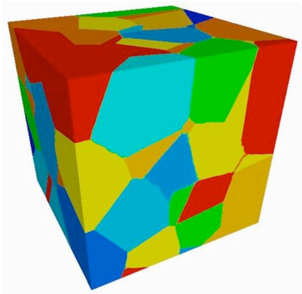
Voronoï method

(Bernacki et al. 2009; Quey et al. 2011; Hitti et al. 2012)

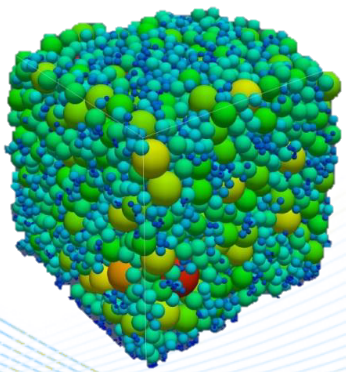






Laguerre-Voronoï method

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



Direct method (packing)

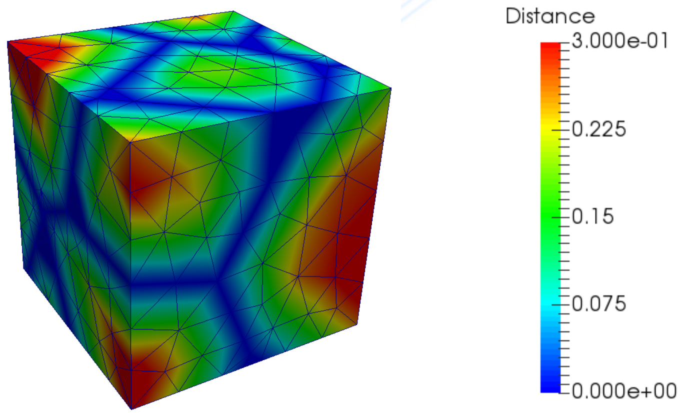
The Level-Set method

Compute the signed distances from each node to its closest interface

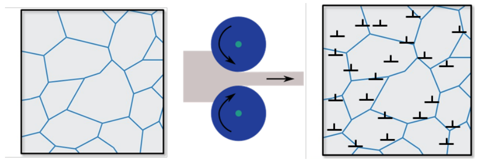
$$\begin{cases} \psi(x,t) = \pm d(x,\Gamma), x \in \Omega, \\ \Gamma(t) = \{x \in \Omega, \psi(x,t) = 0\} \end{cases}$$

$\psi \geq 0$ inside and $\psi \leq 0$ outside

$$\forall x \in \Omega,\ \phi_{glob}(x) = \max_{1 \leq i \leq N} (\phi_i(x)).$$



Non-conform mesh on interfaces



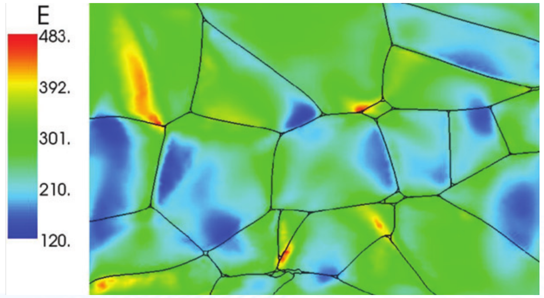
Full field models generally use two kind of approaches to describe hardening and recovery :

- At a local scale with crystal plasticity algorithm (Mellbin et al. 2015; Chen et al. 2015)

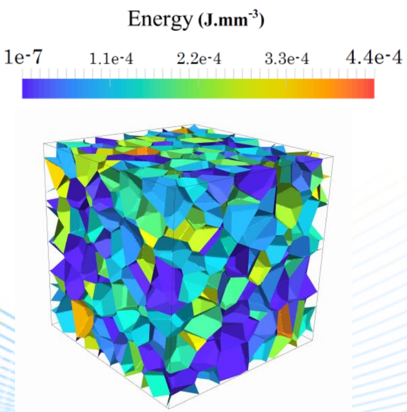
$$\tau^{\alpha} = \bar{\bar{T}}_{\alpha} : \sigma$$

$$\dot{\gamma}_{\alpha} = \dot{\gamma}_0 \left| \frac{\tau^{\alpha}}{\tau_c{}^{\alpha}} \right|^{1/m} sign\,(\tau^{\alpha}).$$

$$\dot{\rho}_{SSD} = \left(\frac{K_1}{M} - \frac{K_2}{M} \rho_{total} \right) V_p$$



- At a macroscopic scale with mean field laws (Mecking and Kocks 1981; Yoshie et al. 1987)



(maire et al. 2016)

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

YLJ law, 1987

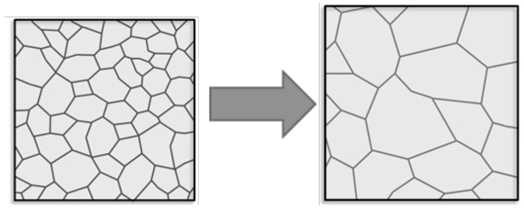
$$\frac{\partial \rho}{\partial \varepsilon} = K_1 \sqrt{\rho} - K_2 \rho$$

Kocks-Mecking law, 1976

$$\frac{\partial \rho}{\partial \varepsilon} = \frac{K_1}{\rho^{\upsilon}}$$

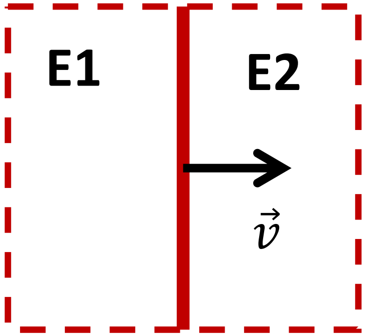
Power law

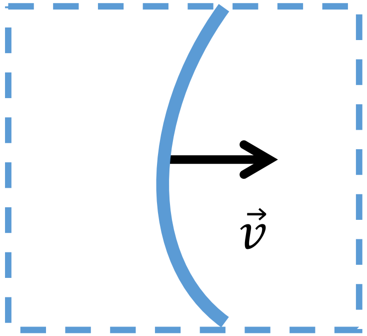
(Montheillet et al. 2009)



Grain boundary migration is due to the stored energy gradients and capillary effects

E1 < E2





$$\cong \Delta \frac{(n-1)}{R}$$

$$\vec{v}_e = M_b \Delta E \nabla \psi$$

$$\vec{v}_{gg} = -M_b \gamma_b \Delta \psi \nabla \psi$$

$$\vec{v} = \vec{v}_{gg} + \vec{v}_e$$

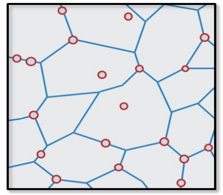
Isotropic

Solving of the transport equation for each LS function

$$\begin{cases} \dfrac{\partial \psi(x,t)}{\partial t} + \vec{v}.\vec{\nabla}\psi(x,t) = 0, \\ \psi(x,t=0) = \psi^0(x), \end{cases}$$

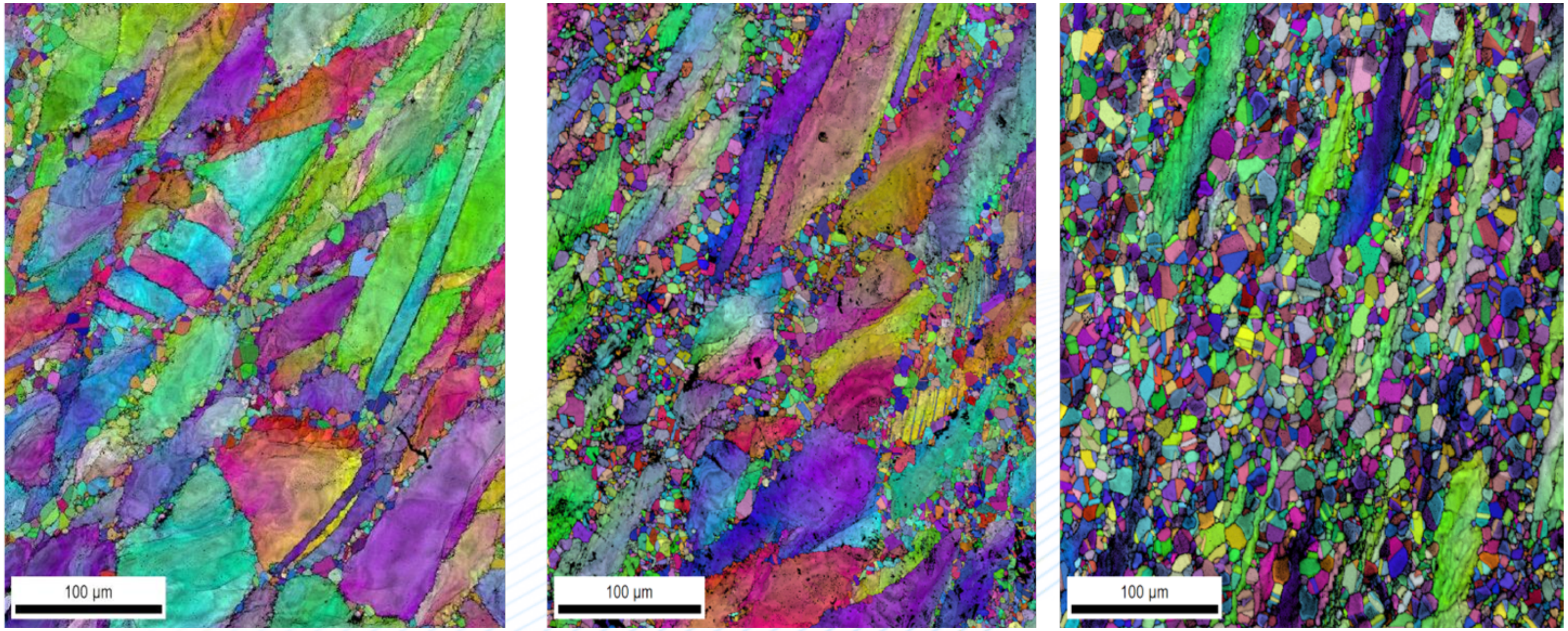
- How to restore the metric property?

$$\|\nabla \psi\| = 1$$



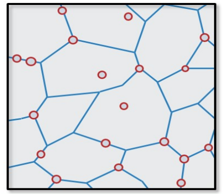
Several kinds of nucleation mechanisms : Subgrains coalescence, sub-boundaries migration, strain induced boundary migration (SIBM)…

- This model is focused on the necklace nucleation mechanism involved in 304L steel



Torsion test *(T, ε, ε̇) following by a quench*

(Inconel718, Thèse M. Zouari)



The nucleation criterion

$$\rho_{cr} = \left[\frac{-2\gamma_b \dot{\varepsilon} \dfrac{K_2}{K_3 \tau}}{\ln\left(1 - \dfrac{K_2}{K_1}\rho_{cr}\right)} \right]^{1/2}$$

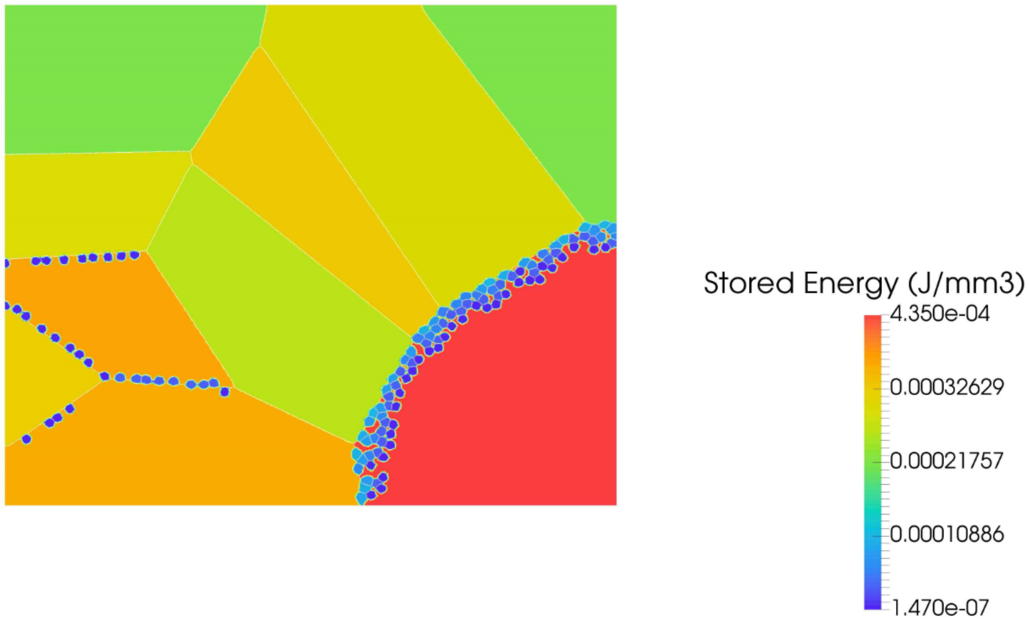
The nucleation rate

(Peczak and Luton, 1993)

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

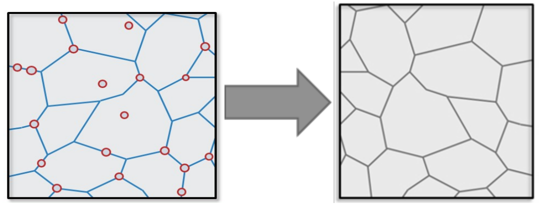
The nucleus size

$$r^* = \omega \frac{2\gamma_b}{\rho_{cr}\tau}$$



Modeling of PDRX

1) Grain growth



$$\vec{v}_{\mathrm{e}} = M_{\mathrm{b}} \Delta E \nabla \psi$$

$$\vec{v}_{\mathrm{gg}} = -M_{\mathrm{b}} \gamma_{\mathrm{b}} \Delta \psi \nabla \psi$$

$$\vec{v} = \vec{v}_{\mathrm{gg}} + \vec{v}_{\mathrm{e}}$$

$$\begin{cases} \dfrac{\partial \psi(x,t)}{\partial t} + \vec{v}.\vec{\nabla}\psi(x,t) = 0, \\ \psi(x,t=0) = \psi^0(x), \end{cases}$$

2) Static recovery

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

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First results and confrontations with experimentations

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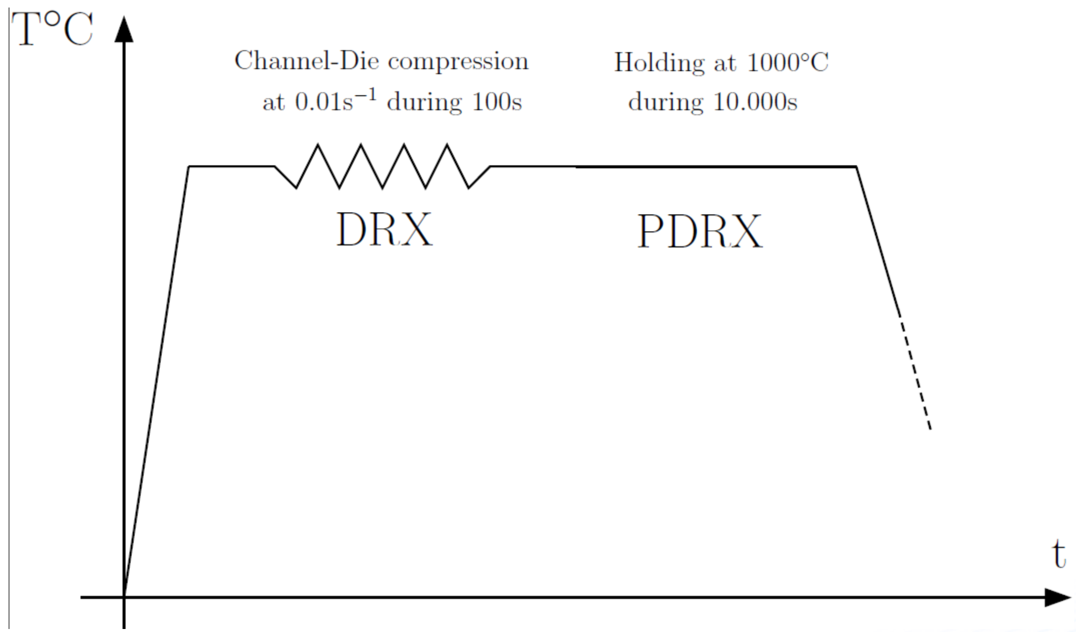
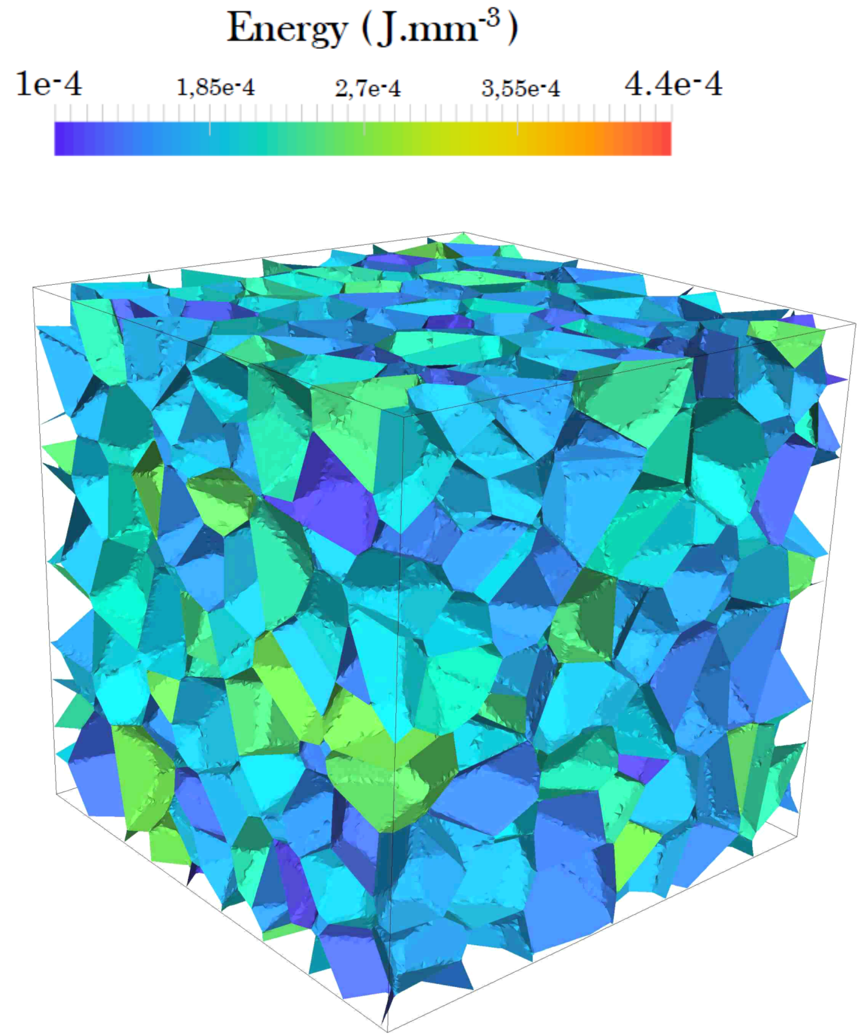
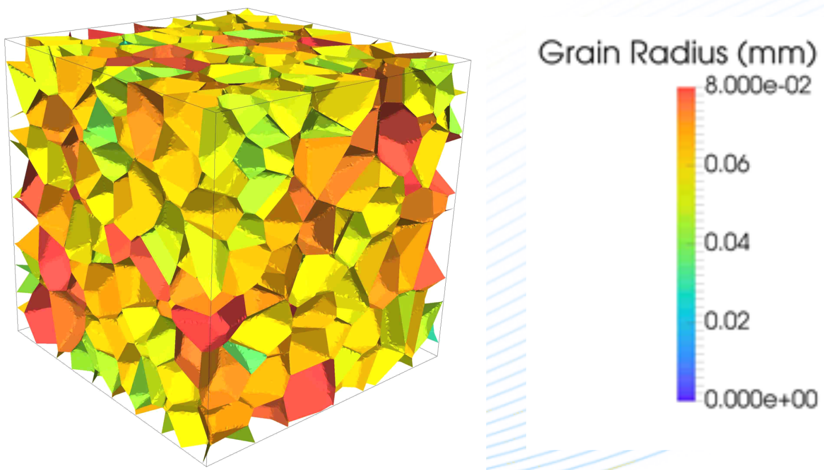
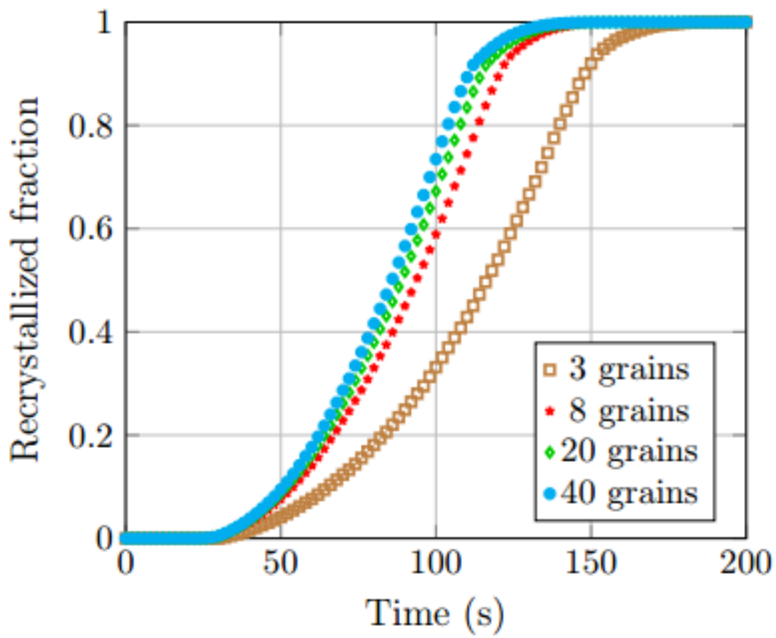


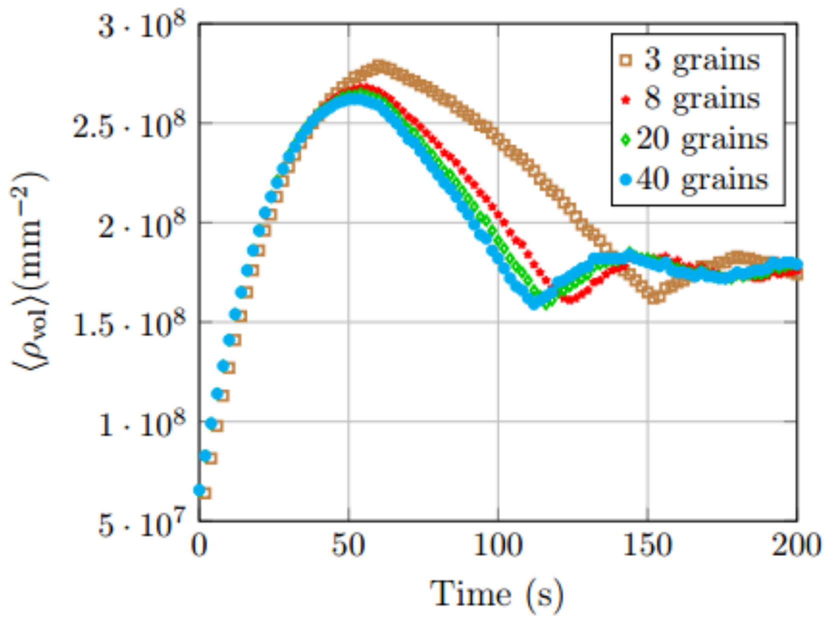


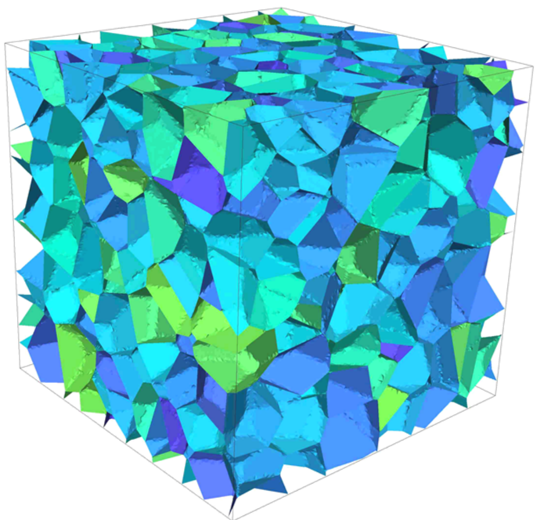


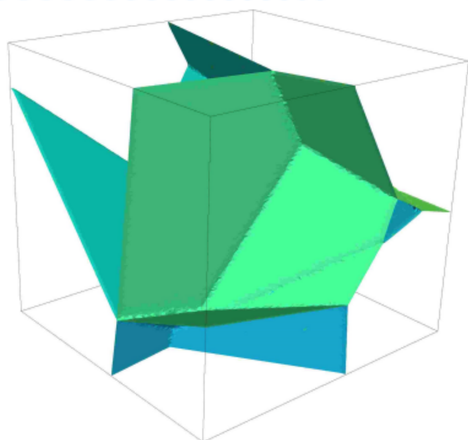
Simulation time
10h on 3*24 procs

DRX : Calibration of the initial number of grains







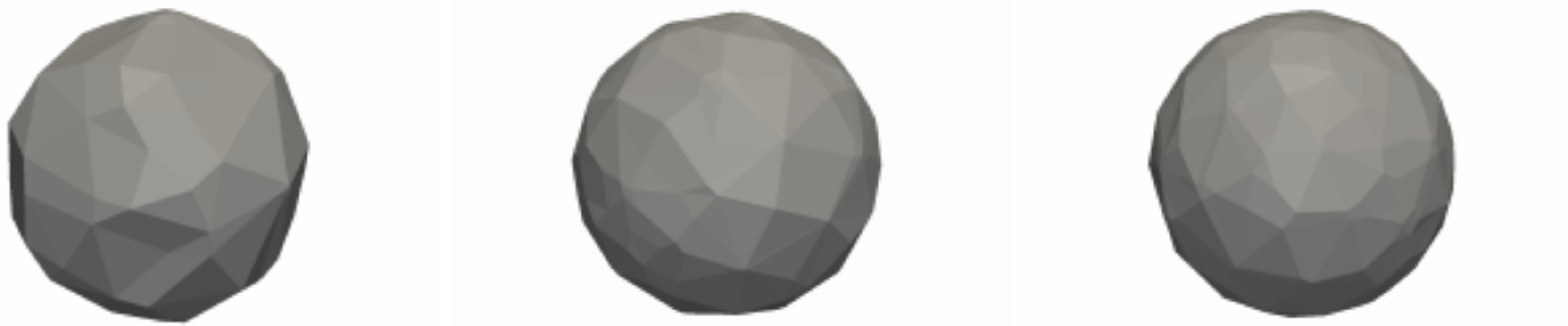


8 initial grains are sufficients

DRX : Calibration of the ideal mesh size

Generation of four nuclei using different mesh sizes

- Ev = L[1] Error on the volume between the numerical nucleus and a spherical nucleus of the same radius



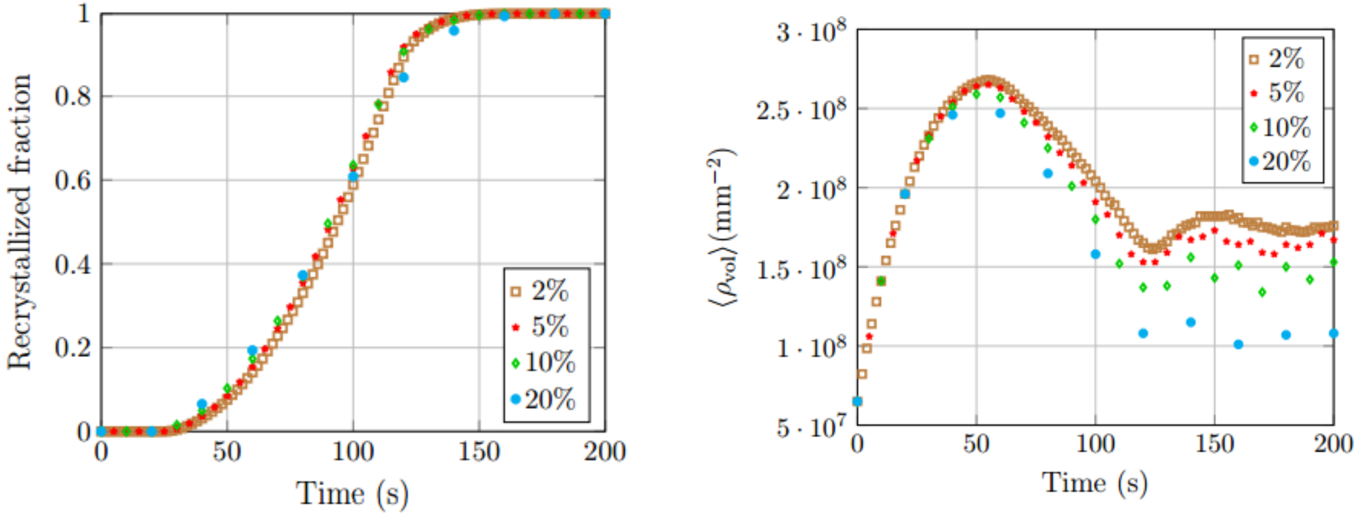
(b) $R = 1.6, E_v = 9\%, E_s = 8\%$ (c) $R = 2, E_v = 3.5\%, E_s = 4,5\%$ (d) $R = 2.7, E_v = 3.5\%, E_s = 2.7\%$

- We note R the number of mesh size in the nucleus radius

R = 2 gives a good representation of the nucleus

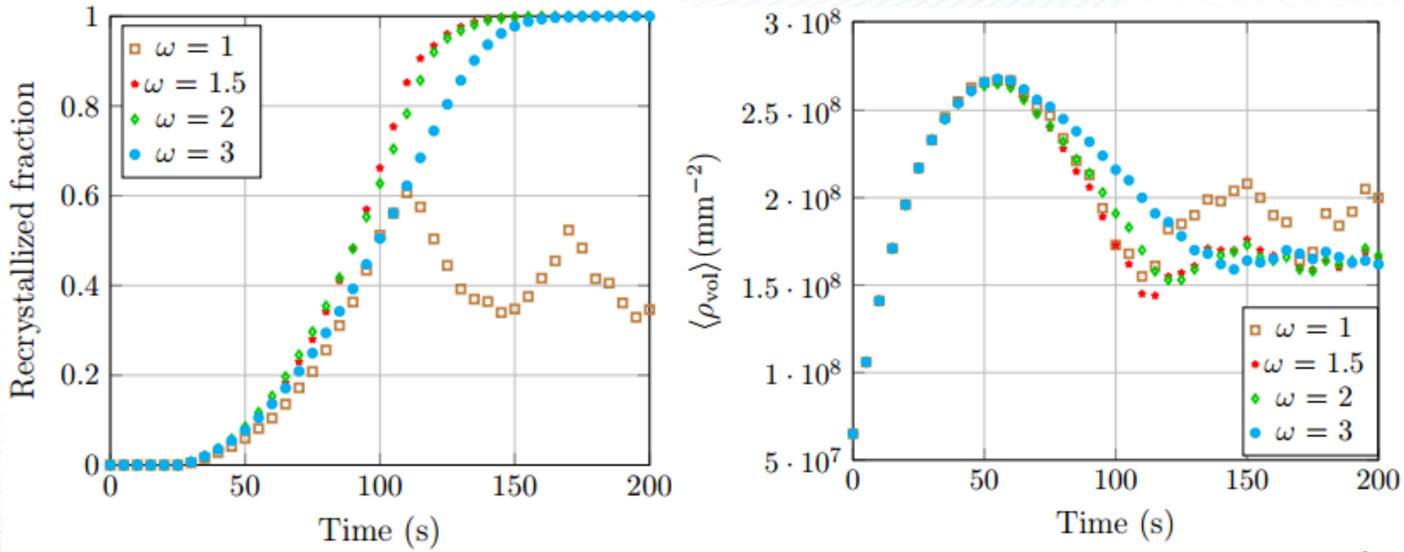
DRX : Calibration of the deformation step and nucleus size

Calibration of the deformation step



Deformation step of 5%

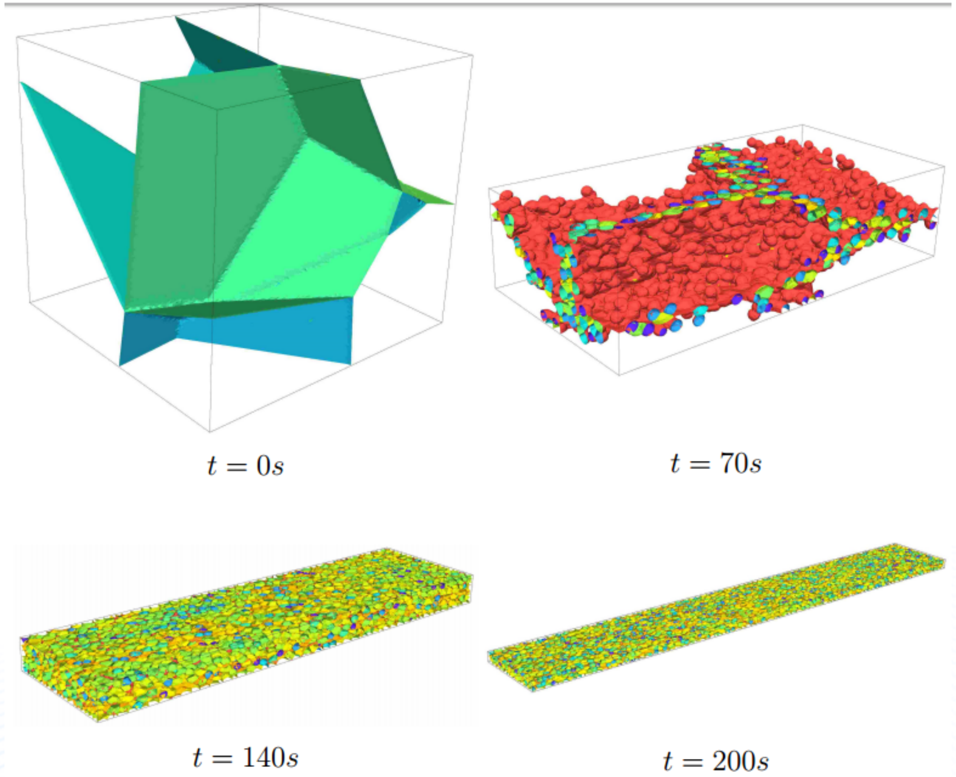
Initial nucleus size = 1,5*Rcr



Ideal parameters of the DRX model

Finally,

- 8 Grains in the initial microstructure
- 2 mesh sizes in the nucleus radius
- A initial nucleus radius equal to 1,5*Rcr
- A deformation step of 5%



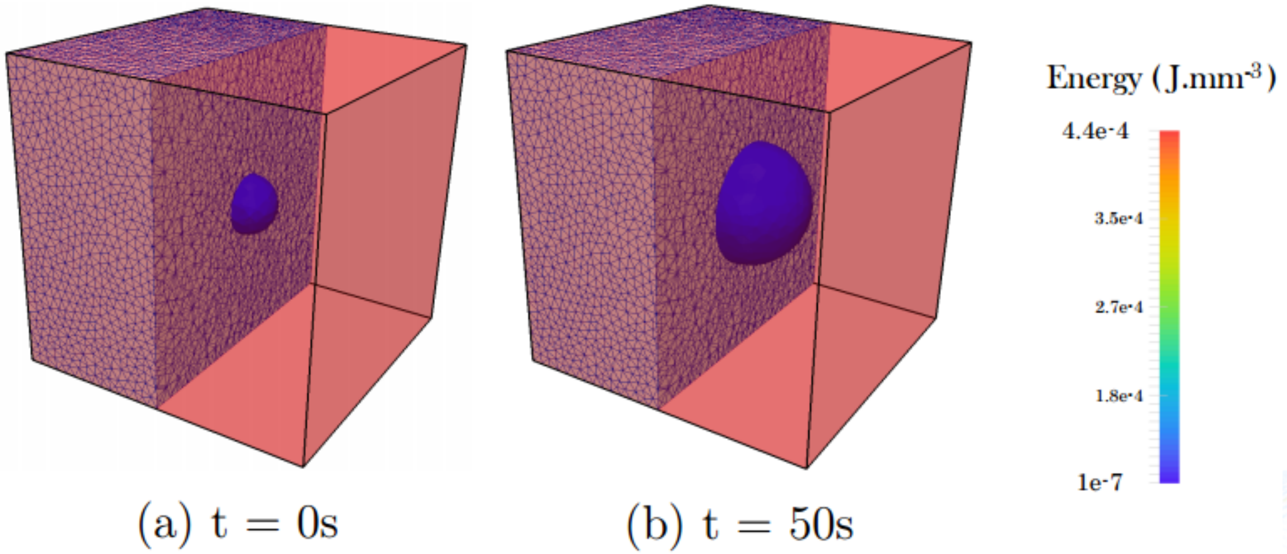
Simulation time before the sensitivity study

10h on 3*24 procs

Simulation time after the sensitivity study

1h30 on 3*24 procs

Grain growth is the preponderant mechanism occuring during PDRX



(a) t = 0s (b) t = 50s

Analytical solution :

$$R^{t+\Delta t} = R^{t} + M_b \Delta t \left(\Delta E - \frac{2\gamma_b}{R^{t}} \right)$$

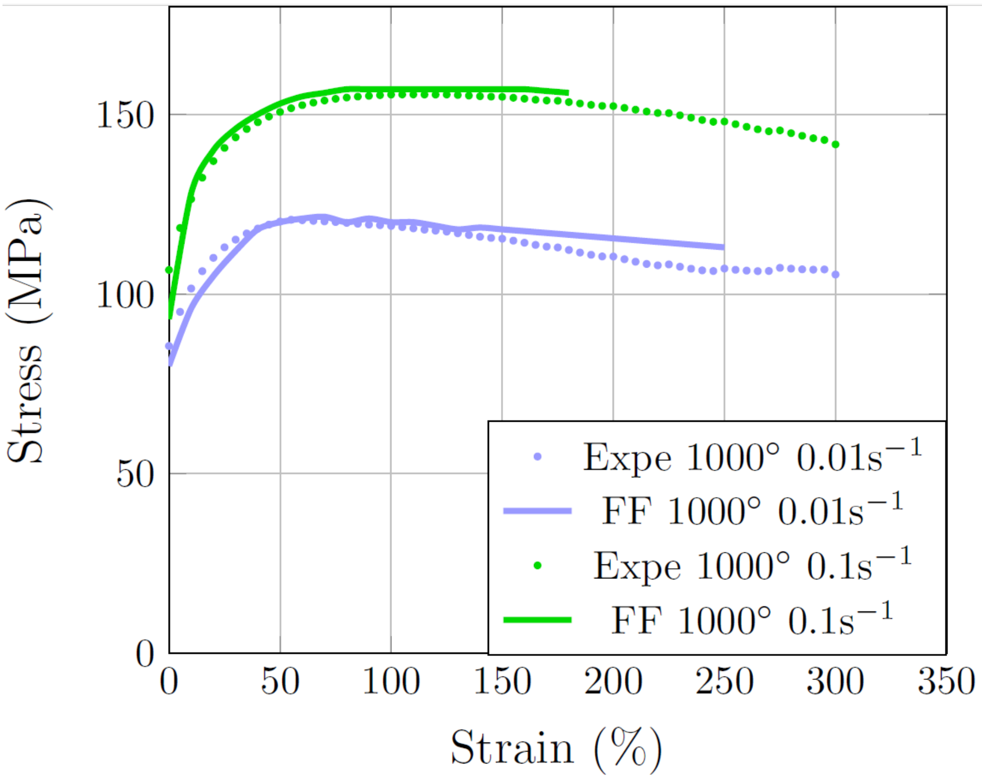
Max displacement of GB:

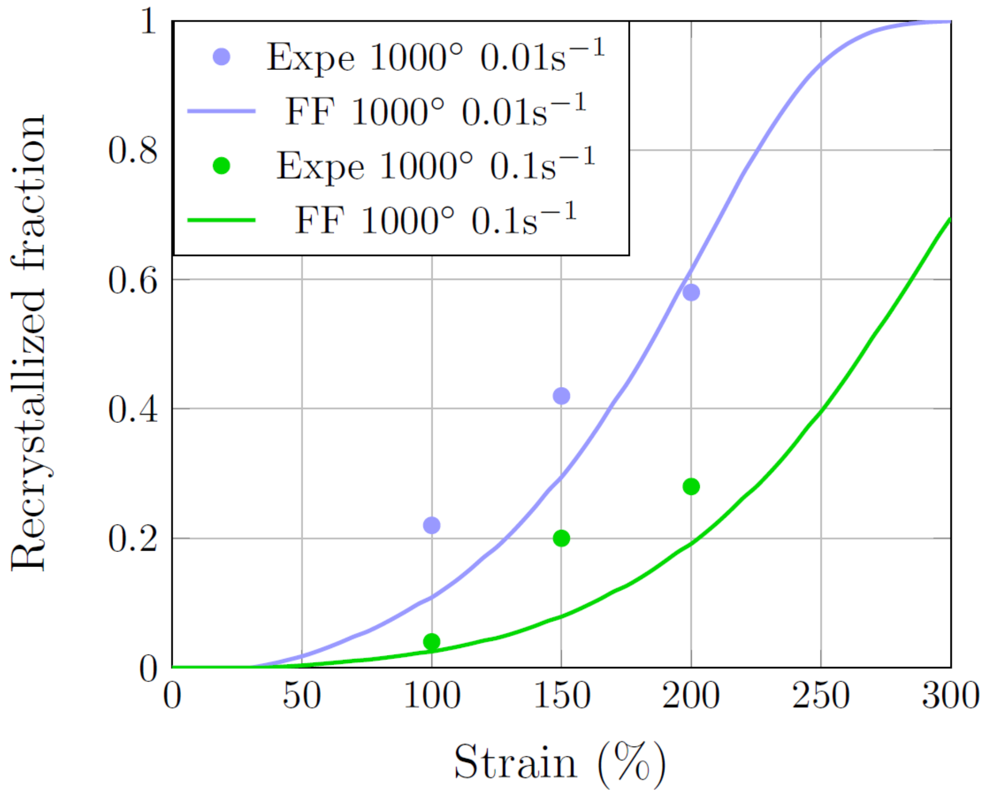
$$d_{max} = \left(\frac{2\gamma_b}{\langle R \rangle} + \Delta E \right) \int_t^{t+\Delta t} M_0 \exp\left(-\frac{Q_m}{R_g T} \right) dt$$

d_{max} = 30% of mesh size gives the best accuracy

First confrontations with experimentations

Confrontations with DRX experimental investigations on 304L steel (Beltran et al, 2015)





Simulation time of FF model
Around 2h on 3*24 procs

Conclusions & Perspectives

- The level-set method coupled to mean field laws leads to an unique resolution schema combining Lagrangian deformation and Eulerian interfaces displacement for modeling DRX and PDRX.

- The developments made in a previous PhD thesis (B. Scholtes, 2013-2016) and a recent sensitivity study concerning the model lead to simulation durations of few hours on 3*24 procs, which is a reasonable time for a 3D DRX model.

Perspectives

- Experimental investigations on 304L steel are in progress for a better identification of model parameters and a validation of this model.
- A next PhD thesis (Digi-μ chair) concerning mesh adaptation in 3D will still lead to lower computational costs.
- An actual PhD thesis (J. Fausty, 2016-2019) aims to consider anisotropic interfacial energies and modeling of twin boundaries in the model.
- Comparisons with a CPFEM full field model will give the limitations of this model.

THANKS

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