# 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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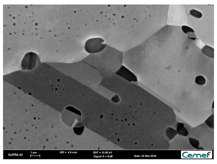
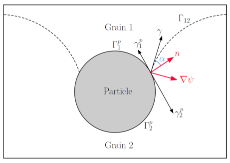
## Context

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]:

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

$\langle R_f \rangle$ – mean grain size, $\langle r_p \rangle$ – 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]:

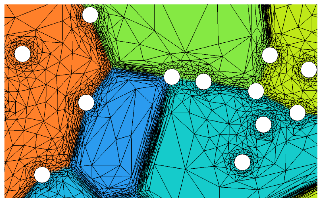
$$\forall t \begin{cases} \psi(x,t) = \pm d(x, \Gamma(t)), \ x \in \Omega, \\ \Gamma(t) = \{x \in \Omega, \psi(x,t) = 0\}, \end{cases}$$

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

$t$ – time, $M$ – mobility, $\gamma$ – 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: $\langle R_0 \rangle$ = 3.35 µm

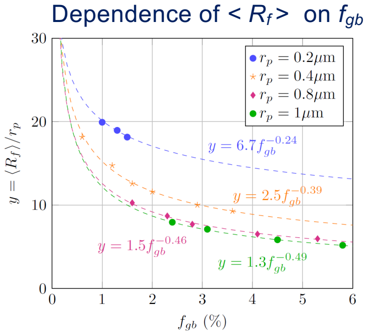
Time step: 0.1 s
16 CPUs (Xeon 1.2 GHz)
(computation time: 1-2 days)

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

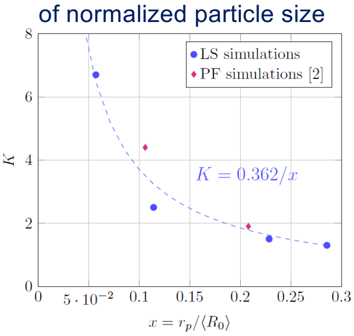
$f_{gb}$ and $\langle R_f \rangle$ are measured at the steady state (when $\langle R_f \rangle$ becomes stable)

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

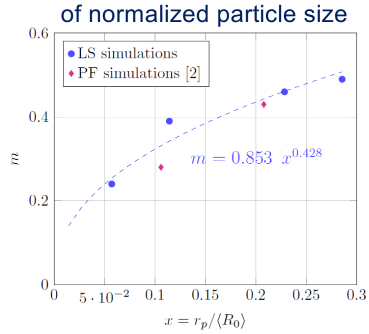
Dependence of $\langle R_f \rangle$ on $f_{gb}$



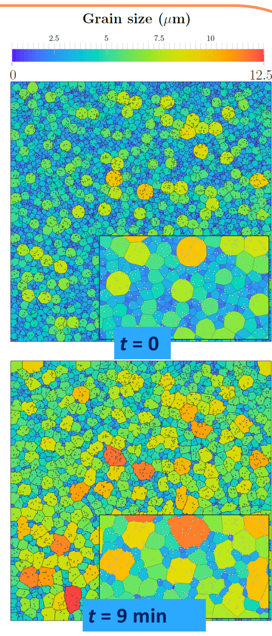

Parameter $K$ as a function of normalized particle size




Parameter $m$ as a function of normalized particle size



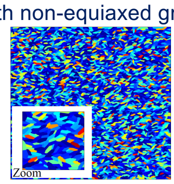

**Expression obtained for the limiting grain size:** $\langle R_f \rangle = 0.362 \langle R_0 \rangle f_{gb}^{-0.853(r_p/\langle R_0 \rangle)^{0.428}}$



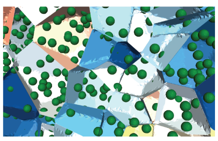

Microstructure at the early and final stages of the simulation ($r_p$ = 0,4 µm, $f$ = 3% )

## Current work

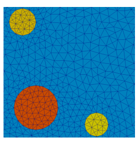
△ Initial microstructures with non-equiaxed grains




△ 3D simulations



△ Evolutive second phase particles



## References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