

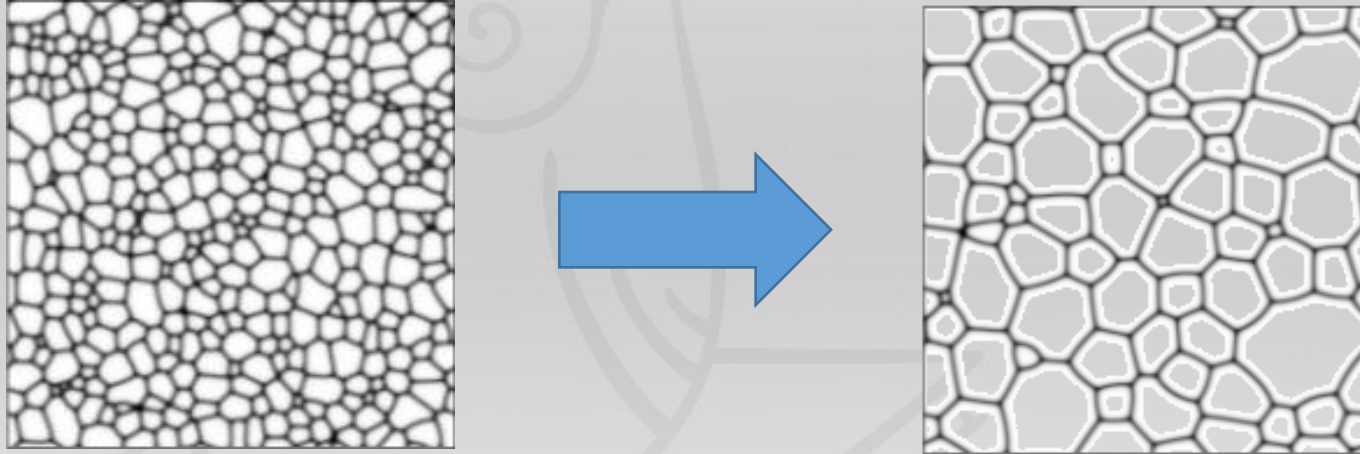
Single class grain growth model in MatCalc 6

(MatCalc 6.01.1000)

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

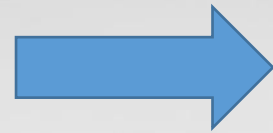
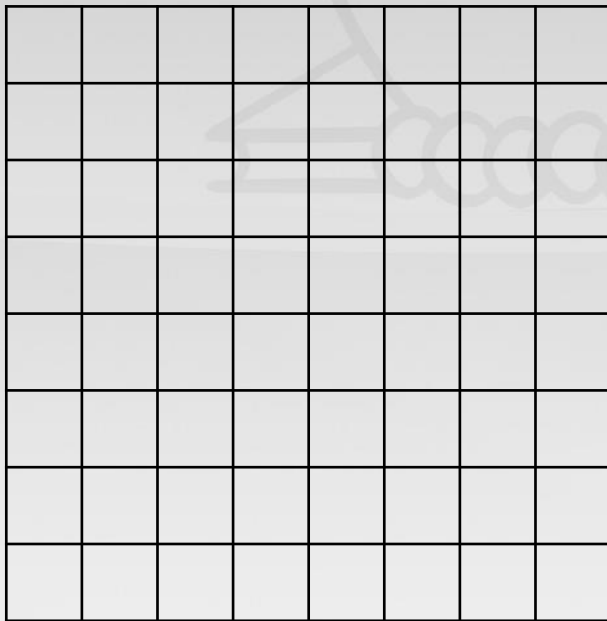
P_D - Driving force/pressure for grain growth

t - Time

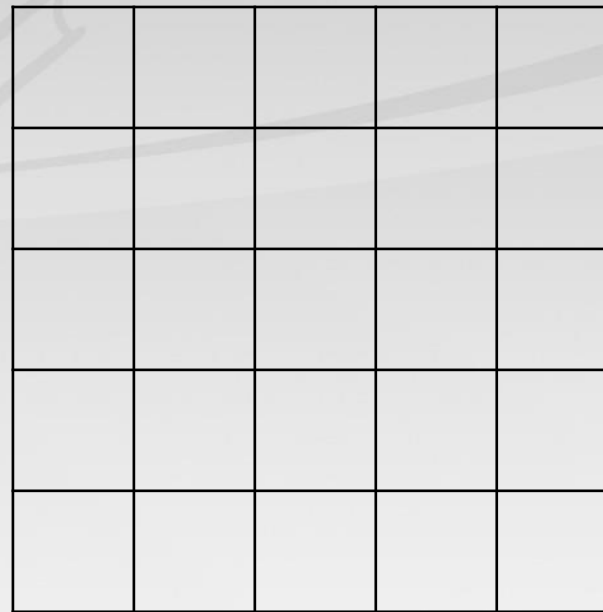
Single class grain growth

- Single quantity: Mean grain size

D_1

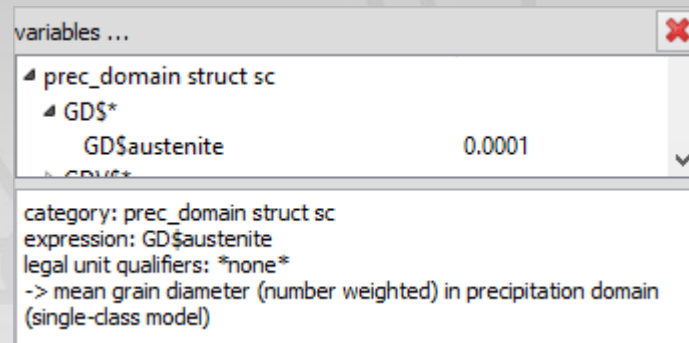


D_2



Single class grain growth

- Single quantity: Mean grain size



Growth driving pressure

- Driving pressure dependent on
 - Grain interface energy
 - Grain size

$$P_D \sim \frac{\gamma_{HA}}{D}$$

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

Growth driving pressure

- Driving pressure dependent on
 - Grain interface energy
 - Grain size

| variables | value |
|--------------------------|-------|
| prec_domain ms evolution | |
| DF_GG\$* | |
| DF_GG\$austenite | 20000 |

category: prec_domain ms evolution
expression: DF_GG\$austenite
legal unit qualifiers: *none*
-> driving force for grain growth of unrecrystallized grains

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor

Growth driving pressure

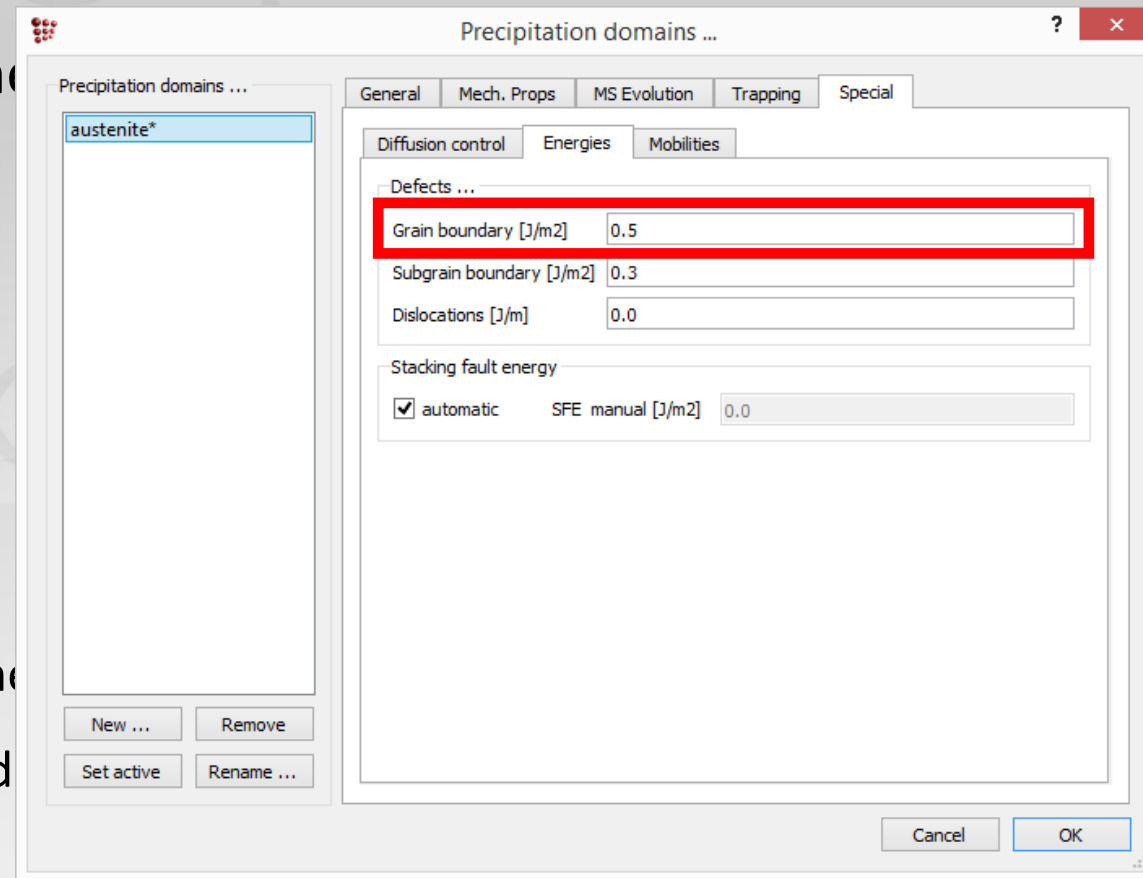
- Driving pressure dependent on
 - Grain interface energy
 - Grain size

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor



Growth driving pressure

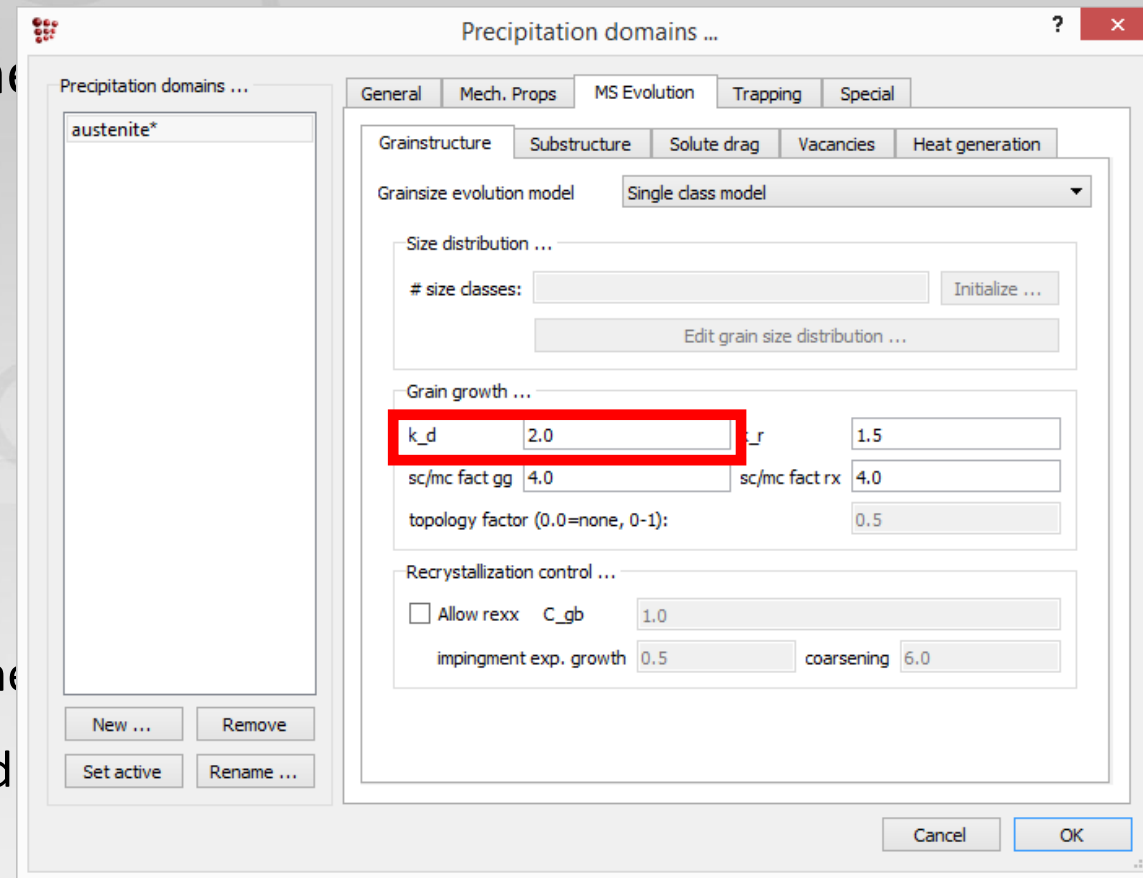
- Driving pressure dependent on
 - Grain interface energy
 - Grain size

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor



Mobility – general approach

- General form

$$M = M_0 \exp(-Q/RT)$$

M - Grain boundary
mobility

M_0 - Mobility pre-factor

Q - Activation energy

R - Gas constant

T - Temperature

Precipitation domains ...

Precipitation domains ...

austenite*

General Mech. Props MS Evolution Trapping Special

Diffusion control Energies Mobilities

Grain boundaries (HAGB) ...

| | | | |
|----------------|--------------------|---|-----|
| intrinsic M0 | 0.01*MOB_HAGB\$@ | Q | 0.0 |
| solute drag M0 | 0.1*GB_MOB_INT\$@ | Q | 0.0 |
| pinned M0 | 0.01*GB_MOB_INT\$@ | Q | 0.0 |

Subgrain boundaries (LAGB) ...

| | | | |
|----------------|---------------------|---|-----|
| intrinsic M0 | 0.01*MOB_LAGB\$@ | Q | 0.0 |
| solute drag M0 | 0.1*SGB_MOB_INT\$@ | Q | 0.0 |
| pinned M0 | 0.01*SGB_MOB_INT\$@ | Q | 0.0 |

New ... Remove

Set active Rename ...

Cancel OK

Mobility – general approach

- General form

$$M = M_0 \exp(-Q/RT)$$

M - Grain boundary
mobility

M_0 - Mobility pre-factor

Q - Activation energy

R - Gas constant

T - Temperature

| variables | value |
|--------------------------|-------------|
| prec_domain ms evolution | |
| GB_MOB_GG\$* | |
| GB_MOB_GG\$austenite | 3.01124e-13 |

category: prec_domain ms evolution
expression: GB_MOB_GG\$austenite
legal unit qualifiers: *none*
-> effective grain boundary mobility for grain growth

No obstacles

$$\dot{D} = M_f P_D$$

$$M_f = \eta_f \frac{\omega D_{GB} V_m}{b^2 RT}$$

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

ω - Grain boundary width
(hard coded - 1 nm)

D_{GB} - Diffusion coefficient
for grain boundary

V_m - Molar volume

b - Burger's vector

R - Gas constant

T - Temperature

η_f, k_d - Scaling factor

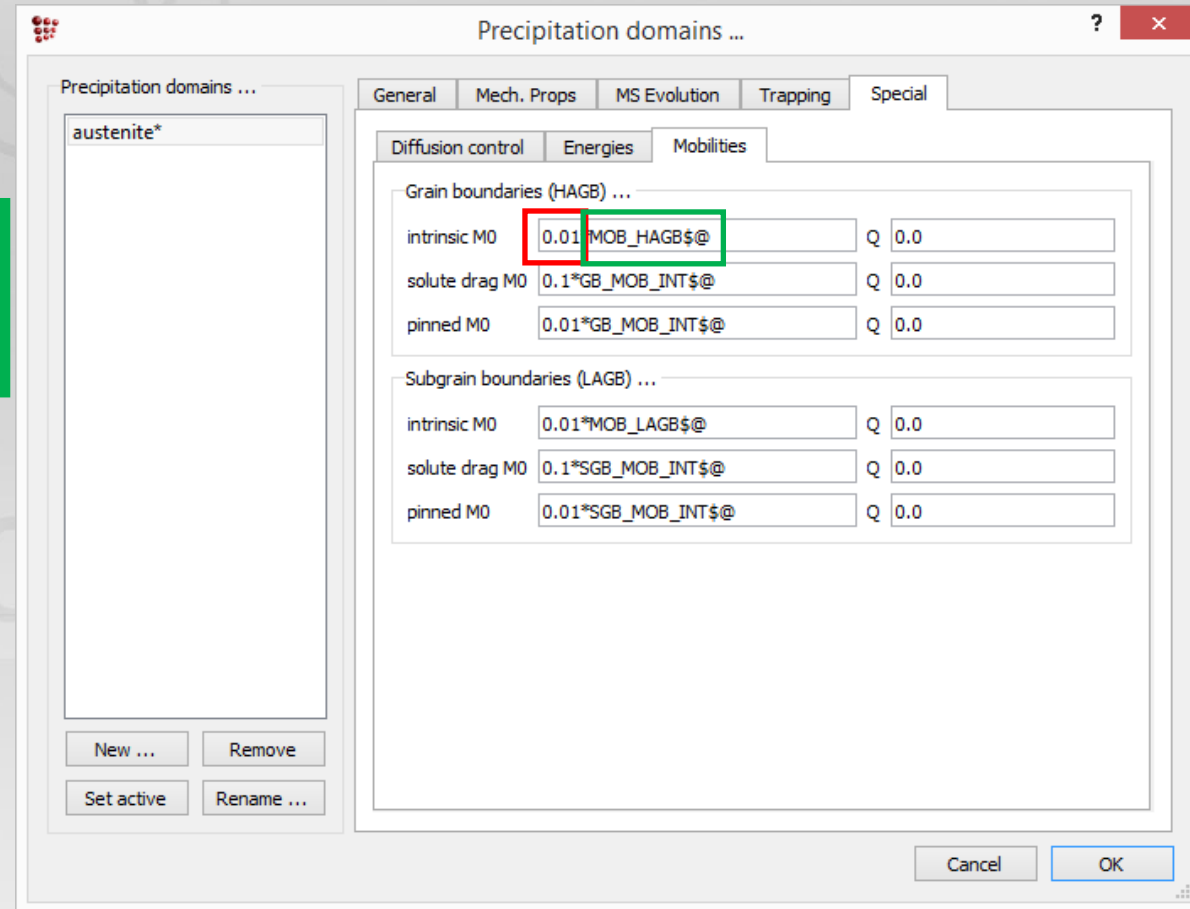
Turnbull D., *Trans. AIME*, 191 (1951), pp. 661-665

No obstacles

$$\dot{D} = M_f P_D$$

$$M_f = \eta_f \frac{\omega D_{GB} V_m}{b^2 RT}$$

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$



| variables | value |
|--------------------------|-------------|
| prec_domain ms evolution | |
| MOB_HAGB\$* | |
| MOB_HAGB\$austenite | 7.40552e-11 |

category: prec_domain ms evolution
expression: MOB_HAGB\$austenite
legal unit qualifiers: *none*
-> mobility of high angle grain boundaries based on gb diffusivities

No obstacles

$$\dot{D} = M_f P_D$$

$$M_f = \eta_f \frac{\omega D_{GB} V_m}{b^2 RT}$$

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

Precipitation domains ...

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Diffusion control Energies Mobilities

Precipitation domains ...

austenite*

Grain boundaries (HAGB) ...

intrinsic M0 0.01 MOB_HAGB\$@ Q 0.0

solute drag M0 0.1*GB_MOB_INT\$@ Q 0.0

pinned M0 0.01*GB_MOB_INT\$@ Q 0.0

Subgrain boundaries (LAGB) ...

intrinsic M0 0.01*MOB_LAGB\$@ Q 0.0

solute drag M0 0.1*SGB_MOB_INT\$@ Q 0.0

pinned M0 0.01*SGB_MOB_INT\$@ Q 0.0

New ... Remove

Set active Rename ...

Cancel OK

variables ...

| variables | value |
|--------------------------|-------------|
| prec_domain ms evolution | |
| GB_MOB_INT\$austenite | 7.40552e-13 |

category: prec_domain ms evolution
expression: GB_MOB_INT\$austenite
legal unit qualifiers: *none*
-> intrinsic grain boundary mobility

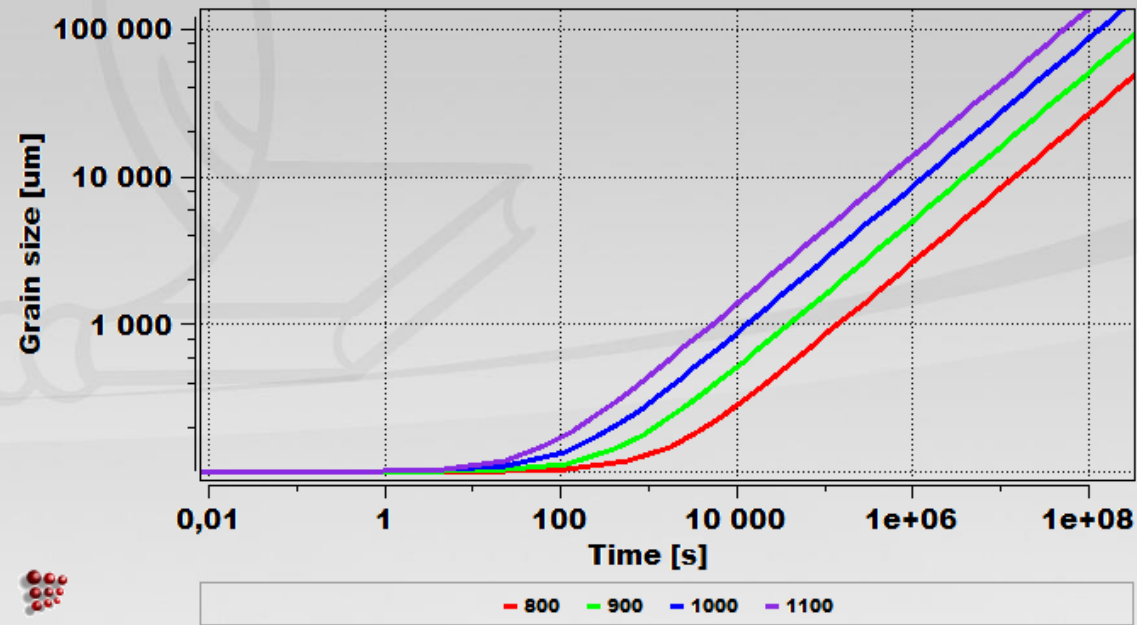
No obstacles

$$\dot{D} = M_f P_D$$

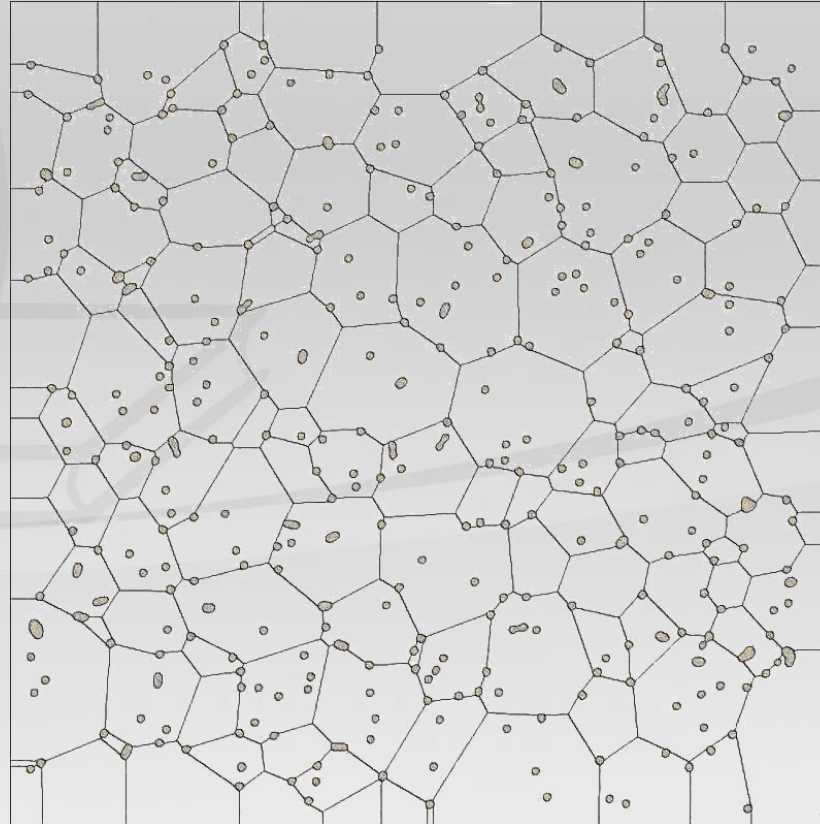
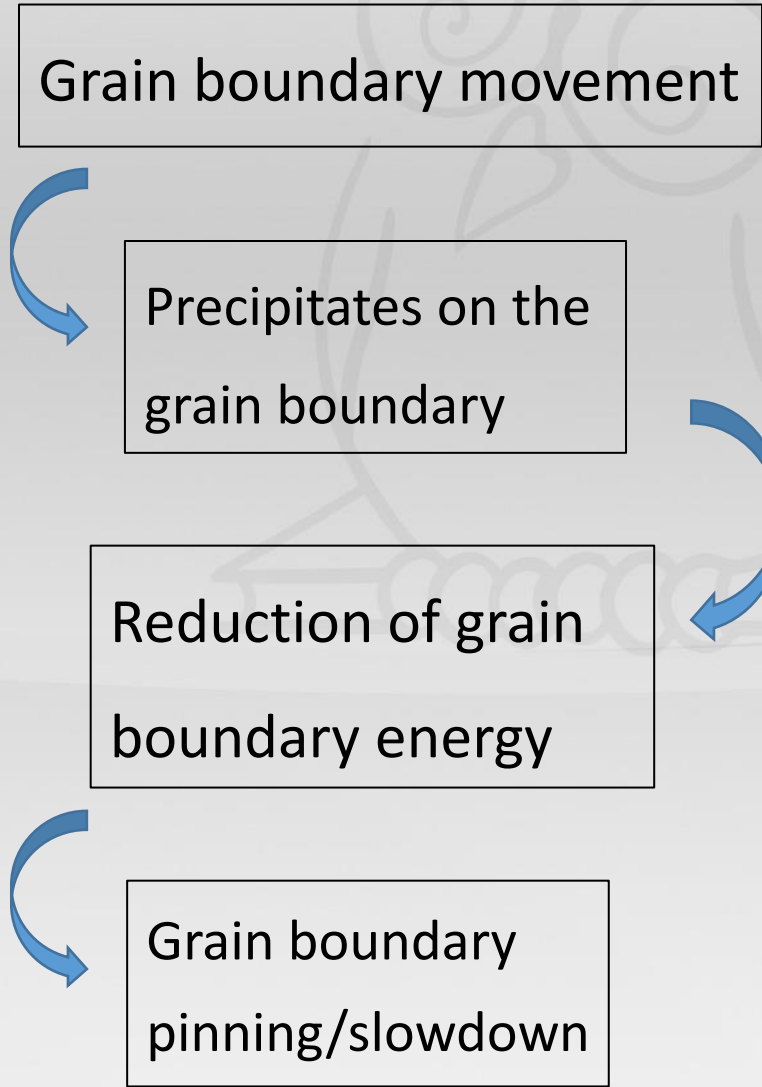
$$M_f = \eta_f \frac{\omega D_{GB} V_m}{b^2 RT}$$

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

$$D \sim \sqrt{t}$$



System with precipitates



https://i.ytimg.com/vi/8EET_T6LWY/maxresdefault.jpg

System with precipitates

- Growth retarding pressure dependent on
 - Precipitate phase fraction
 - Precipitate radius

P_Z - Pinning force (Zener force)

$f_{i,j}$ - Phase fraction of class j of precipitate i

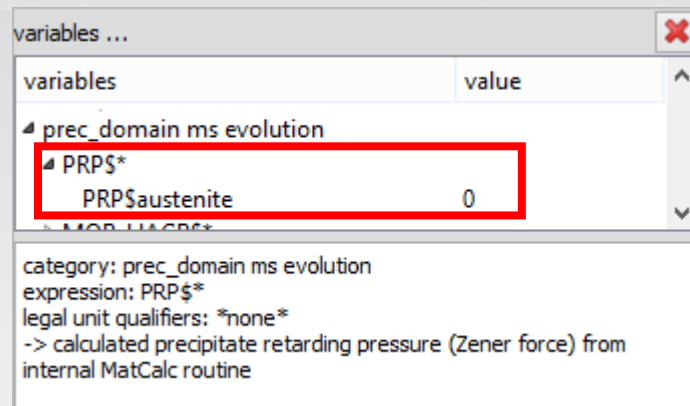
$r_{i,j}$ - Mean radius of class j of precipitate i

k_r - Scaling factor

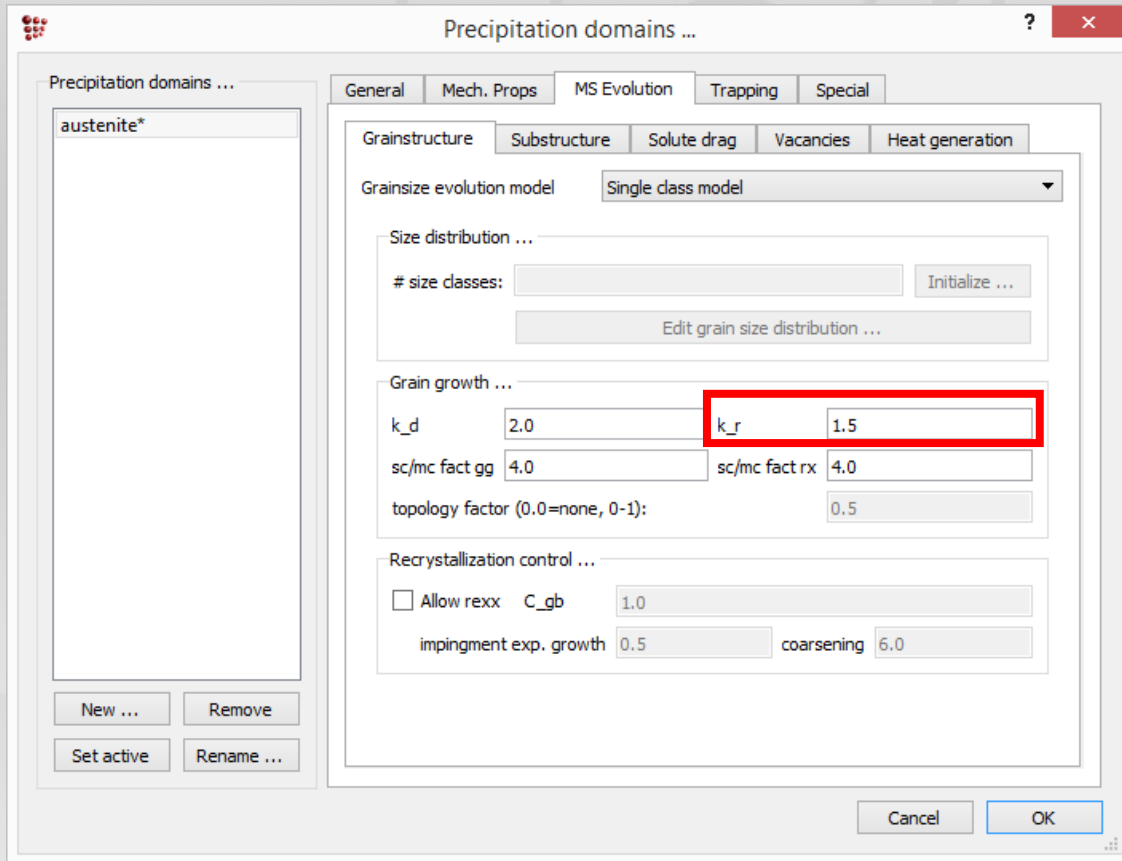
α_i - Pinning factor of precipitate i

β_i - Pinning exponent of precipitate i

$$P_Z = \frac{k_r \gamma_{HA}}{2} \sum_i \left[\alpha_i f_i^{(\beta_i - 1)} \sum_j \frac{f_{i,j}}{r_{i,j}} \right]$$



System with precipitates



dependent on

P_Z - Pinning force (Zener force)

$f_{i,j}$ - Phase fraction of class j of precipitate i

$r_{i,j}$ - Mean radius of class j of precipitate i

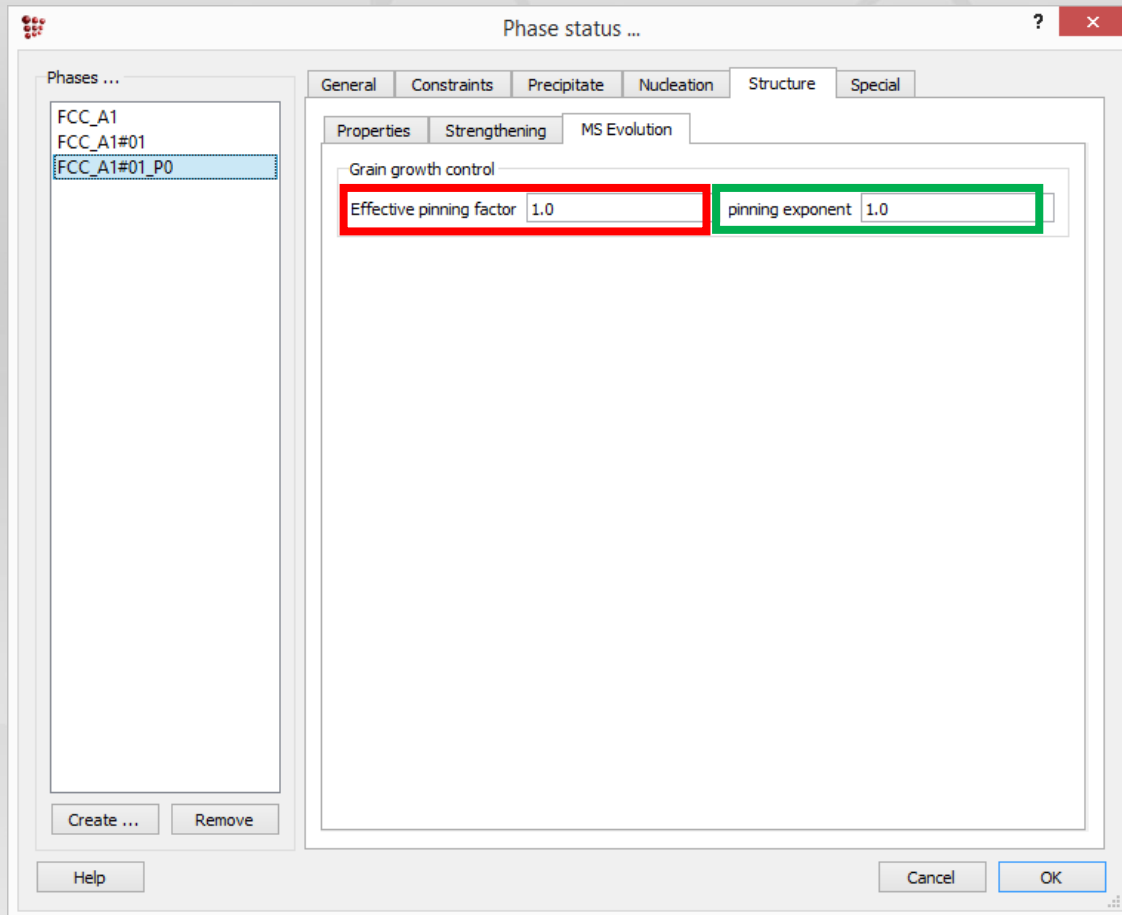
k_r - Scaling factor

α_i - Pinning factor of precipitate i

β_i - Pinning exponent of precipitate i

$$P_Z = \frac{k_r \gamma_{HA}}{2} \sum_i \left[\alpha_i f_i^{(\beta_i - 1)} \sum_j \frac{f_{i,j}}{r_{i,j}} \right]$$

System with precipitates



dependent on

P_Z - Pinning force (Zener force)

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$$P_Z = \frac{k_r \gamma_{HA}}{2} \sum_i \left[\alpha_i f_i^{\beta_i - 1} \sum_j \frac{f_{i,j}}{r_{i,j}} \right]$$

System with precipitates

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

$$P_Z \geq P_D$$

$$P_Z < P_D$$

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

M_{prec} - Grain boundary mobility for matrix with precipitates

M_p - Grain boundary mobility for pinned interface

η_p - Scaling factor

$$\dot{D} = M_{prec} P_D$$

System with precipitates

$$M_{prec} = \begin{cases} M_p \\ M_p \frac{P_Z}{P_D} + M_j \left(\dots P_Z \right) \end{cases}$$

$$P_Z \geq P_D$$

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

$$\dot{D} = M_{prec} P_D$$

Precipitation domains ...

austenite*

General Mech. Props MS Evolution Trapping Special

Diffusion control Energies Mobilities

Grain boundaries (HAGB) ...

| | | | |
|----------------|--------------------|---|-----|
| intrinsic M0 | 0.01*MOB_HAGB\$@ | Q | 0.0 |
| solute drag M0 | 0.1*GB_MOB_INT\$@ | Q | 0.0 |
| pinned M0 | 0.01*GB_MOB_INT\$@ | Q | 0.0 |

Subgrain boundaries (LAGB) ...

| | | | |
|----------------|---------------------|---|-----|
| intrinsic M0 | 0.01*MOB_LAGB\$@ | Q | 0.0 |
| solute drag M0 | 0.1*SGB_MOB_INT\$@ | Q | 0.0 |
| pinned M0 | 0.01*SGB_MOB_INT\$@ | Q | 0.0 |

New ... Remove

Set active Rename ...

Cancel OK

variables ...

| variables | value |
|--------------------------|-------------|
| prec_domain ms evolution | |
| GB_MOB_PREC\$* | |
| GB_MOB_PREC\$austenite | 7.40552e-15 |

category: prec_domain ms evolution
expression: GB_MOB_PREC\$*
legal unit qualifiers: *none*
-> pinned (Zener drag) grain boundary mobility

System with precipitates

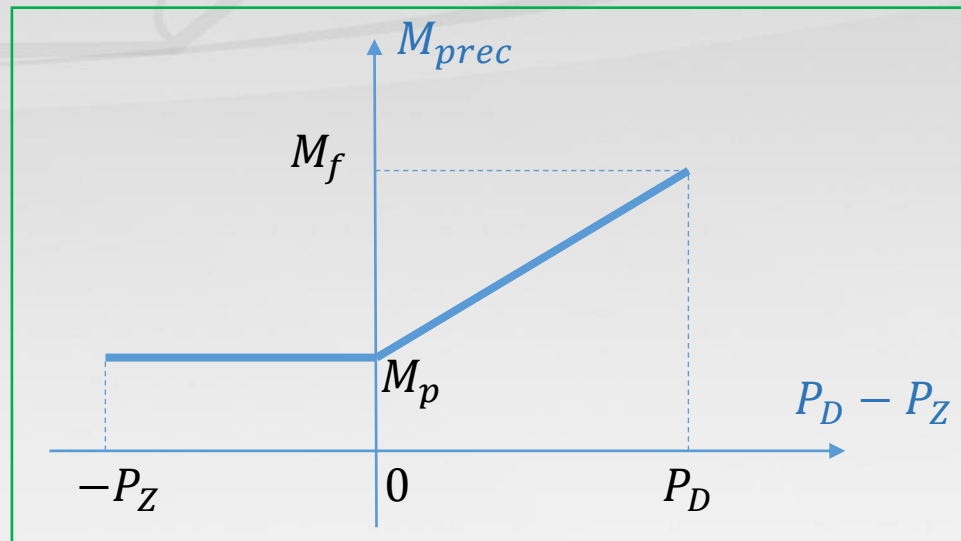
$$M_{prec,0} = \begin{cases} M_p & P_Z \geq P_D \\ M_p \frac{P_Z}{P_D} + M_f \left(1 - \frac{P_Z}{P_D}\right) & P_Z < P_D \end{cases}$$

$$P_Z \geq P_D$$

$$P_Z < P_D$$

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

$$\dot{D} = M_{prec} P_D$$



System with precipitates

$$\dot{D} = M_{prec} P_D$$

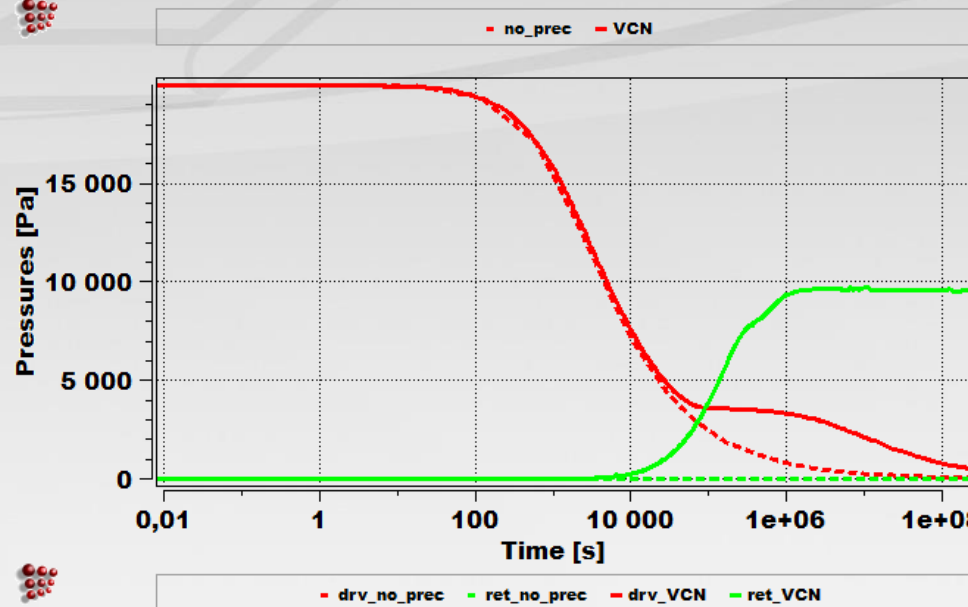
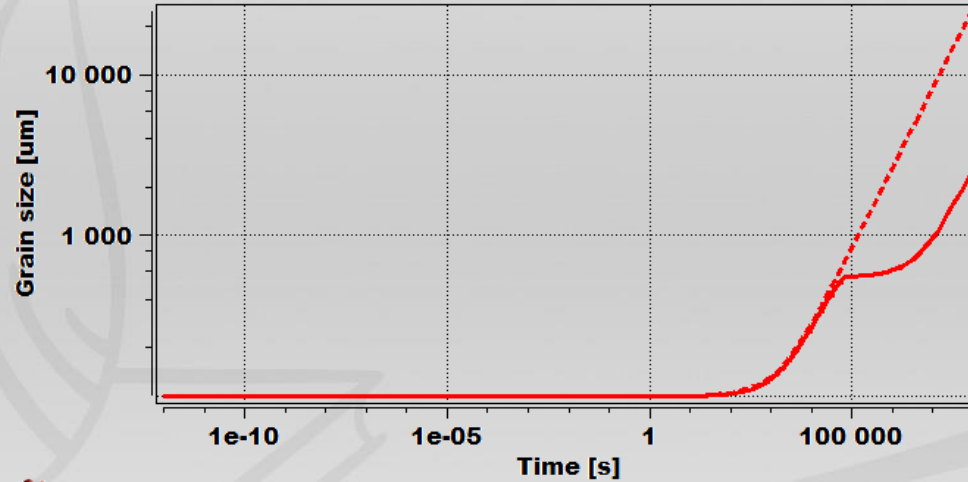
$$M_{prec} = \begin{cases} M_p & P_Z \geq P_D \\ M_p \frac{P_Z}{P_D} + M_f \left(1 - \frac{P_Z}{P_D}\right) & P_Z < P_D \end{cases}$$

$$P_Z \geq P_D$$

$$P_Z < P_D$$

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

$$P_Z = \frac{k_r \gamma_{HA}}{2} \sum_i \left[\alpha_i f_i^{(\beta_i - 1)} \sum_j \frac{f_{i,j}}{r_{i,j}} \right]$$

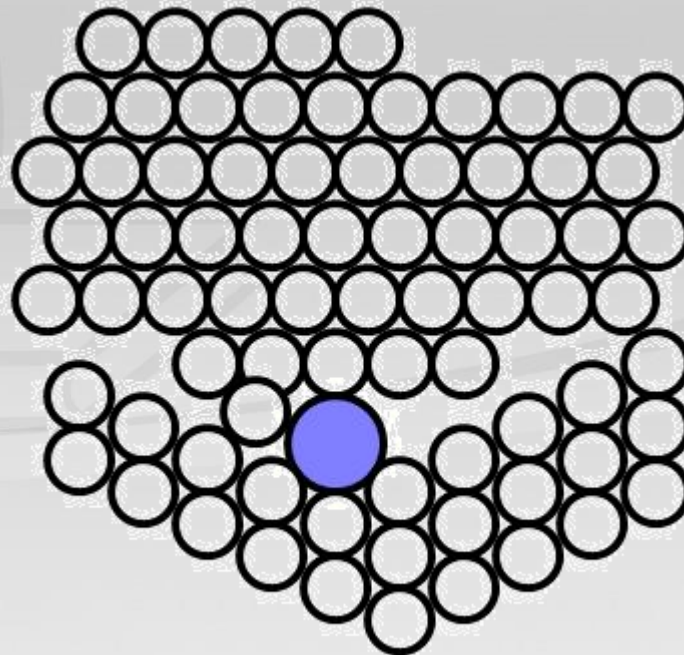


Case with solute drag

Solutes on the
grain boundary

Reduction of grain
boundary energy

Grain boundary
pinning/slowdown



<http://slideplayer.com/slide/227236/>

Case with solute drag

$$\dot{D} = M_{eff} P_D$$

M_{eff} - Effective grain
boundary mobility

M_{sd} - Grain boundary
mobility with solute
drag

$$\frac{1}{M_{eff}} = \frac{1}{M_{prec}} + \frac{1}{M_{sd}}$$

$$M_{eff} = \frac{M_{prec} M_{sd}}{M_{prec} + M_{sd}}$$

Cahn impurity drag

- Evaluation of critical velocity $v_{crit,i}$ for each solute element

$$v_{crit,i} = \frac{3D_i}{b} \theta$$

D_i - Diffiusion coefficient of element i

b - Burgers vector

θ - Scaling factor

- Comparison of current grain boundary velocity \dot{D} with critical velocities
 - $\dot{D} \geq v_{crit,i}$ - „fast branch“, grain boundary is faster than the pinning solute i
 - $\dot{D} < v_{crit,i}$ - „slow branch“, grain boundary cannot escape from the pinning solute i

Cahn impurity drag

- Evaluation of critical velocity

$$v_{crit,i} = \frac{3D_i}{b} \theta$$

- Comparison of current grain growth rate

- $\dot{D} \geq v_{crit,i}$ - „fast branch
- $\dot{D} < v_{crit,i}$ - „slow branch

The screenshot shows the 'Precipitation domains' dialog box in MatCalc. The 'Solute drag' tab is active, and the 'Solute drag model' is set to 'Cahn: impurity drag (transient)'. Below this, a table titled 'Solute drag interaction energies ...' lists parameters for elements C, Fe, N, and V. The 'trans_theta' column is highlighted with a red box.

| Element | Inter. energy [J/mol] | CB diff factor | trans_eta | trans_theta | fast_branch | eff_sol_X |
|---------|-----------------------|----------------|-----------|-------------|-------------|-----------|
| C | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |
| Fe | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |
| N | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |
| V | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |

Cahn impurity drag

$$M_{sd} = \left(\sum_i \alpha_i c_i f_{i,b} \right)^{-1}$$

$$f_{i,b} = \begin{cases} 1 & \text{Element in fast branch} \\ \eta \exp\left(\frac{E_i}{RT}\right) & \text{Element in slow branch} \end{cases}$$

$$\alpha_i = \frac{\omega(RT)^2}{E_i D_{CB} V_m} \left(\sinh\left(\frac{E_i}{RT}\right) - \left(\frac{E_i}{RT}\right) \right)$$

M_{eff} - Effective grain boundary mobility

M_{sd} - Grain boundary mobility with solute drag

α_i - Inverse mobility

c_i - Solute concentration on the grain boundary

η - Scaling factor

E_i - Grain boundary/solute interaction energy

D_{CB} - Cross boundary diffusion coefficient

Cahn impurity drag

$$M_{sd} = \left(\sum_i \alpha_i c_i f_{i,b} \right)^{-1}$$

$$f_{i,b} = \begin{cases} 1 & \text{Element } i \text{ is active} \\ \eta \exp\left(\frac{E_i}{RT}\right) & \text{Element } i \text{ is inactive} \end{cases}$$

$$\alpha_i = \frac{\omega(RT)^2}{E_i D_{CB} V_m} \left(\sinh\left(\frac{E_i}{RT}\right) \right)$$

Precipitation domains ...

General Mech. Props MS Evolution Trapping Special

Grainstructure Substructure Solute drag Vacancies Heat generation

Solute drag model Cahn: impurity drag (transient)

Solute drag interaction energies ...

| Element | Inter. energy [J/mol] | CB diff factor | trans_eta | trans_theta | fast_branch | eff_sol_X |
|---------|-----------------------|----------------|-----------|-------------|-------------|-----------|
| C | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |
| FE | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |
| N | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |
| V | 0.0 | 2.0 | 1.0 | 1.0 | 1 | 0 |

New ... Remove

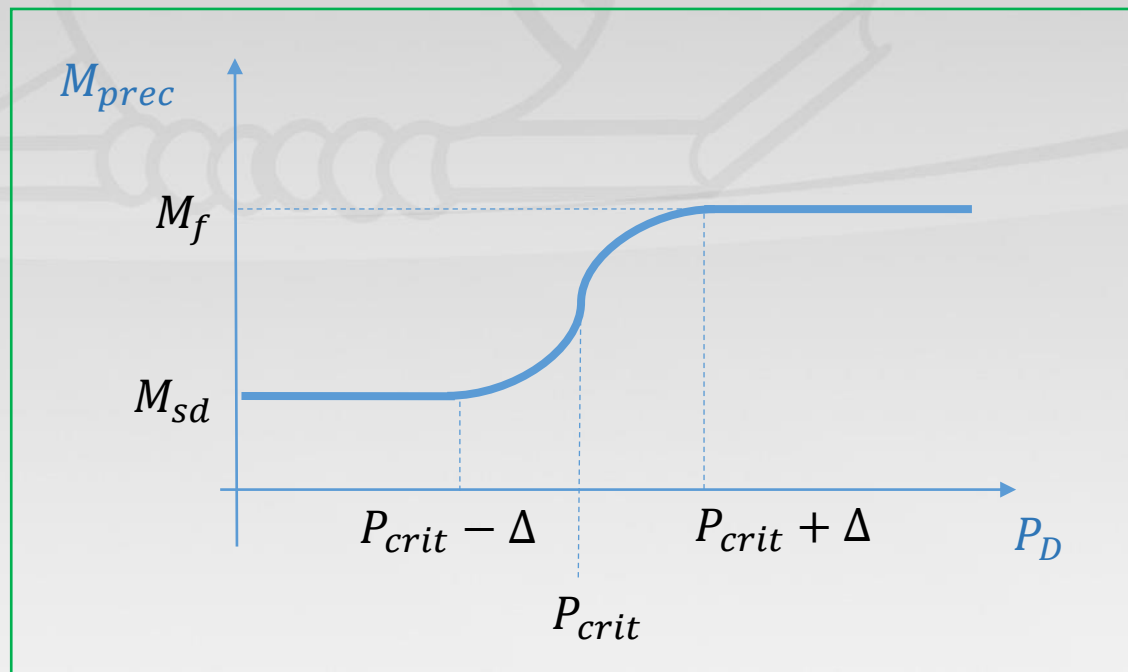
Set active Rename ...

Cancel OK

coefficient

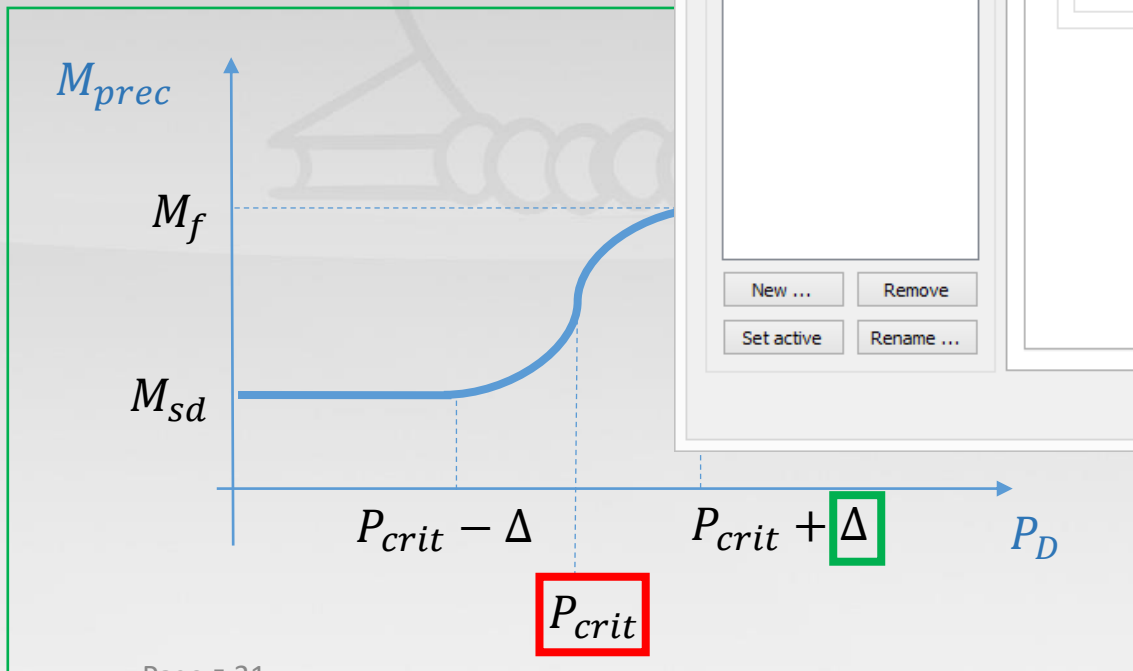
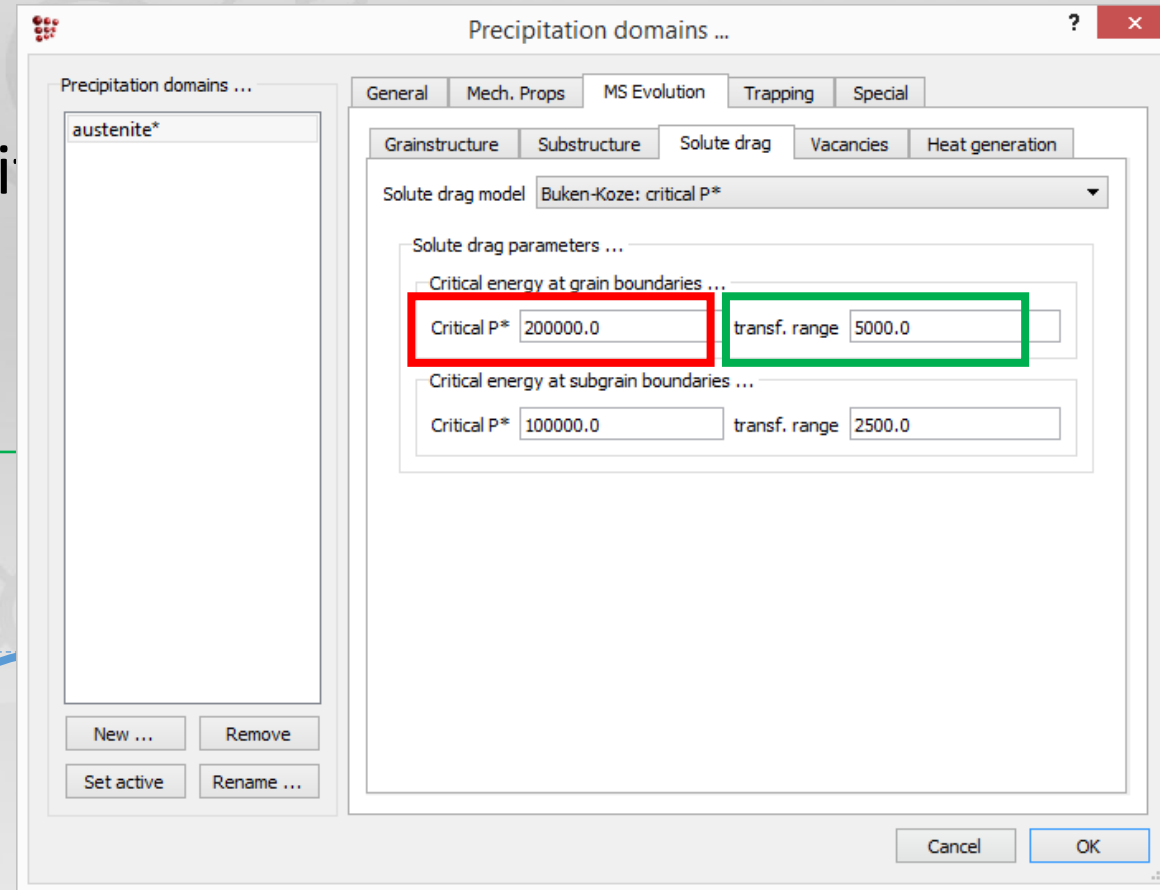
Buken-Kozeschnik critical pressure

- Continuous mobility change dependent on the driving pressure.



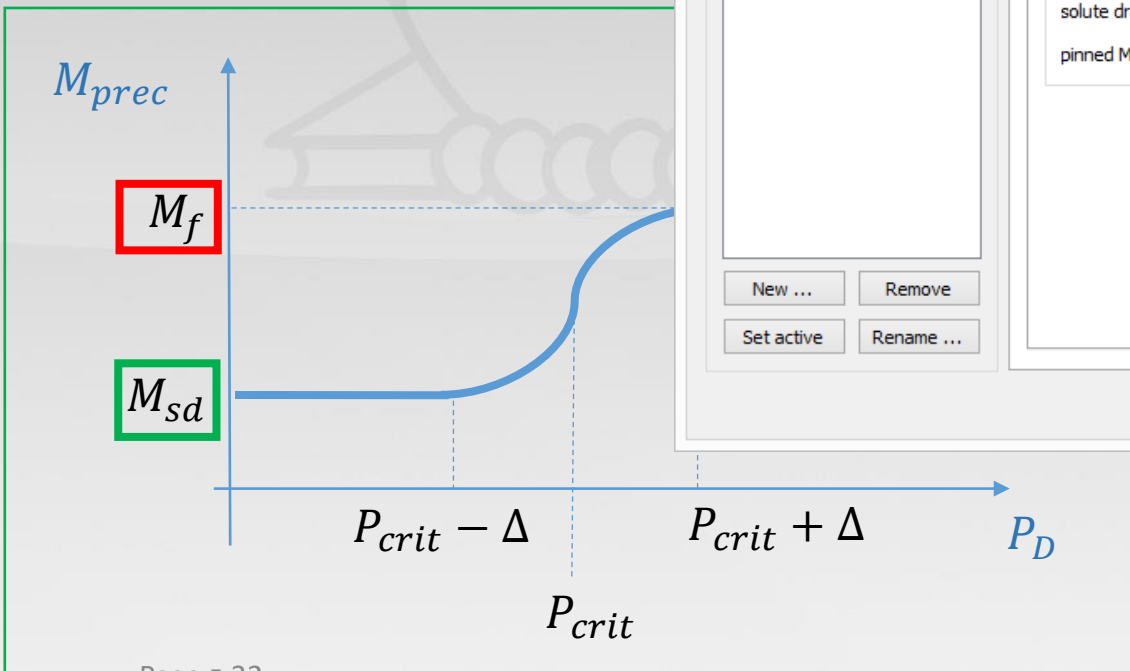
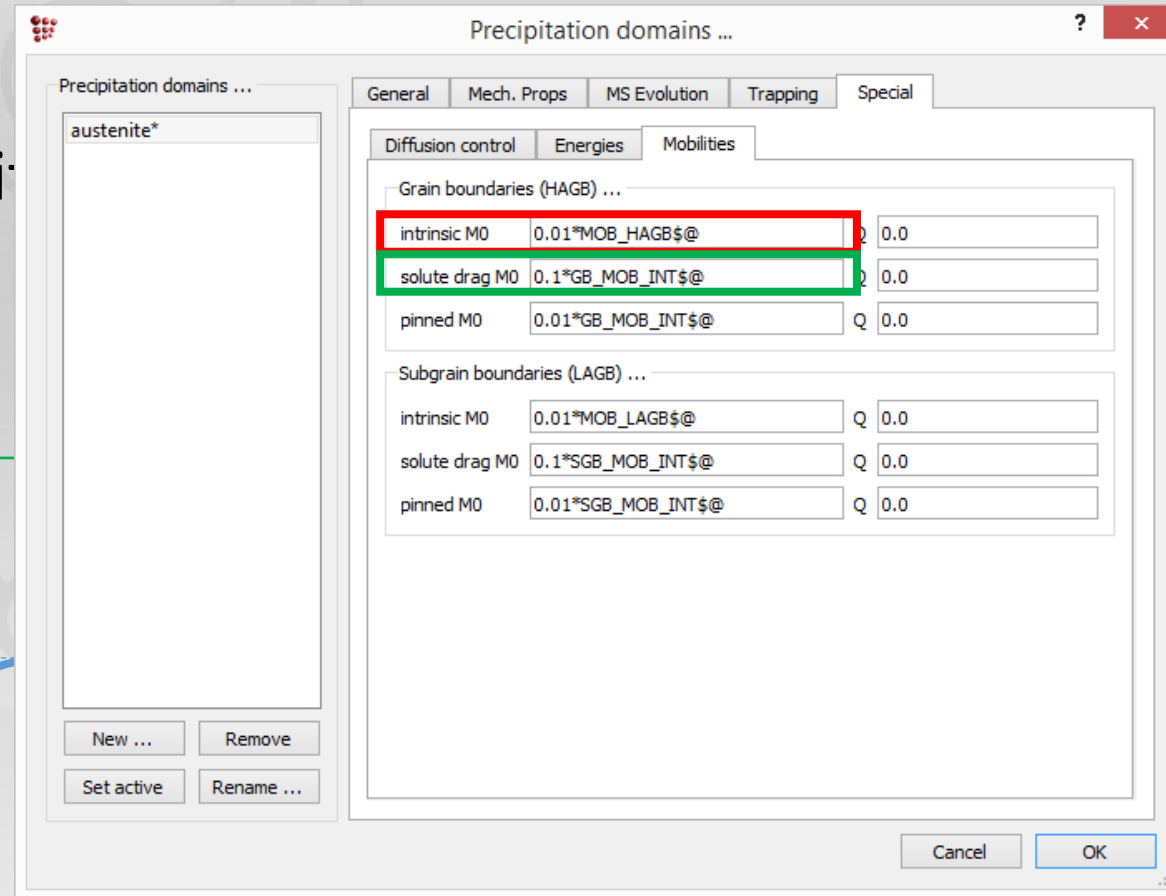
Buken-Kozeschnik critical pressure

- Continuous mobility pressure.



Buken-Kozeschnik critical pressure

- Continuous mobility pressure.



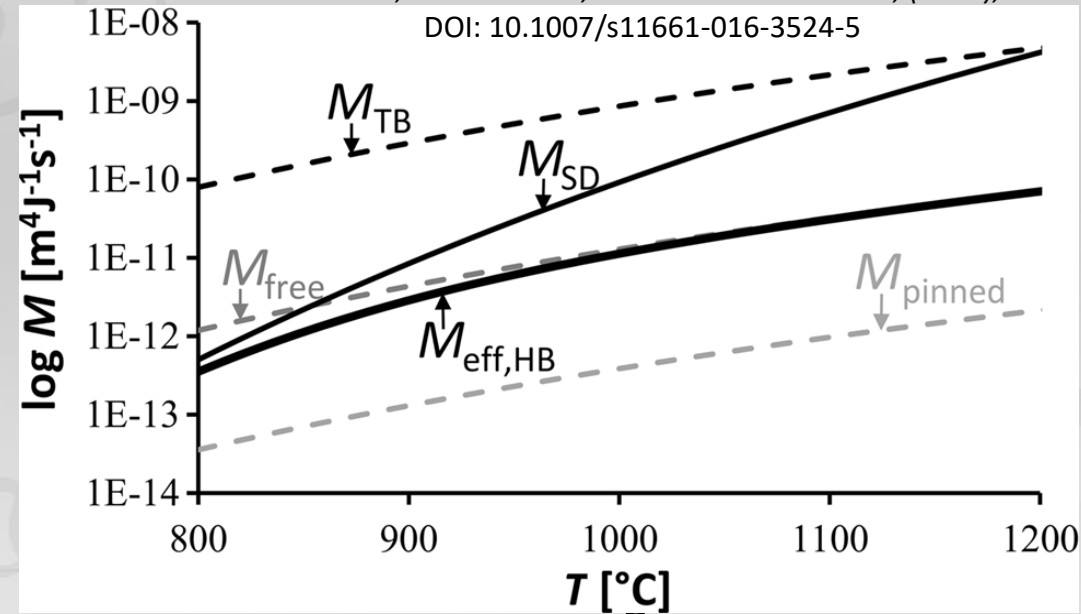
Case with solute drag

$$\dot{D} = M_{eff} P_D$$

$$\frac{1}{M_{eff}} = \frac{1}{M_{prec}} + \frac{1}{M_{sd}}$$

$$M_{eff} = \frac{M_{prec} M_{sd}}{M_{prec} + M_{sd}}$$

Buken H., Kozeschnik E., Metall. Mater. Trans. A, (2016),
DOI: 10.1007/s11661-016-3524-5



| variables | value |
|--------------------------|-------------|
| prec_domain ms evolution | |
| GB_MOB_SD\$ | |
| GB_MOB_SD\$austenite | 7.40552e-14 |
| GB_MOB_\$ | |

category: prec_domain ms evolution
expression: GB_MOB_SD\$austenite
legal unit qualifiers: *none*
-> pinned (solute drag) grain boundary mobility

Acknowledgments

- Heinrich Buken
- Philipp Retzl
- Yao Shan



MatCalc

Engineering

