Full field modeling in a level set framework of Zener pinning phenomenon - discussion of classical limit mean grain size equation.

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Full-field Modeling of the Zener Pinning Phenomenon in a Level Set Framework - Discussion of Classical Limiting Mean Grain Size Equation

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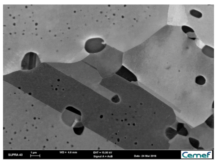
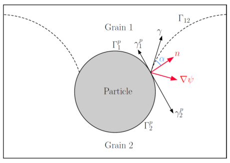
Context

Pinning of grain boundaries by second phase particles is widely used to control the grain size during forming process of superalloys.



BSE image of precipitates in nickel based superalloy (S.Vernier, CEMEF, France)



$\sin(\alpha) = (\gamma_2^p - \gamma_1^p)/\gamma$

Classical Zener pinning law predicting the limiting mean grain size [1]:

$$\langle R_f \rangle = K \frac{\langle r_p \rangle}{f^m}$$

$< R_f >$ – mean grain size, $< r_p >$ – mean particle radius, f – volume fraction of particles; K, m – parameters depending on the assumptions.

Relation to the volume fraction of particles located at grain boundaries f_{gb} [2]:

$$\langle R_f \rangle = K \frac{\langle r_p \rangle}{f_{gb}^m}$$

Numerical model

Level Set Framework:
LS function ψ is defined over a domain Ω as the signed distance to the interface Γ [3]:

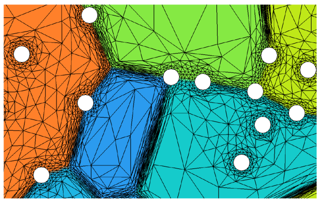
$$\forall t \begin{cases} \psi(x,t) = \pm d(x, \Gamma(t)), \ x \in \Omega, \\ \Gamma(t) = \{x \in \Omega, \psi(x,t) = 0\}, \end{cases}$$

$$\begin{cases} \frac{\partial \psi_i(x,t)}{\partial t} - M\gamma \Delta \psi_i(x,t) + \vec{v}_e \cdot \nabla \psi_i(x,t) = 0, \\ \psi_i(x, t=0) = \psi_i^0(x), \end{cases}$$

t – time, M – mobility, γ – interface energy, $\vec{v}_e$ – velocity due to stored energy gradient

Boundary condition at precipitate/matrix interface:

$$\frac{\nabla \psi}{\|\nabla \psi\|} \cdot \vec{n} = \nabla \psi \cdot \vec{n} = \sin(\alpha)$$



- **Adaptive metric based meshing remeshing tool [4] was used.**
- **New direct and parallel reinitialization algorithm [5] was incorporated.**
- **Recoloring scheme [6] was used to reduce the number of LS functions needed to represent the polycrystal**

Simulation parameters:

Material: Inconel 718
$M = 2.3 \times 10^{-23}$ m^4/(Js)
$\gamma = 0.6$ J/m^2

$\alpha = 0°$ (incoherent precipitates)
Particle radii r_p: 0.2, 0.4, 0.6, 0.8 μm
Area fraction f: 1-8 %

Domain size: 0.3 × 0.3 mm^2,
Number of grains: 2600
Initial mean grain size: $<R_0>$ = 3.35 μm

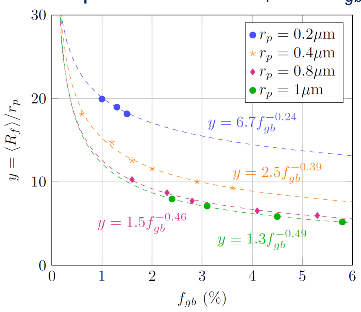
Time step: 0.1 s
16 CPUs (Xeon 1.2 GHz)
(computation time: 1-2 days)

2D simulation results for grain growth: New mean field model for the limiting mean grain size

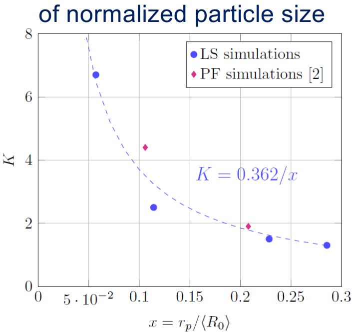
f_{gb} and $< R_f >$ are measured at the steady state (when $< R_f >$ becomes stable)

1) The radius of precipitates (for a given f) affects drastically the grain growth kinetics
2) K and m were found to depend on $r_p / <R_0>$ (see figures for K and m)

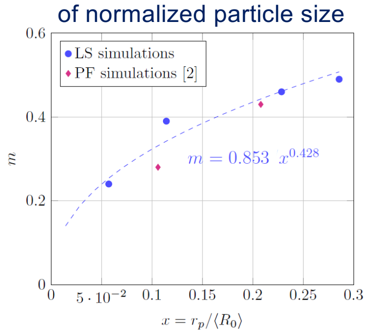
Dependence of $< R_f >$ on f_{gb}



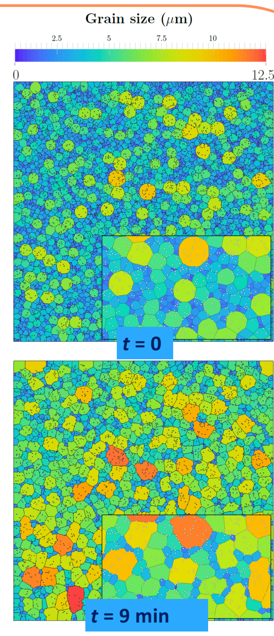
Parameter K as a function of normalized particle size



Parameter m as a function of normalized particle size



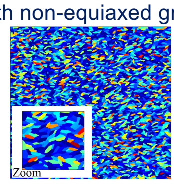
Expression obtained for the limiting grain size: $\langle R_f \rangle = 0.362 \langle R_0 \rangle f_{gb}^{-0.853 (r_p/\langle R_0 \rangle)^{0.428}}$



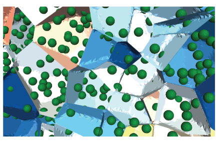
Microstructure at the early and final stages of the simulation (r_p = 0,4 μm, f = 3%)

Current work

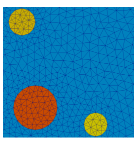
△ Initial microstructures with non-equiaxed grains



△ 3D simulations



△ Evolutive second phase particles



References

[1] C. Zener - C. S. Smith, Trans. AIME 175, 15, (1948).
[2] N. Moelans, B. Blanpain, P. Wollants, Acta Mater 54, 1175-1184, (2006).
[3] A. Agnoli, N. Bozzolo, R. Logé, J.-M. Franchet, J. Laigo, M. Bernacki, Comput Mater Sci 89, 233-241, (2014).
[4] H. Resk, L. Delannay, M. Bernacki, T. Coupez, R. Logé, Modelling Simul Mater Sci Eng 17, 075012, (2009).
[5] M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki, Appl Math Model 39 (23-24), 7291-7302, (2015).
[6] B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, M. Bernacki, Comput Mater Sci 109, 388-398, (2015).