Multi class grain growth model in MatCalc 6

(MatCalc 6.00.0200)

P. Warczok
Grain growth

- Tendency - to minimize:
  - grain surface area
  - specific grain boundary energy
Grain growth kinetics

- General idea: Mobility & Driving force

\[
\dot{D} = \frac{dD}{dt} = MP_D
\]

- \(\dot{D}\): Grain size growth rate
- \(M\): Grain boundary mobility
- \(P_D\): Driving force/pressure for grain growth
- \(t\): Time
Single class grain growth

• Single quantity: Mean grain size

\[ D_1 \rightarrow D_2 \]
Various grain sizes need to be followed simultaneously...
Multi Class Grain Model (MCGM)

• Class representation – as for precipitates
• Each class has identical:
  - size (diameter)
  - accumulated strain
  - dislocation densities
  - subgrain size
  - etc.
MCGM - selection
MCGM – class definition
MCGM – class definition
MCGM – class inspection
MCGM – class inspection
MCGM – class inspection

<table>
<thead>
<tr>
<th>D</th>
<th>D_dot</th>
<th>N</th>
<th>X_N_av</th>
<th>acc_eps</th>
<th>dd_ex_internal</th>
<th>dd_ex_wall</th>
<th>dd_ex_int_dot</th>
<th>dd_ex_wall_dot</th>
<th>dd_ex_internal_set</th>
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<th>sgd_dot</th>
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<table>
<thead>
<tr>
<th>grain_orientation_x</th>
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<th>grain_orientation_z</th>
<th>aspect_ratio_x</th>
<th>aspect_ratio_y</th>
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<th>dfm_gg</th>
<th>gb_mob</th>
<th>N_dot_rexo_gb</th>
<th>N_dot_rexo_psn</th>
<th>X_N_av_dct</th>
<th>D_rexo</th>
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</table>

<table>
<thead>
<tr>
<th>D_mean_class</th>
<th>gg_wf_class</th>
<th>rexo_class_index</th>
<th>reo_h_i_factor</th>
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</thead>
<tbody>
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<td>0</td>
<td>0.644838..</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0.644838..</td>
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</tbody>
</table>
MCGM – class generation
MCGM – class export/import
MCGM – relevant windows
MCGM – size distribution histogram
Mean grain sizes

Single class

Multi class
# Grain growth kinetics model

<table>
<thead>
<tr>
<th>Single class</th>
<th>Multi class</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{D} = \frac{dD}{dt} = MP_D$</td>
<td>$\dot{D}<em>i = \frac{dD_i}{dt} = MP</em>{D,i}$</td>
</tr>
</tbody>
</table>

- $\dot{D}$ - Grain size growth rate
- $M$ - Grain boundary mobility
- $P_D$ - Driving force/pressure for grain growth
- $t$ - Time
- $\dot{D}_i$ - Grain size growth rate for class i
- $P_{D,i}$ - Driving force/pressure for grain growth relevant to class i
Grain growth driving pressure

**Single class**

\[ P_D = 2k_d \frac{\gamma_{HA}}{D} \]

- \(\gamma_{HA}\) - Grain interface energy
- \(D\) - Mean grain size (diameter)
- \(k_d\) - Scaling factor

**Multi class**

\[ P_{i,D} = 2\eta_H k_d \gamma_{HA} \left( \frac{1}{D_i} - \frac{1}{D_m} \right) \]

- \(D_i\) - Grain size (diameter) for class \(i\)
- \(D_m\) - Mean grain size (diameter), number weighted
- \(\eta_H\) - Scaling factor
Grain growth driving pressure

\[ P_{i,D} = 2\eta_H k_d \gamma_{HA} \left( \frac{1}{D_i} - \frac{1}{D_m} \right) \]

- \( D_i \) - Grain size (diameter) for class \( i \)
- \( D_m \) - Mean grain size (diameter), number weighted
- \( \eta_H \) - Scaling factor
Grain boundary mobility

\[ \dot{D} = M_{\text{eff}} P_D \]

\[ \frac{1}{M_{\text{eff}}} = \frac{1}{M_{\text{prec}}} + \frac{1}{M_{\text{sd}}} \]

\[ M_{\text{prec}} = \begin{cases} M_p & P_Z \geq P_D \\ M_p \frac{P_Z}{P_D} + M_f \left(1 - \frac{P_Z}{P_D}\right) & P_Z < P_D \end{cases} \]

\[ M_p = \eta_p M_f = \eta_p \eta_f \frac{\omega D_{GB} V_m}{b^2 RT} \]

- **\( M_{\text{eff}} \)** - Effective grain boundary mobility
- **\( M_{\text{sd}} \)** - Grain boundary mobility with solute drag
- **\( M_{\text{prec}} \)** - Grain boundary mobility for matrix with precipitates
- **\( M_p \)** - Grain boundary mobility for pinned interface
Grain boundary mobility

\[ \dot{D} = M_{eff} P_D \]

\[ \frac{1}{M_{eff}} = \frac{M_p}{P_D} + M_f \left( 1 - \frac{P_D}{P_D} \right) \]

Grain boundary mobility is the same for both grain size representations (single and multi class)!

\[ M_{p \text{prec}} = \begin{cases} 
M_p \frac{1}{P_D} + M_f \left( 1 - \frac{P_D}{P_D} \right) & P_Z < P_D 
\end{cases} \]

\[ M_p = \eta_p M_f = \eta_p \eta_f \frac{\omega D_{GB} V_m}{b^2 RT} \]

\[ M_{eff} \] - Effective grain boundary mobility

\[ M_{p} \] - Grain boundary mobility for pinned interface

\[ M_{p\text{prec}} \] - Grain boundary mobility for matrix with precipitates
### Grain growth driving pressure

<table>
<thead>
<tr>
<th>Single class</th>
<th>Multi class</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Volume conservation by grain number adjustment</td>
<td>• Volume conservation by grain size adjustment – Lagrange control volume approach</td>
</tr>
</tbody>
</table>
Grain growth kinetics

No obstacles
Grain growth kinetics

Single class

Multi class
(volume weighted)

No obstacles
Grain growth kinetics

When performing multiple calculation with multi class model:
- Save a calc-state before the start of the first calculation (to save the generated grain size distribution)
- Start every calculation with the saved calc-state as the starting condition

No obstacles
Acknowledgments

- Heinrich Buken
- Yao Shan