The effect of ellipsoid second-phase particles on grain growth studied by three-dimensional phase field simulations

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Grain growth in presence of second-phase particles

- polycrystalline materials
- study of grain growth: increase of mean grain size
- control grain size by addition of impurities
- pinning effect depends on volume fraction, particle shape
Zener pinning

Analytical theories

Calculation of the pinning force $F_Z$:

- **one particle**: analytical calculation based on
  1. position of the grain boundary
  2. particle shape and size
  3. interface energy

- **distribution of particles**: complex!
  - difficult to state how many second-phase particles lie at grain boundaries when grain growth is arrested

[Moelans et al., 2007]
Zener pinning
Analytical theories

**Macroscopic effect:** Zener pinning arrests normal grain growth when a limiting mean grain radius $\bar{R}_{\text{lim}}$ is reached:

$$\frac{\bar{R}_{\text{lim}}}{r} = K \left( \frac{f_b}{f_V} \right)$$

- second-phase particle radius $r$
- volume fraction $f_V$ of second-phase particles
- parameter values $K$ and $b$ varies among the different theories
Zener pinning

Computational studies

Results and conclusions so far:

- Monte Carlo Potts, front tracking-type and phase field simulations
- **mostly 2D simulations:**
  - most particles are in contact with a grain boundary
  - Zener relation is obeyed, with $b = 0.5$
- **3D simulations:**
  - many particles not in contact with a grain boundary
  - no agreement on parameter values in Zener relation
- **mostly sphere-shaped particles**
Phase field model for grain growth

- set of phase field variables [Chen et al., 1994]
  \[ \eta_i(r, t), \quad i = 1, \ldots, p \]
- inside grain \( i \)
  \[ (\eta_1, \ldots, \eta_i, \ldots, \eta_p) = (0, \ldots, \pm1, \ldots, 0) \]
- parameter \( \phi \) for the second-phase particles [Moelans et al., 2005]
  - \( \phi = 1 \) inside particles
  - \( \phi = 0 \) else
Phase field model for grain growth

- kinetic equations
  \[
  \frac{\partial \eta_i}{\partial t} = -L \frac{\delta F}{\delta \eta_i}, \quad i = 1, \ldots, p
  \]

- free energy
  \[
  F = \int_V \left( f_0(\eta_1, \eta_2, \ldots, \eta_p) + \sum_{i=1}^{p} \kappa (\nabla \eta_i)^2 \right) dV
  \]

- homogeneous free energy density
  \[
  f_0(\eta_1, \eta_2, \ldots, \eta_p) = \sum_{i=1}^{p} \left( \frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \sum_{i=1}^{p} \sum_{j>i}^{p} \eta_i^2 \eta_j^2 + \phi^2 \sum_{i=1}^{p} \eta_i^2
  \]
Phase field model for grain growth

Grain growth model

\[ \frac{\partial \eta_i}{\partial t} = L \kappa \nabla^2 \eta_i - L (\eta_i^3 - \eta_i + 2 \eta_i \sum_{j \neq i} \eta_j^2 + 2 \eta_i \phi^2), \quad i = 1, \ldots, p \]

Ellipsoid particles

Spheroid particles

- long axis radius \( l \), short axis radius \( s \)
- characterize shape by aspect ratio \( r_a = \frac{l}{s} \)
- aspect ratios \( r_a = 1, 2 \) and \( 3 \), with the same volume
Second-phase particles

(a) $r_a = 1$
   $l = s = 4$ grid points

(b) $r_a = 2$
   $l = 7$ g.p., $s = 3$ g.p.

(c) $r_a = 3$
   $l = 9$ g.p., $s = 3$ g.p.

After discretisation:
- approximately equal volume
- the third shape is little bit larger than the other two shapes
Discretisation

\[
\frac{\eta_i^{n+1} - \eta_i^n}{\Delta t} = \left[ \left( \kappa \nabla^2 \eta \right)^{n+1} + \left( \eta_i^3 + \eta_i - 2 \eta_i \left( \sum_j \eta_j^2 + \phi_j^2 \right) \right) \right]_i,
\]

\(i = 1, \ldots, p\)

- finite difference scheme
  - spatial derivative is discretised with second order central differences
  - time derivative is discretised using a first order semi-implicit scheme
- periodic boundary conditions are assumed
Bounding box algorithm

Basic elements

- A grain is a set of connected grid points $r$ where $|\eta(r)| > \epsilon$
- For each grain, the corresponding bounding box is the smallest cuboid containing the grain

Algorithm

- Solve the equations only locally, inside bounding boxes
- Only values inside boxes are kept in memory
- Boxes grow or shrink with grain

Parallel computing

Model equations

\[ \frac{\partial \eta_i}{\partial t} = L \left( \kappa \nabla^2 \eta_i + \eta_i^3 + \eta_i - 2 \eta_i \left( \sum_{j} \eta_j^2 + \phi^2 \right) \right), \quad i = 1, \ldots, p \]

Distribution of memory and work load

▶ bounding boxes spread over processors
  ▶ every processor \( P_k \) handles set of bounding boxes
▶ communication
  ▶ every processor \( P_k \) computes partial sum \( S_k = \sum_{j=a_k}^{b_k} \eta_j^2 \)
  ▶ summation of \( S_k \) through MPI_Allreduce-operation

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Effect of second-phase particles on grain growth
Parallel computing

Model equations

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  - summation of \( S_k \) through \texttt{MPI\_Allreduce-operation}
Initialisation: grains and particles

- for every $\eta_i$, with $i = 1, \ldots, p$
  1. choose grid point $g$ according to uniform distribution
  2. create sphere-shaped grain with centre $g$ and radius $s$
  3. determine bounding box

- add particles until $f_V$ is obtained:
  1. choose grid point $g$ according to uniform distribution
  2. choose orientation according to uniform distribution over three orientations: parallel with x-, y- or z-axis
  3. generate spheroid particle with centre $g$: set $\phi = 1$
     inside particle volume

- set up data structure
Simulation parameters

- system size
  - $256 \times 256 \times 256$ grid
  - $p = 25000$
- discretisation parameters
  - $\Delta x = 1, \Delta t = 0.2$
  - $\epsilon = 10^{-5}$
- material parameters
  - $\kappa = 0.5, L = 1$
  - volume fractions $f_V = 6\%, 8\%, 10\%$ and $12\%$
  - aspect ratios $r_a = 1, 2$ and $3$
- for every parameter combination: three simulation runs
- parallel computing: 12 processors
Growth kinetics

- for higher $f_V$, limiting grain size is reached sooner
- particles with $r_a = 3$ have strongest pinning effect
- smaller difference between $r_a = 1$ and $r_a = 2$
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Effect of second phase particles on grain growth

Cross-sections

$f_V = 6\%$
$r_a = 2$

$f_V = 6\%$
$r_a = 3$

$f_V = 12\%$
$r_a = 2$

$f_V = 12\%$
$r_a = 3$
Particle location

- fraction of particles $\phi_{101}$ located at boundaries subdivided into four types:
  - $\phi_2$: at grain faces
  - $\phi_3$: where three grains meet
  - $\phi_4$: where four grains meet
  - $\phi_n$: where more than four grains meet

(a) $r_a = 1$  (b) $r_a = 2$  (c) $r_a = 3$
Particle location

(a) \( r_a = 1 \)  
(b) \( r_a = 2 \)  
(c) \( r_a = 3 \)

- For \( r_a = 1 \) and \( r_a = 2 \):
  - \( \phi_{\text{tot}} \) increases with \( f_v \), mainly due to increase of \( \phi_3 \) and \( \phi_4 \)
  - \( \phi_2 \) more or less independent of \( f_v \)
  - \( \phi_n \) negligible

- For \( r_a = 3 \):
  - \( \phi_2 \) decreases with \( f_v \)
  - Strong increase of \( \phi_n \) with \( f_v \)
Zener relation fit

The presence of second-phase particles inhibits grain growth when a limiting mean grain size radius $\bar{R}_{\text{lim}}$ is reached:

$$\frac{\bar{R}_{\text{lim}}}{r} = K \frac{1}{f_V^b}$$

- replace particle radius $r$ by parameter $m$ and apply
  - $m = s$: short axis radius
  - $m = l$: long axis radius
  - $m = (ls^2)^{1/3}$: geometric average
- Ideally, for the relation to have predictive value, the graphs of the three aspect ratios should coincide.
Zener relation fit

The presence of second-phase particles inhibits grain growth when a limiting mean grain size radius $\bar{R}_{\text{lim}}$ is reached:

$$\frac{\bar{R}_{\text{lim}}}{m} = K \frac{1}{f_b}$$

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  - $m = s$: short axis radius
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Zener relation fit

(a) $m = s$

(b) $m = l$

(c) $m = (ls^2)^\frac{1}{3}$

Fig. (a): graphs surprisingly close to each other
Fig. (b): graphs distinctly separated
Fig. (c): graphs for $r_a = 1$ and $r_a = 2$ almost coincide; graph for $r_a = 3$ lower
Comparison with other studies

- Experimental graphs below graphs for spherical particles
- Data points $r_a = 1$
  - Coincide with MC results
  - Slightly below PFM results
- Data points $r_a = 3$ closer to experiments
Conclusions

Effect of particles with a spheroid shape on grain growth

- particles with $r_a = 1$ and $r_a = 2$: similar behaviour
- particles with $r_a = 3$: stronger pinning effect
  - at higher $f_V$: tendency to lie where more than two grains meet rather than at grain boundary faces
  - larger impact on topology