Improvement of 3-D mean field models for capillarity driven grain growth based on full field simulations

(Maire & al, submitted in JMS, 2016)

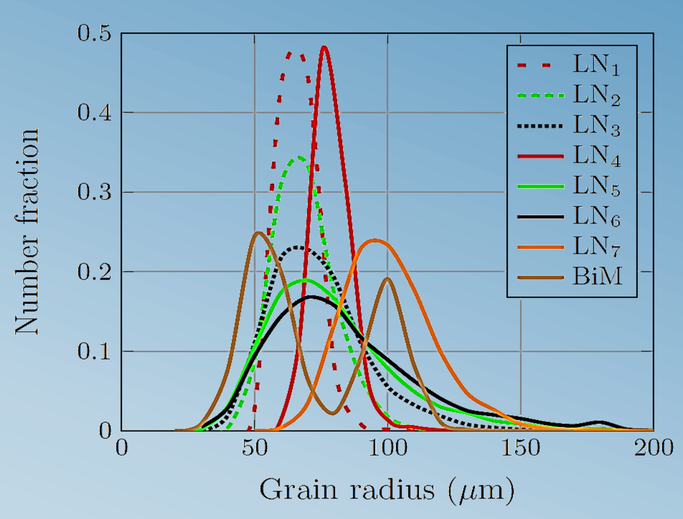
L. Maire[a], B. Scholtes[a], C. Moussa[a], N. Bozzolo[a], D. Pino Muñoz[a], M. Bernacki[a]

[a] *Mines ParisTech, CEMEF – Centre de mise en forme des matériaux, CNRS UMR 7635, CS 10207 rue Claude Daunesse, 06904 Sophia Antipolis cedex, France*

Heat treatment and initial parameters

Eight initial grain size distributions:

- 7 log-normal and 1 bimodal



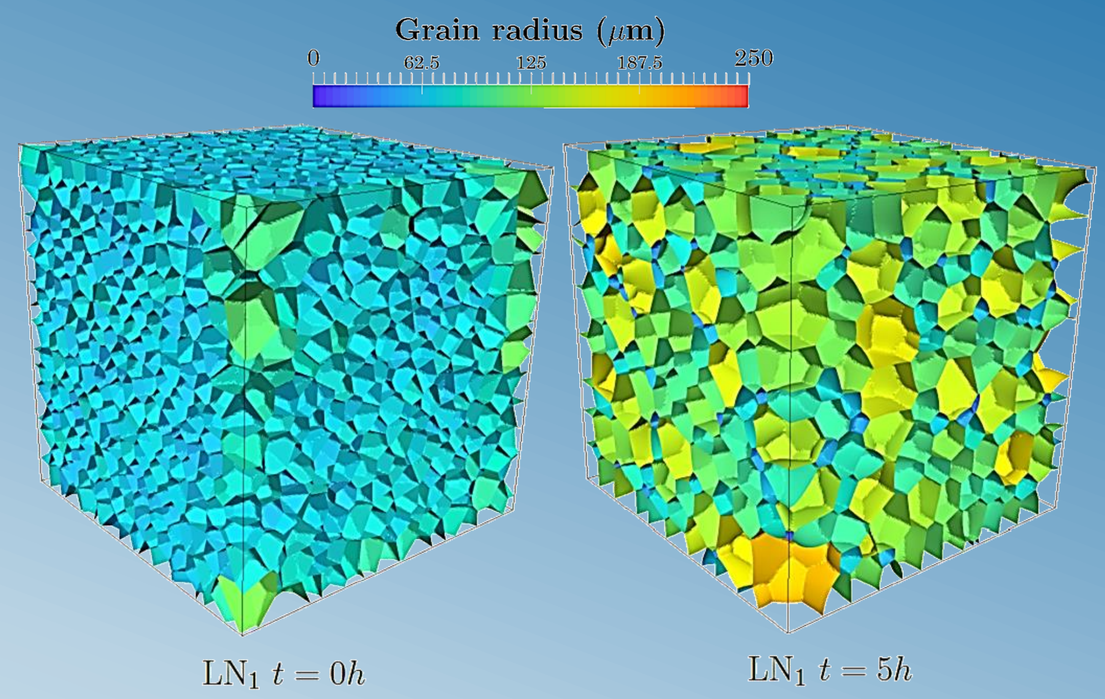
Full field simulations as references:

- Immersed volume method using level set functions
- VER composed of 8000 grains
- 25M of tetrahedral elements

(Scholtes & al, 2015, CMS
Scholtes & al, 2016, CMS,
Bernacki & al., 2009, MSMSE, 17 , 064006.
Bernacki & al., 2011, Scripta Mat., 64, 6.)

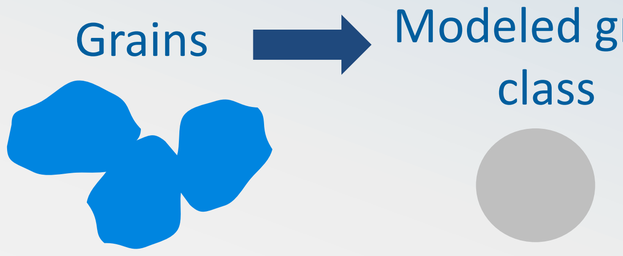
Heat treatment :

- T = 1050° C ; t = 5h
- Isotropic grain boundary energy and mobility
- No second-phase particles



Confrontation of full field results with mean field model predictions

Hillert model: (Hillert, 1965, Acta Metall Mater 13:227)



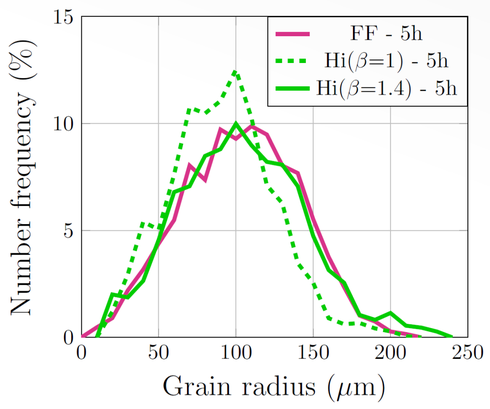
Spherical grain (3D) :
- Number of grains N_i
- Equivalent size R_i

$$v_i = \beta M \gamma \left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right)$$

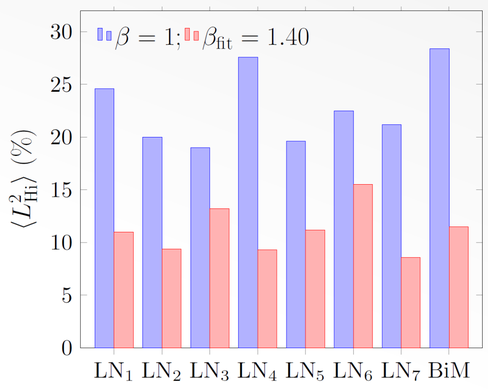
Fitting parameter close to unity **(Hillert, 1965, Acta Metall Mater 13:227)**

Optimisation of the β value by minimisation of the L^2_{Hi} error on the grain size distribution predictions :

Comparison of the grain size distributions with the classical (β=1) and new (β =1.4) Hillert model



L^2_{Hi} error measured on grain size distributions predicted by full field and Hillert model



Improvement of the Hillert model :

$$v_i = 1.4 M \gamma \left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right)$$

Classical B&T law : (Burke & Turnbull, 1952, Prog Met Phys 3:220)

$$\langle R \rangle^2 - \langle R_0 \rangle^2 = \delta M \gamma t$$

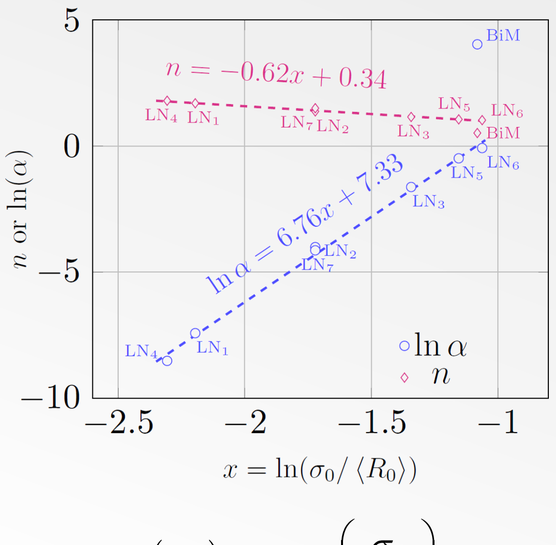
Fitting parameter close to 0.5 **(Burke1952, Kamachali2012)**

Proposition of a new B&T formulation :

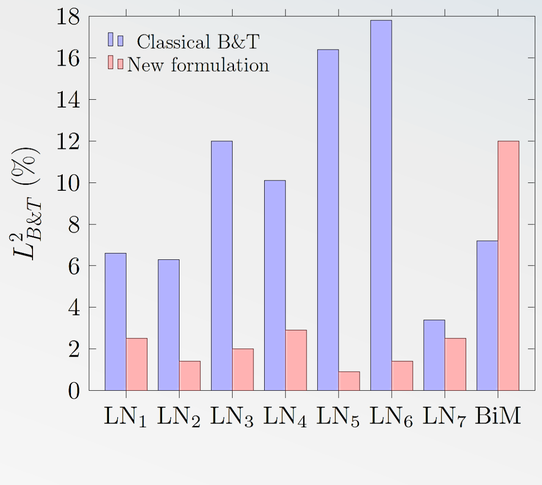
(Fabiano & al., 2014, Comp. Mater. Sci., 92.)

$$\langle R \rangle^2 - \langle R_0 \rangle^2 = \alpha M \gamma t^n$$

Determination of α and n by inverse analyses



$L^2_{B\&T}$ error measured on the evolution of $\langle R \rangle$ predicted by full field and B&T model



$$\ln(\alpha_{fit}) = 6.76 \ln\left(\frac{\sigma_0}{\langle R_0 \rangle} \right) + 7.33 \qquad n_{fit} = -0.62 \ln\left(\frac{\sigma_0}{\langle R_0 \rangle} \right) + 0.34$$

$$\langle R \rangle^2 - \langle R_0 \rangle^2 = \exp^{7.33} \left(\frac{\sigma_0}{\langle R_0 \rangle} \right)^{6.76} M \gamma t^{-0.62 \ln\left(\frac{\sigma_0}{\langle R_0 \rangle} \right) + 0.34}$$