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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.

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

\[
\langle R_f \rangle = K \frac{\langle r_p \rangle}{f_{gb}}
\]

\(< R_f >\) 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]:

\[
\langle R_f \rangle = K \frac{\langle r_p \rangle}{f_{gb}}
\]

\(\gamma\) = 0° (incoherent precipitates)

Material: Inconel 718

\(M = 2.3 \times 10^{-23}\) m\(^3\)J/(J/s)

\(\gamma\) = 0.6 J/m\(^2\)

Particle radii \(r_p\): 0.2, 0.4, 0.6, 0.8 µm

Area fraction \(f\): 1-8%

Domain size: 0.3 \(\times\) 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)

**Numerical model**

LS function \(\varphi\) is defined over a domain \(\Omega\) as the signed distance to the interface \(\Gamma\) [3]:

\[
\varphi(x, t) = \pm \delta(x, \Gamma(t)), x \in \Omega,
\]

\[
\Gamma(t) = \{ x \in \Omega: \varphi(x, t) = 0 \}.
\]

\(\delta\) is the Dirac delta function.

Level Set Framework:

\(M\gamma^{-1}\mathbf{v}_{gb} - M_{gb}^{\delta(\varphi)} + \mathbf{v}_b - \nabla \psi_b(x, t) = 0,\)

\(\psi_b(x, t) = \psi_b^0(x),\)

\(J\) - time, \(M\) - mobility, \(\varphi\) - interface energy, \(\mathbf{v}_b\) - velocity due to stored energy gradient

Boundary condition at precipitate/matrix interface:

\[
\nabla \varphi \cdot \mathbf{t} = \nabla \psi \cdot \mathbf{t} = \sin(\alpha)
\]

- 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\(^3\)J/(J/s)
- \(\gamma\) = 0.6 J/m\(^2\)
- \(\mathbf{v}_{gb}\) 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 \(r_p, f_{gb}\) (see figures for \(K\) and \(m\))

**2D simulation results for grain growth:**

New mean field model for the limiting mean grain size

Expression obtained for the limiting grain size:

\[
\langle R_f \rangle = 0.362 \langle R_0 \rangle f_{gb}^{-0.853} (r_p / \langle R_0 \rangle)^{0.428}
\]

Current work

- Initial microstructures with non-eqixed grains
- 3D simulations
- Evolutive second phase particles

**References**