

Single class grain growth model in MatCalc 6

(MatCalc 6.00.0206)

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

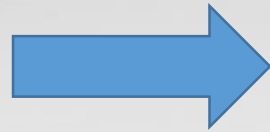
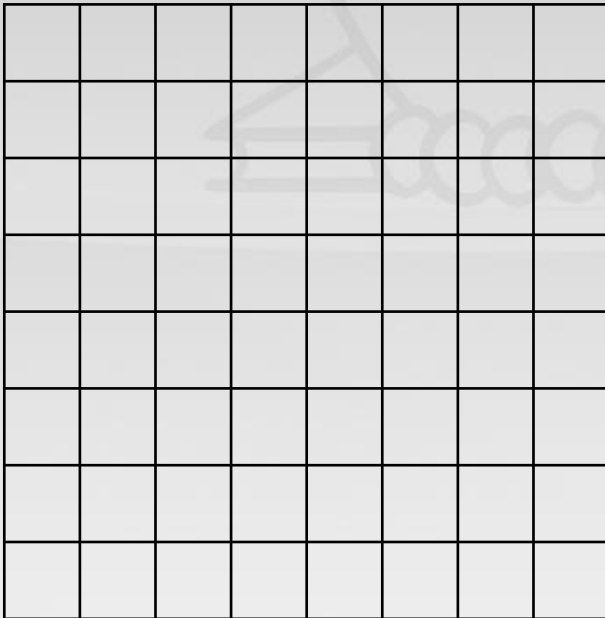
P_D - Driving force/pressure for grain growth

t - Time

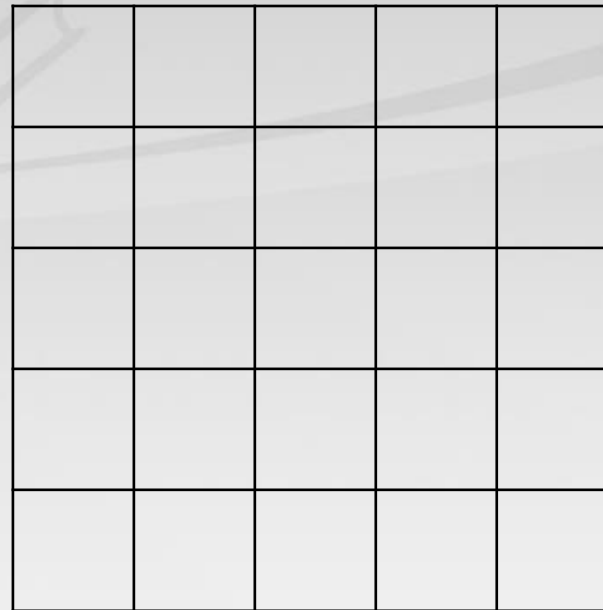
Single class grain growth

- Single quantity: Mean grain size

D_1

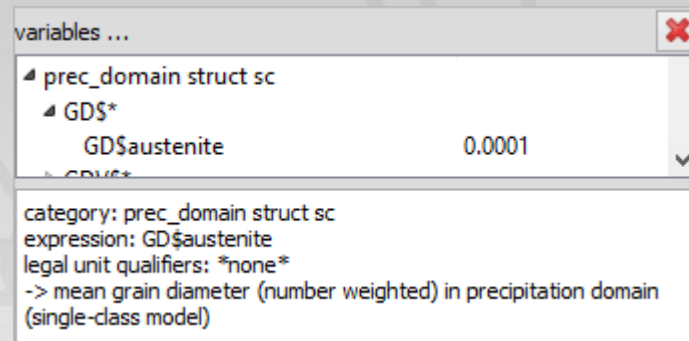


D_2



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

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

variables ...	
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	

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor

Growth driving pressure

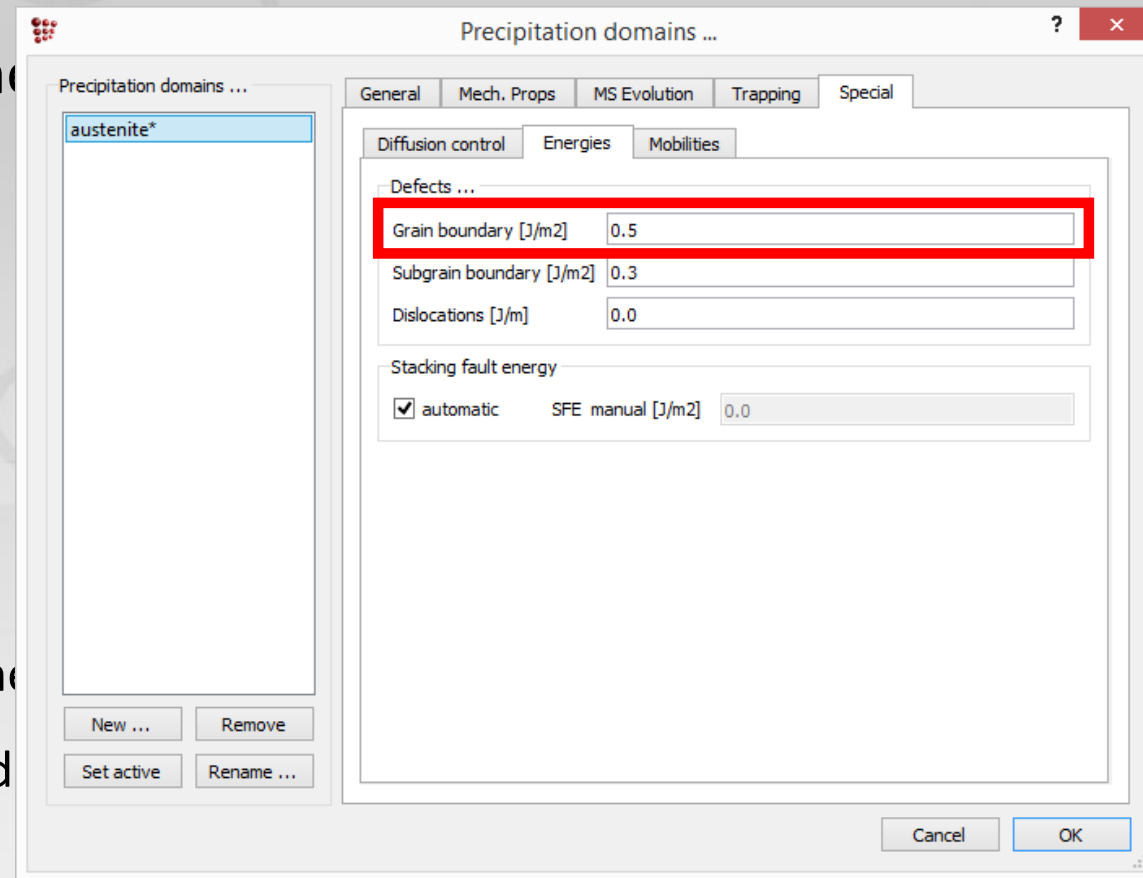
- Driving pressure dependent on
 - Grain interface energy
 - Grain size

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

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor



Growth driving pressure

- Driving pressure dependent on

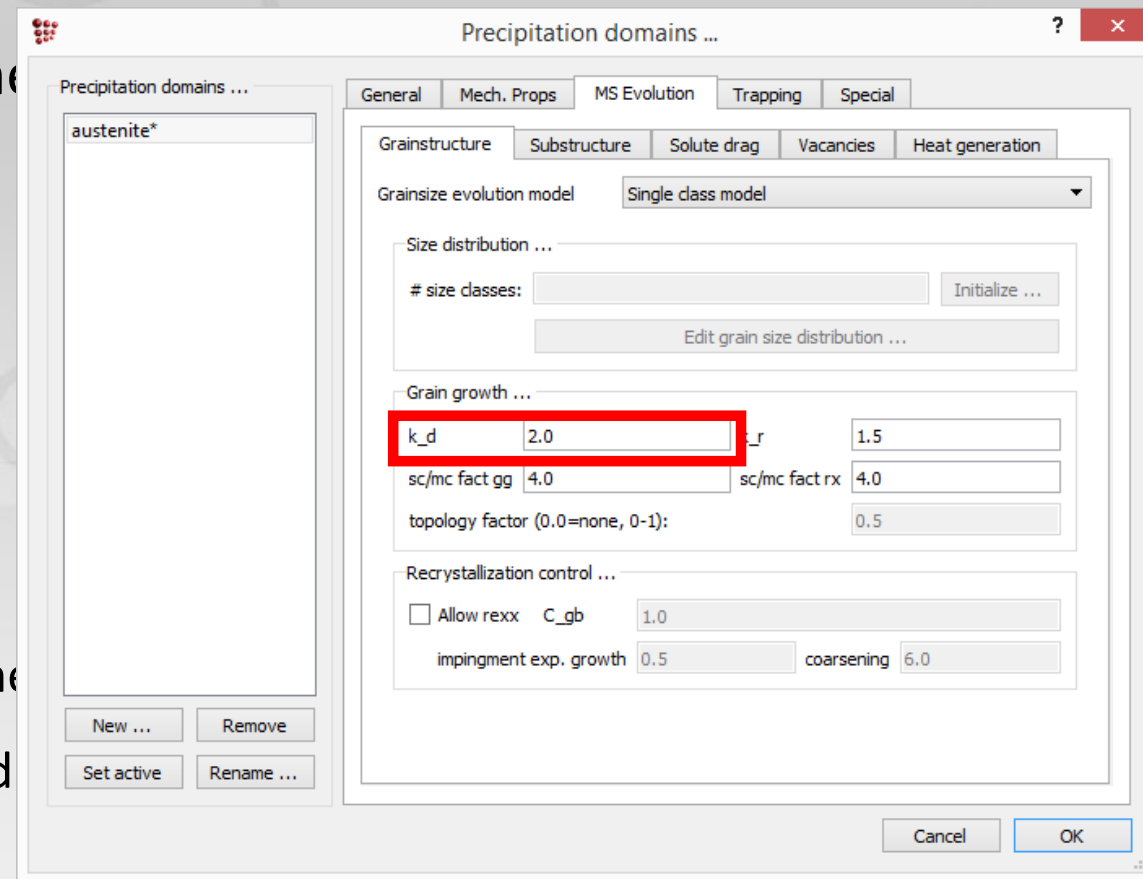
- Grain interface energy
- Grain size

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

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 ...

General Mech. Props MS Evolution Trapping Special

Diffusion control Energies Mobilities

Precipitation domains ...

austenite*

New ... Remove Set active Rename ...

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

Cancel OK

Mobility – general approach

- General form

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

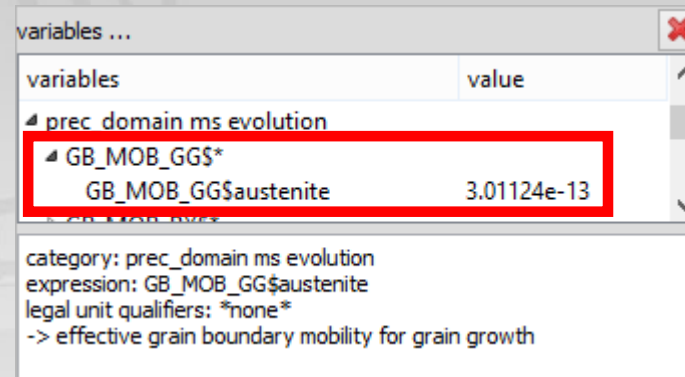
M - Grain boundary
mobility

M_0 - Mobility pre-factor

Q - Activation energy

R - Gas constant

T - Temperature



variables	value
prec_domain ms evolution	
GB_MOB_GG\$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 ...	
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	

Precipitation domains ...

austenite*

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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

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\$*	
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

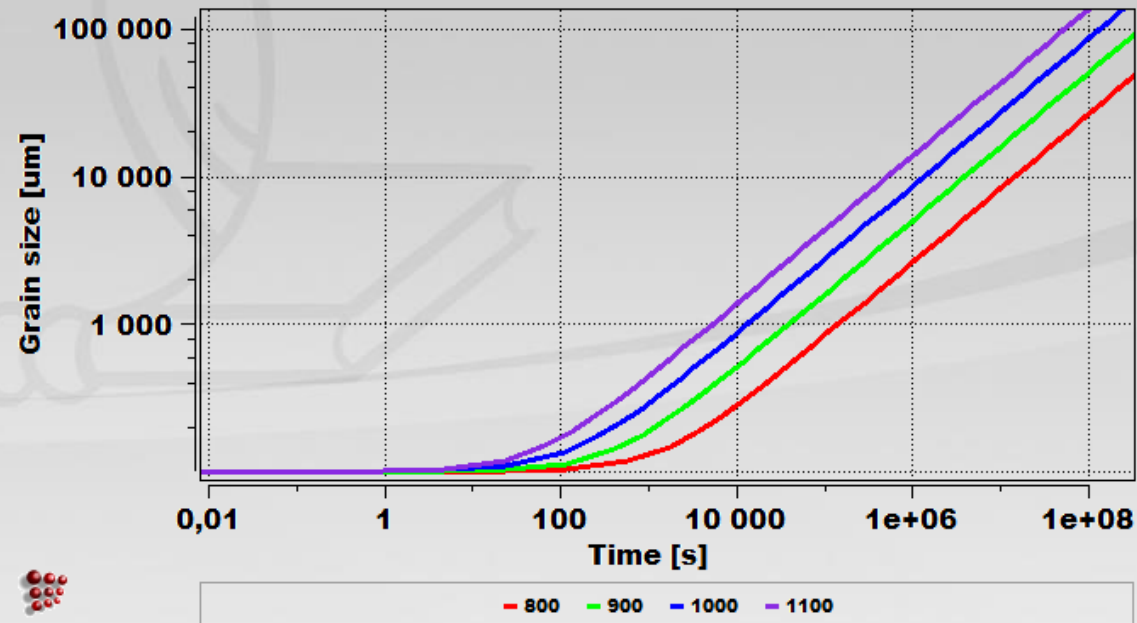
No obstacles

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

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

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

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



System with precipitates

Grain boundary movement



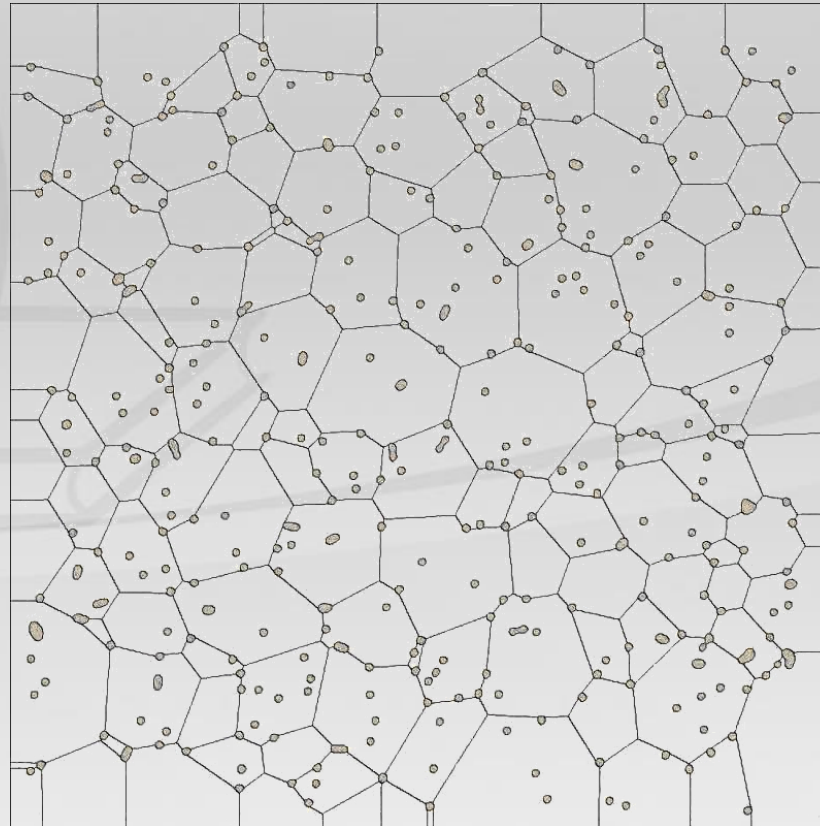
Precipitates on the
grain boundary



Reduction of grain
boundary energy



Grain boundary
pinning/slowdown



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

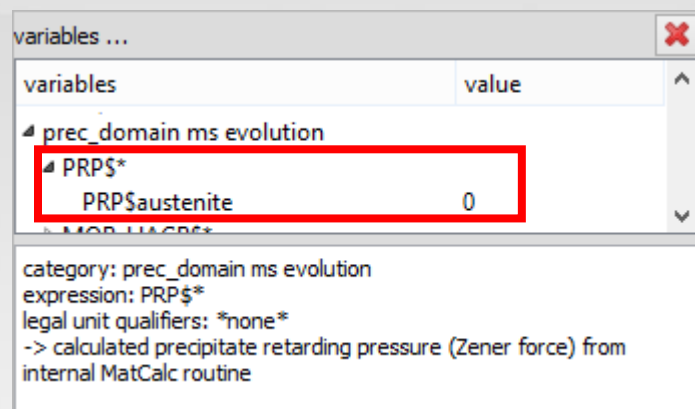
$r_{i,j}$ - Mean radius of class j of precipitate i

k_r - Scaling factor

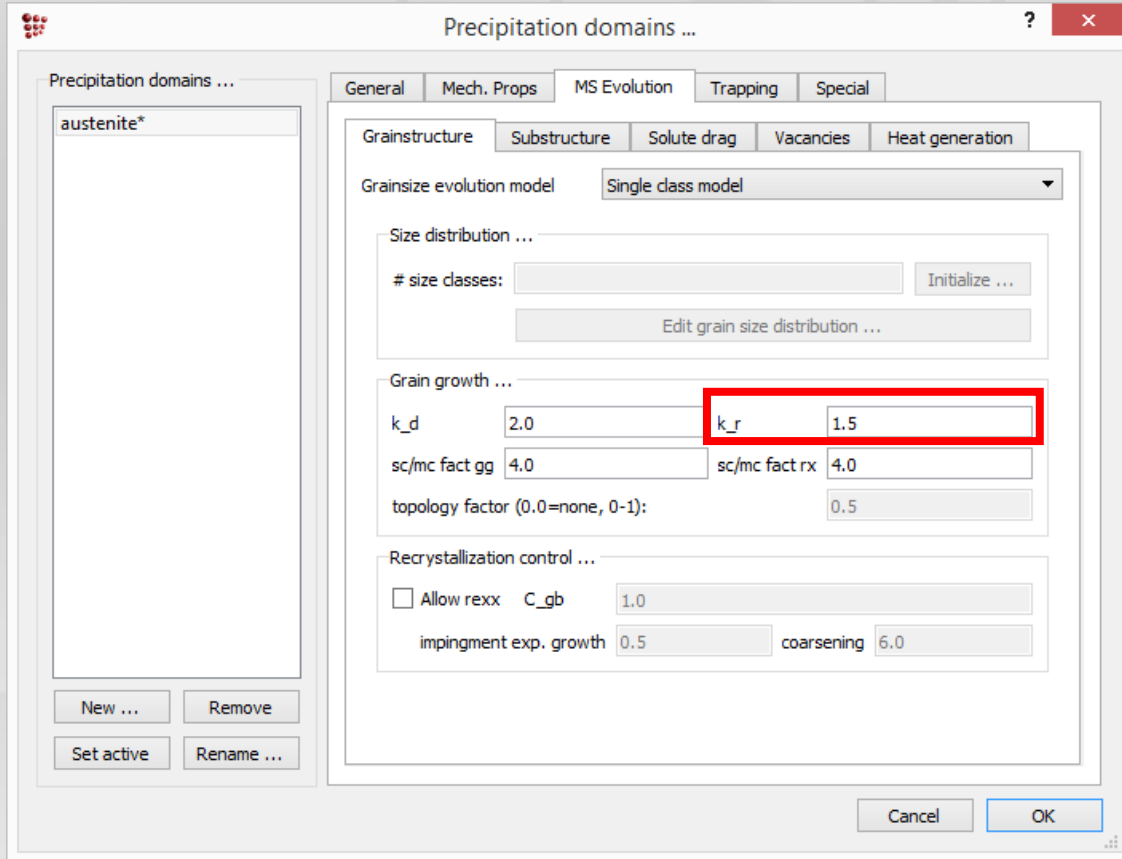
α_i - Pinning factor of precipitate i

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

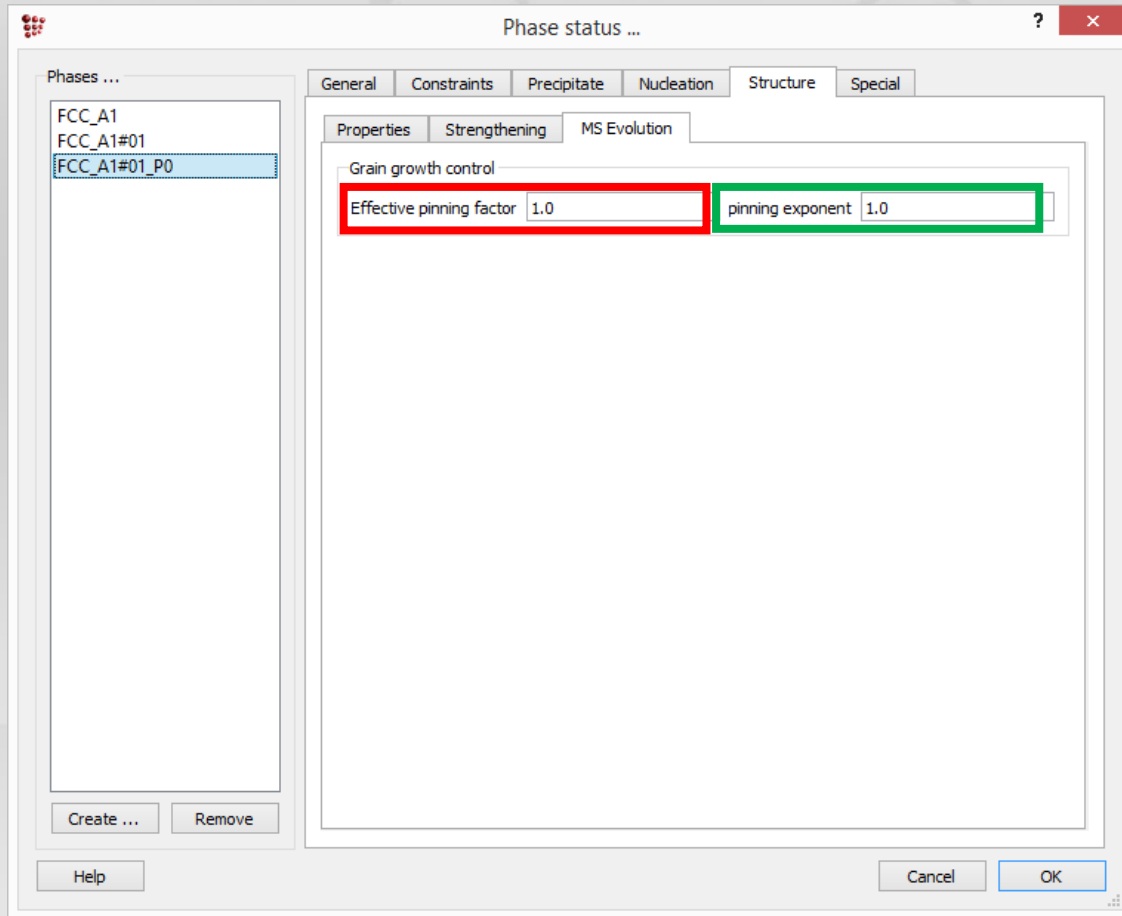
k_r - Scaling factor

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)

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

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k_r - Scaling factor

α_i - Pinning factor of precipitate i

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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

$$P_Z \geq P_D$$

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

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

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

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

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 ...

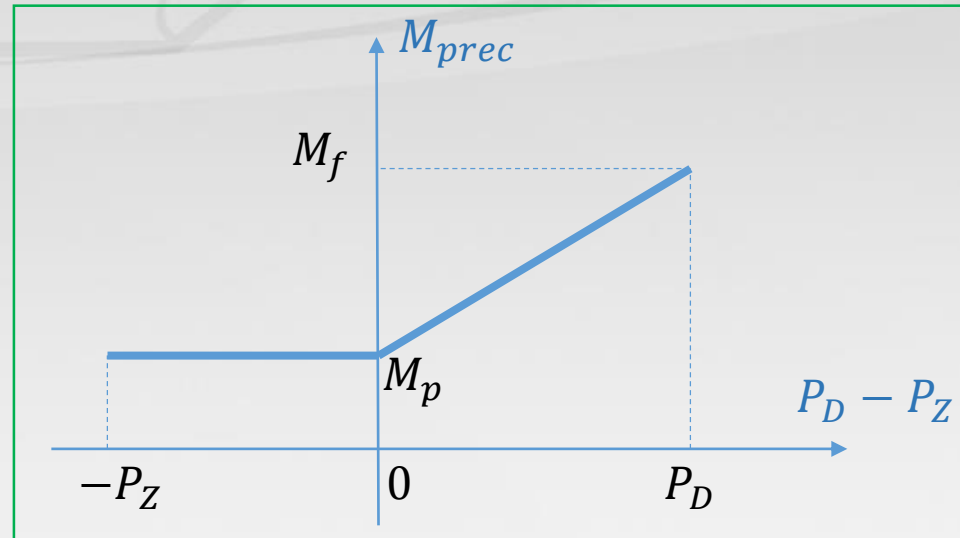
Cancel OK

System with precipitates

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

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

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



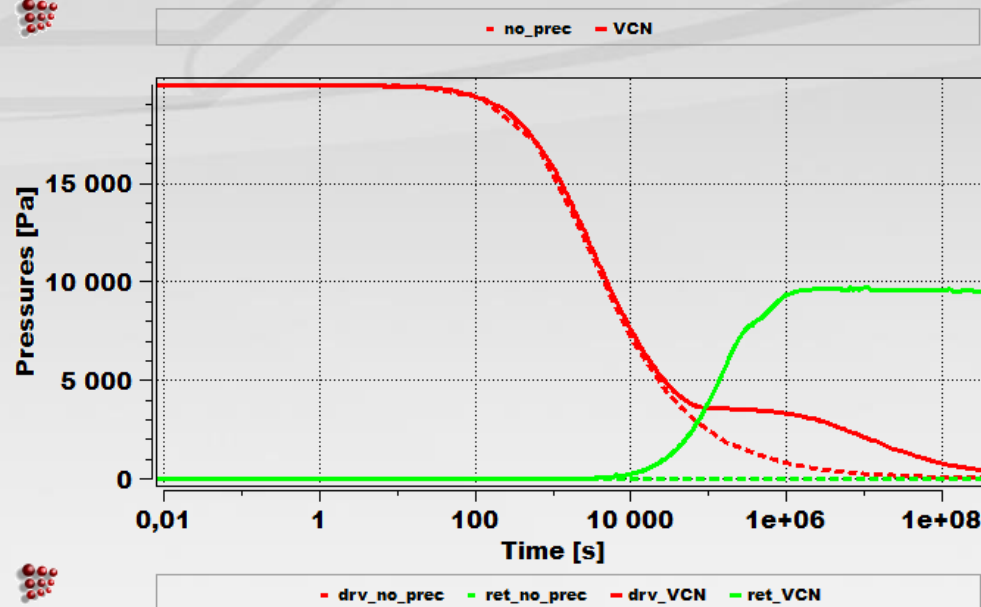
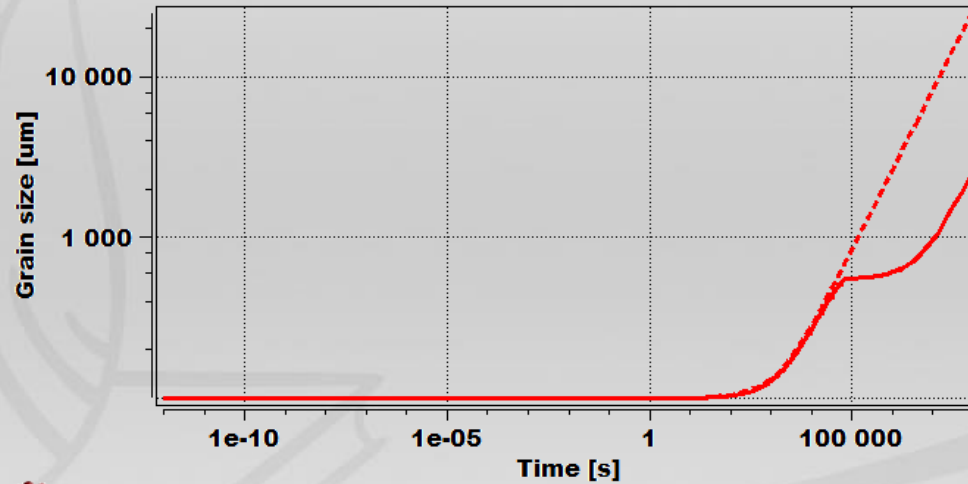
System with precipitates

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

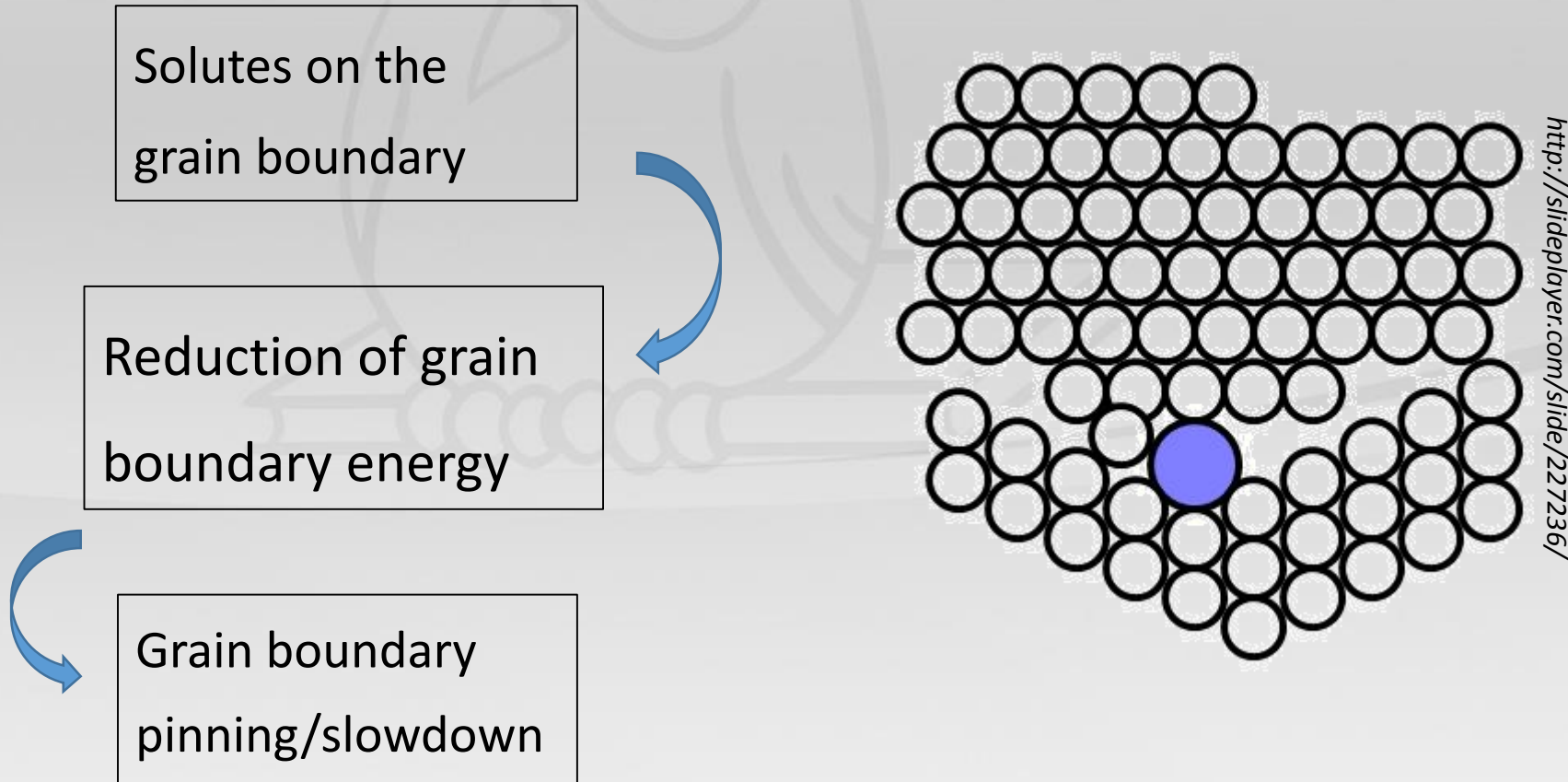
$$M_{prec} = \begin{cases} M_p & P_Z \geq P_D \\ M_p \frac{P_Z}{P_D} + M_f \left(1 - \frac{P_Z}{P_D}\right) & P_Z < P_D \end{cases}$$

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

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



Case with solute drag



Case with solute drag

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

M_{eff} - Effective grain
boundary mobility

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

M_{sd} - Grain boundary
mobility with solute
drag

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

Cahn impurity drag

$$M_{sd} = \sum_i (\alpha_i c_i)^{-1}$$

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

M_{eff} - Effective grain boundary mobility

M_{sd} - Grain boundary mobility with solute drag

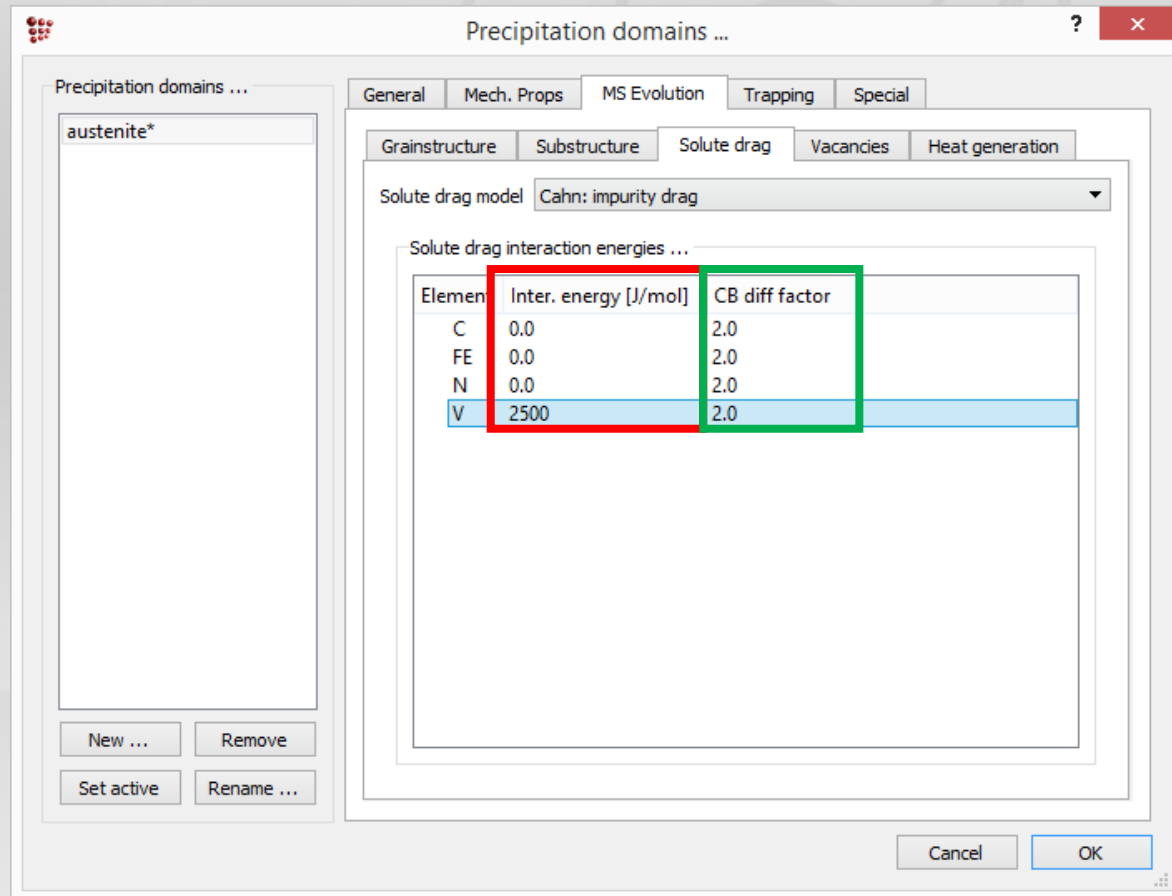
α_i - Inverse mobility

c_i - Solute concentration on the grain boundary

E_i - Grain boundary/solute interaction energy

D_{CB} - Cross boundary diffusion coefficient

Cahn impurity drag



α_{eff} - Effective grain boundary mobility

α_{sd} - Grain boundary mobility with solute drag

α_i - Inverse mobility

c_i - Solute concentration on the grain boundary

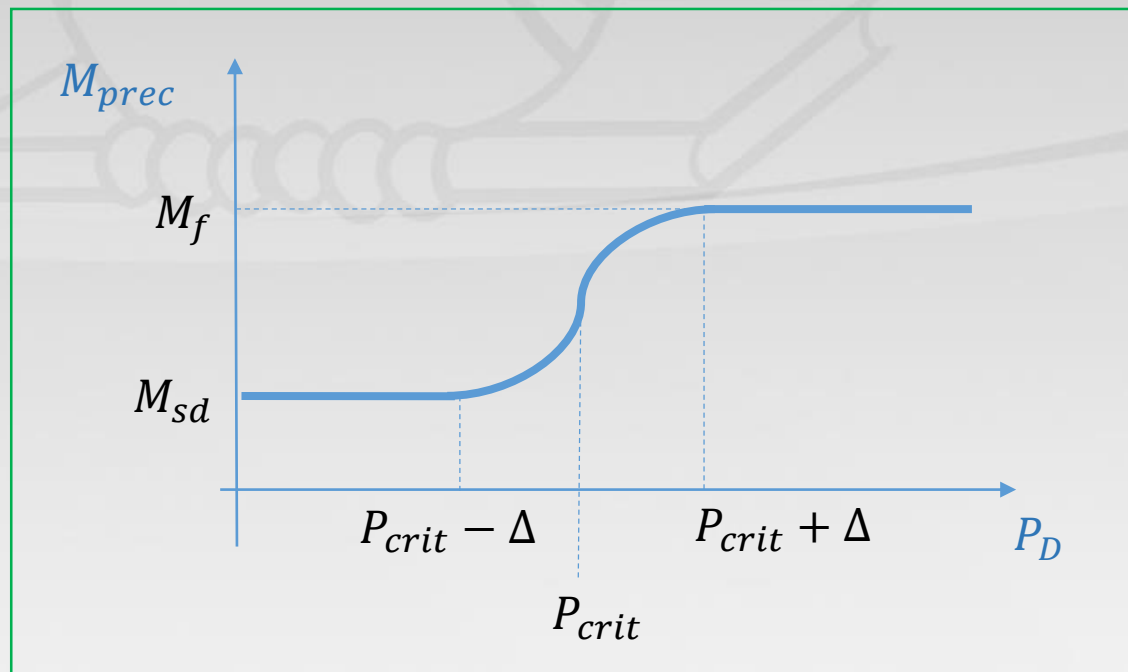
E_i - Grain boundary/solute interaction energy

D_{CB} - Cross boundary diffusion coefficient (~tracer diff.)

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

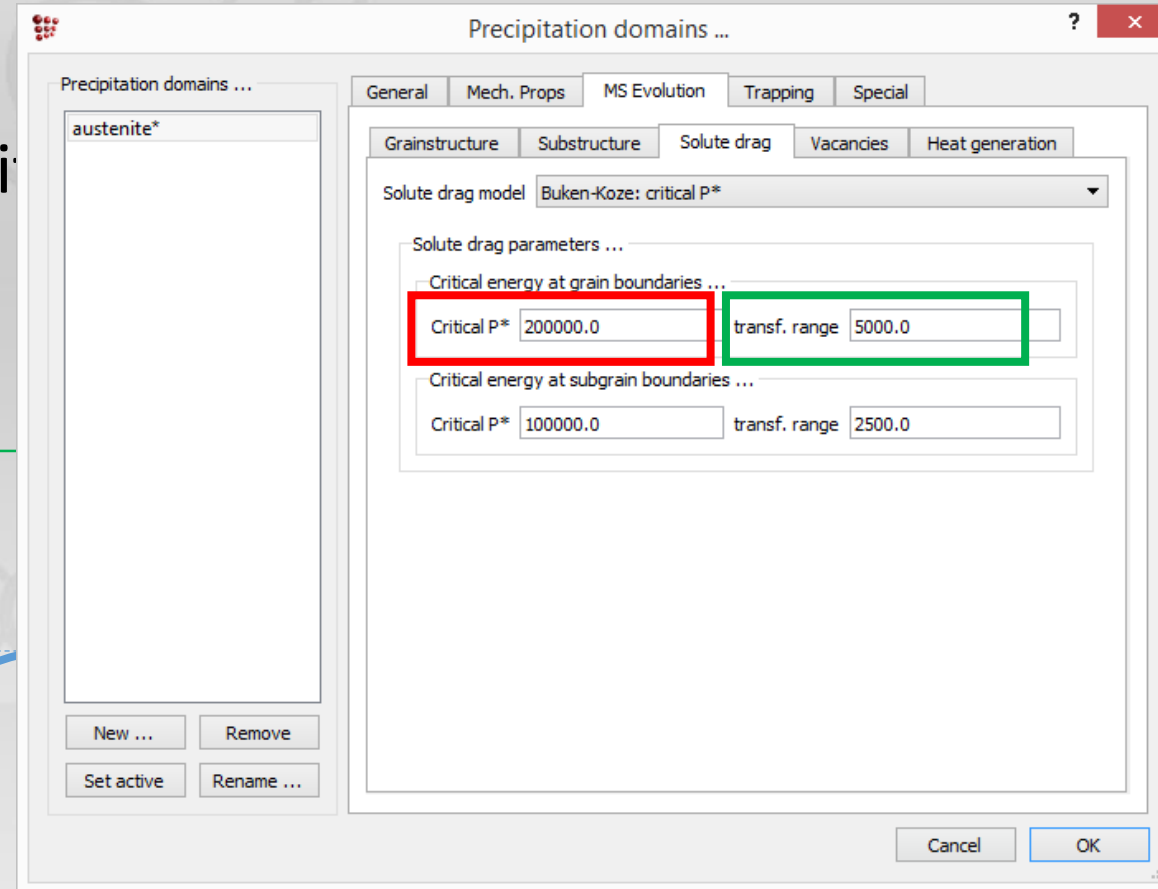
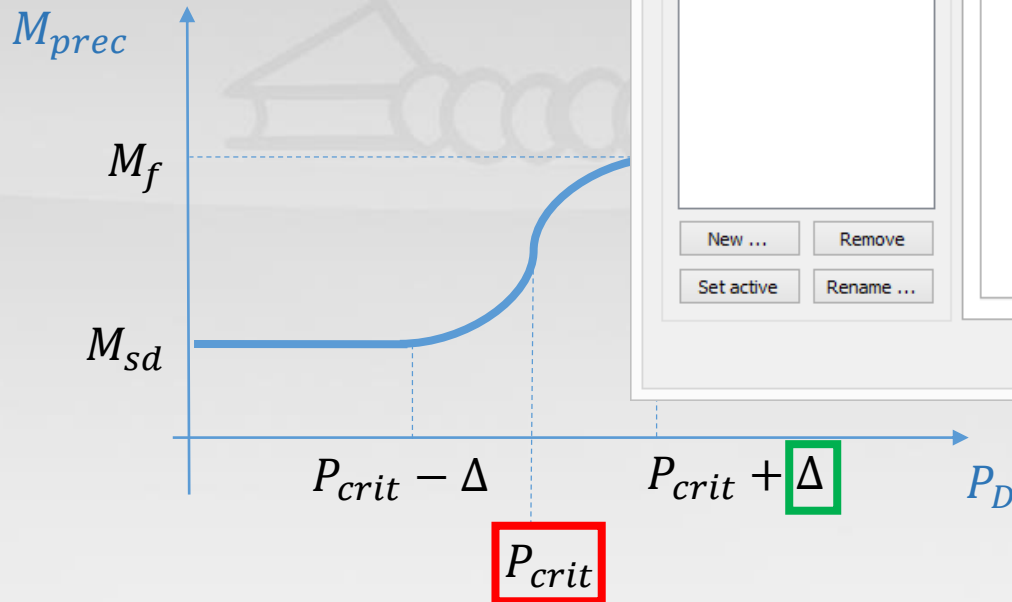
Buken-Kozeschnik critical pressure

- Continuous mobility change dependent on the driving pressure.



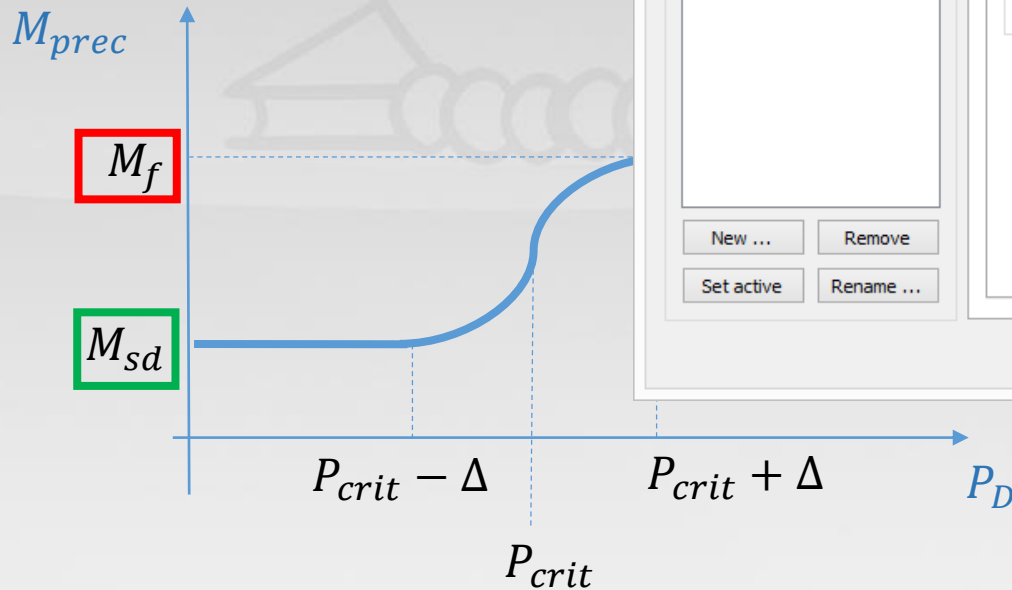
Buken-Kozeschnik critical pressure

- Continuous mobility pressure.



Buken-Kozeschnik critical pressure

- Continuous mobility pressure.



Precipitation domains ...

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 ...

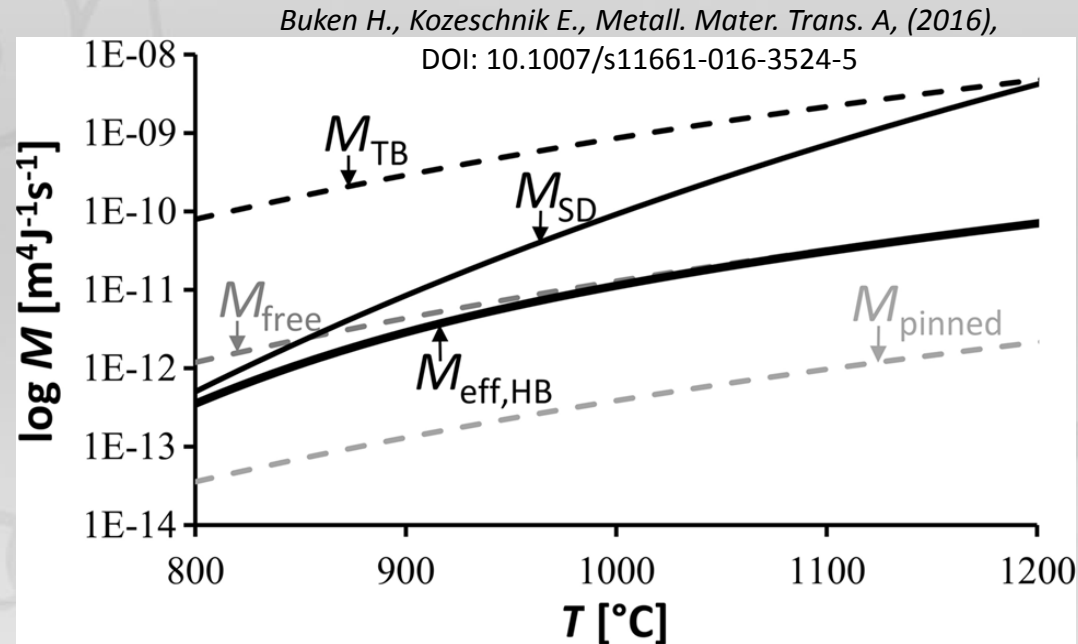
Cancel OK

Case with solute drag

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

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

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



variables ...	
variables	value
prec_domain ms evolution	
GB_MOB_SD\$	
GB_MOB_SD\$austenite	7.40552e-14
category: prec_domain ms evolution	
expression: GB_MOB_SD\$austenite	
legal unit qualifiers: *none*	
-> pinned (solute drag) grain boundary mobility	

Acknowledgments

- Heinrich Buken
- Yao Shan

