MatCalc
Engineering

Single class grain growth model in MatCalc 6

(MatCalc 6.00.0206)

P. Warczok

Grain growth

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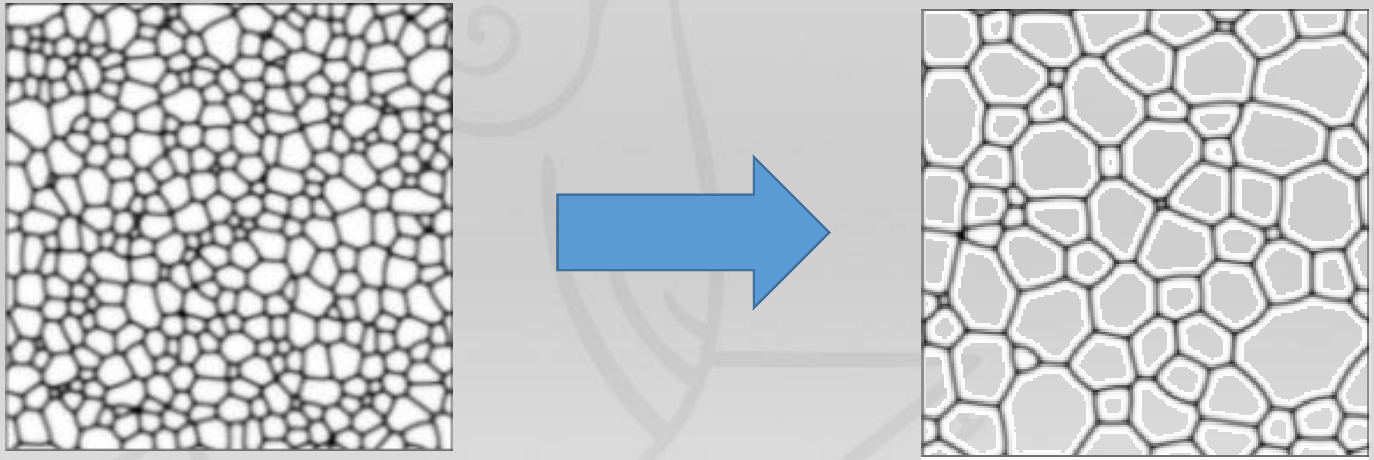

- Tendency - to minimize:
  - grain surface area
  - specific grain boundary energy

Grain growth kinetics

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- General idea: Mobility & Driving force

$$\dot{D} = \frac{dD}{dt} = MP_D$$

$\dot{D}$ - Grain size growth rate

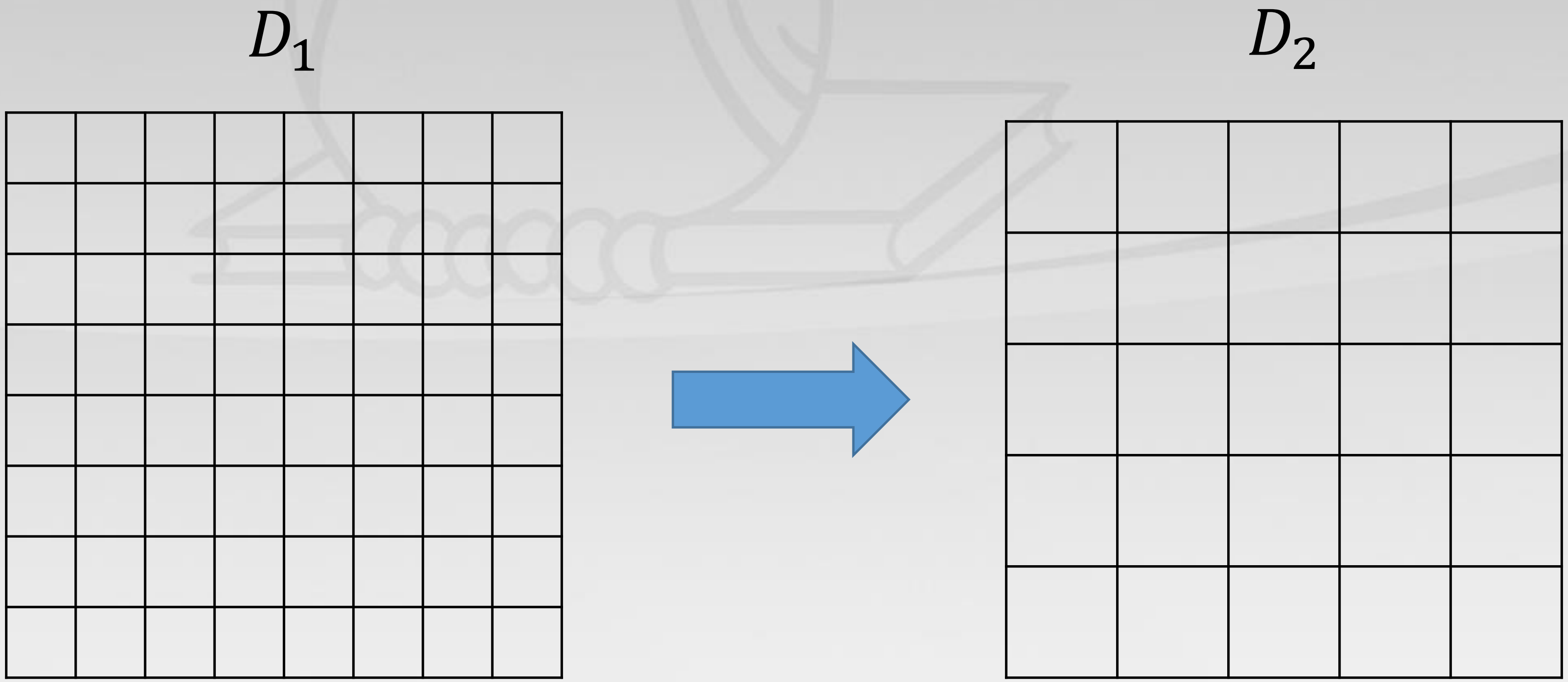
M - Grain boundary mobility

P_D - Driving force/pressure for grain growth

t - Time

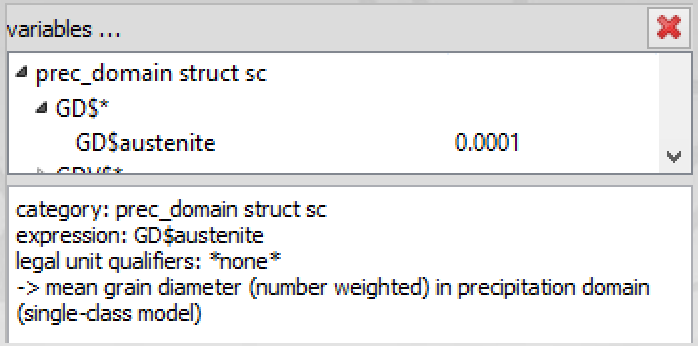
Single class grain growth

- Single quantity: Mean grain size



Single class grain growth

- Single quantity: Mean grain size



Growth driving pressure

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- 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

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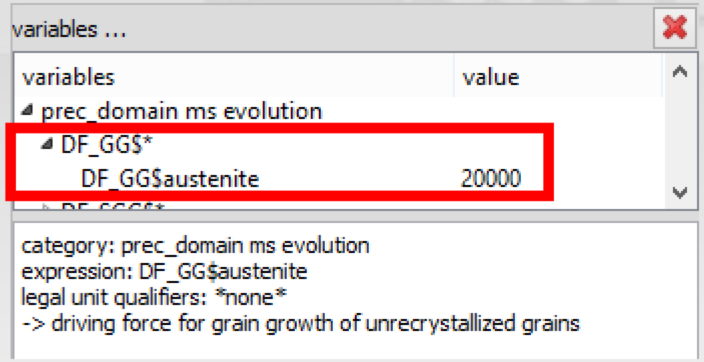
- Driving pressure dependent on
  - Grain interface energy
  - Grain size



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

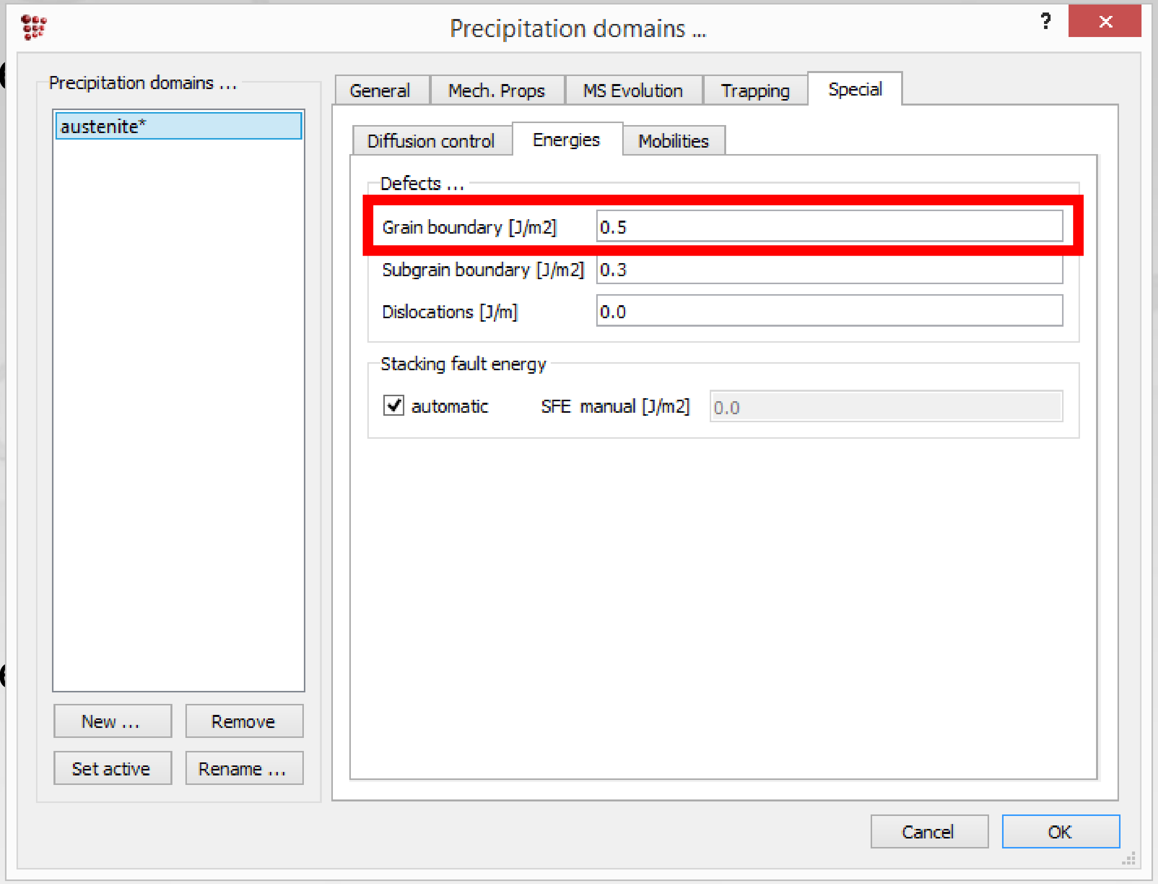
γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor

Growth driving pressure

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



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Growth driving pressure

MatCalc Engineering

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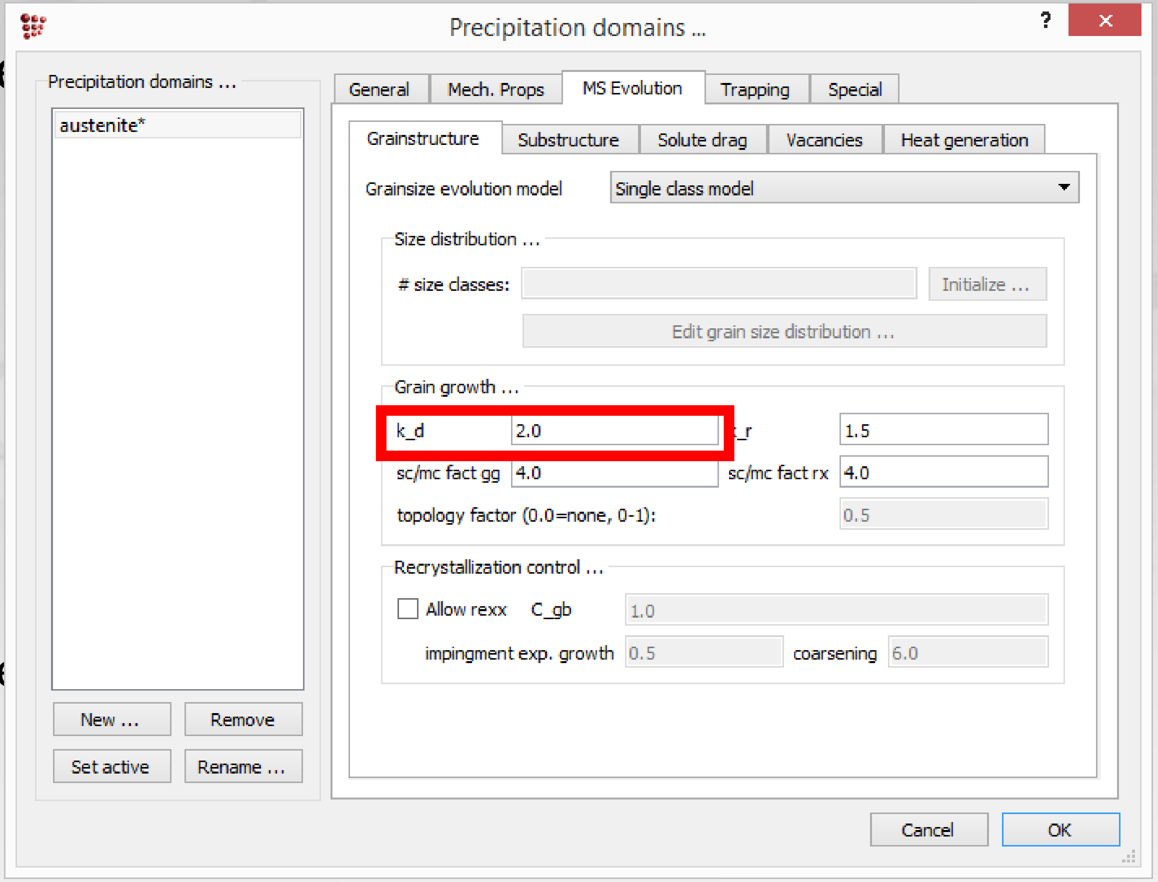

$$P_D = 2\boxed{k_d}\frac{\gamma_{HA}}{D}$$

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Mobility – general approach

MatCalc Engineering

- General form $$M = \boxed{M_0} exp(-\boxed{Q}/RT)$$

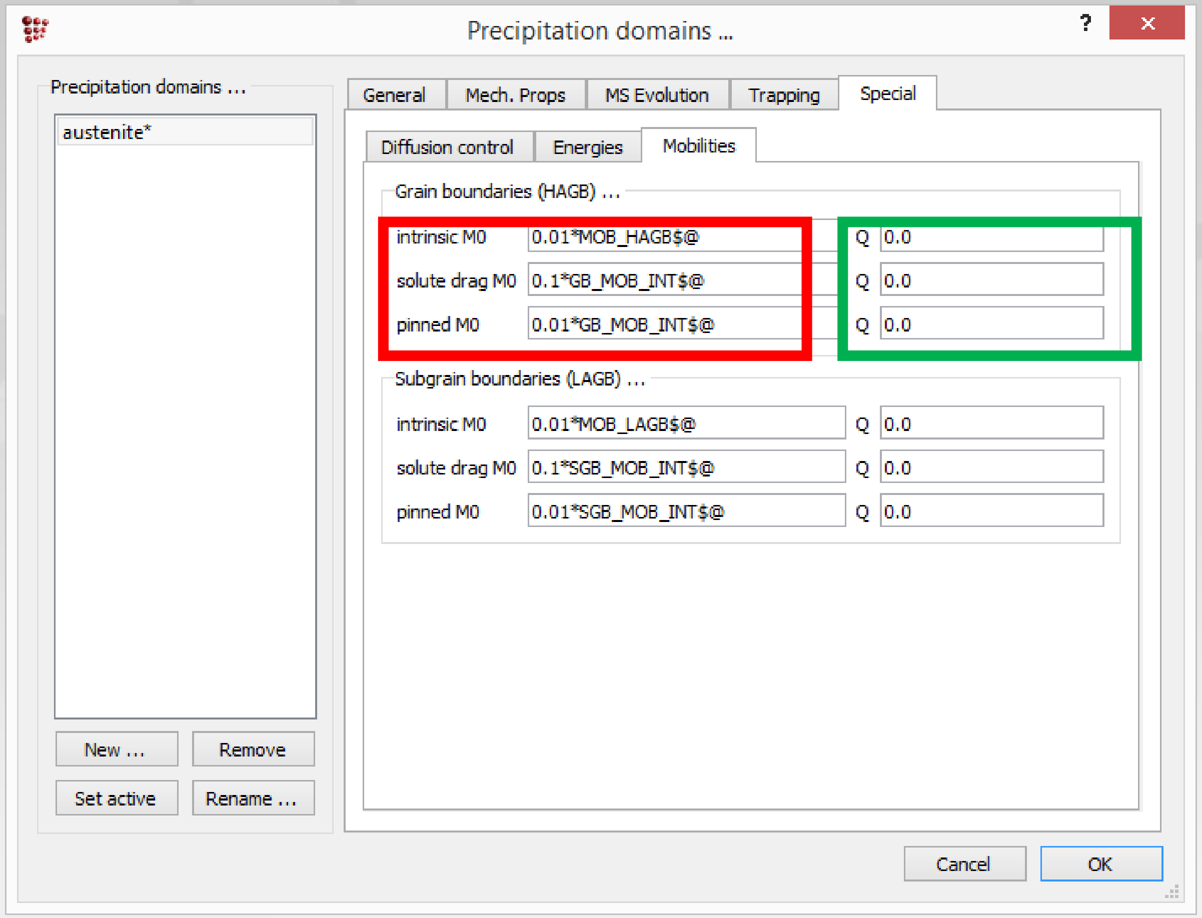
M - Grain boundary mobility

M_0 - Mobility pre-factor

Q - Activation energy

R - Gas constant

T - Temperature



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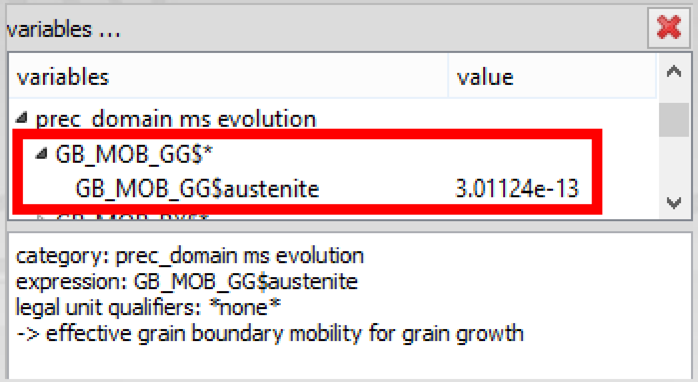

No obstacles

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

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

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

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

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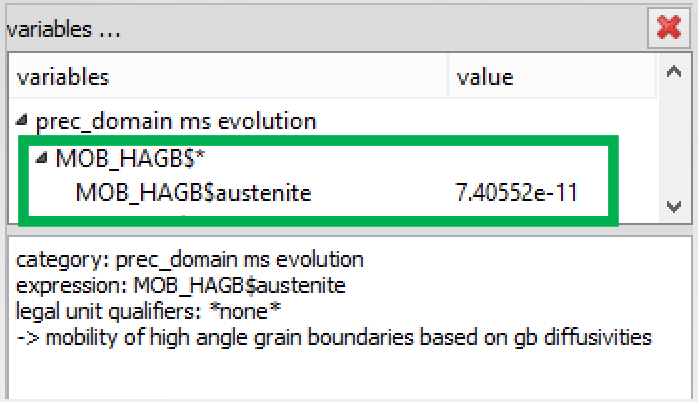

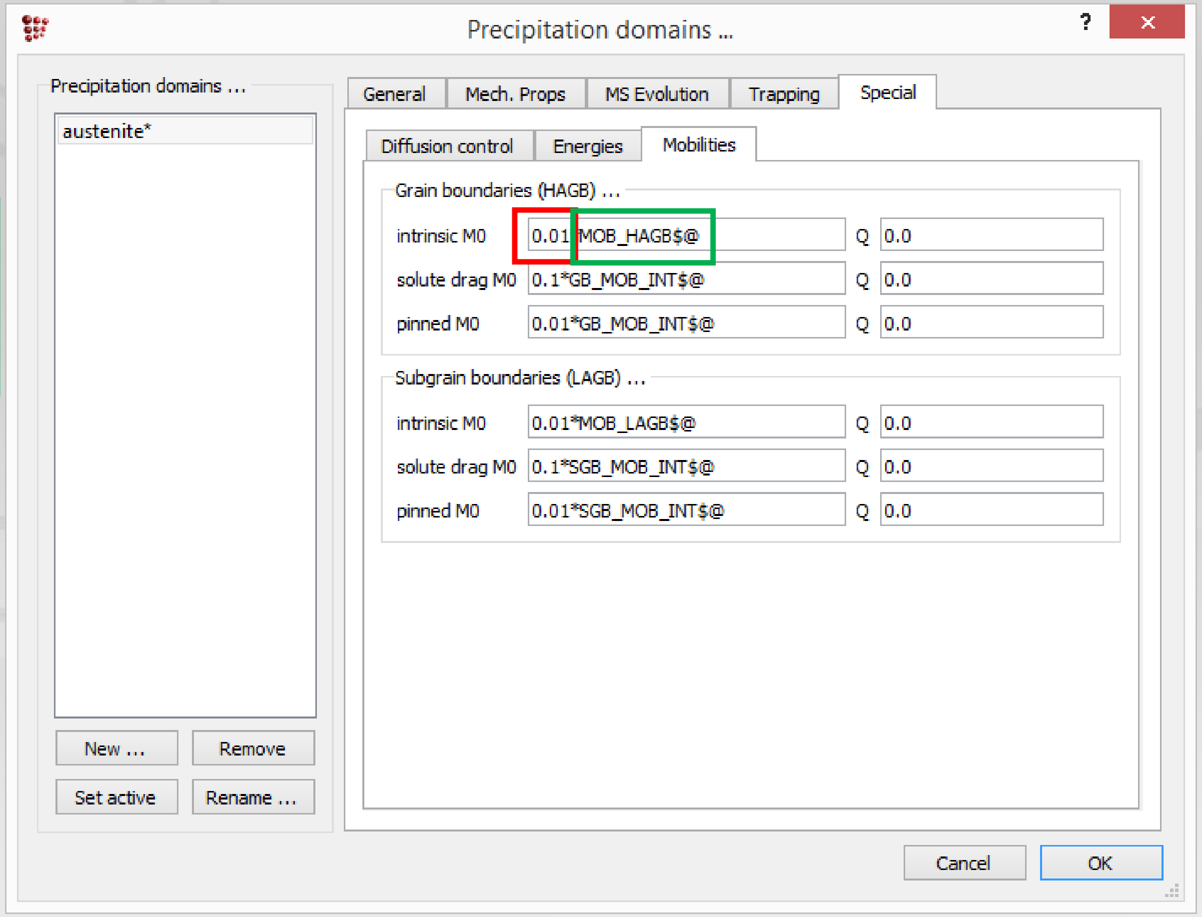

No obstacles

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

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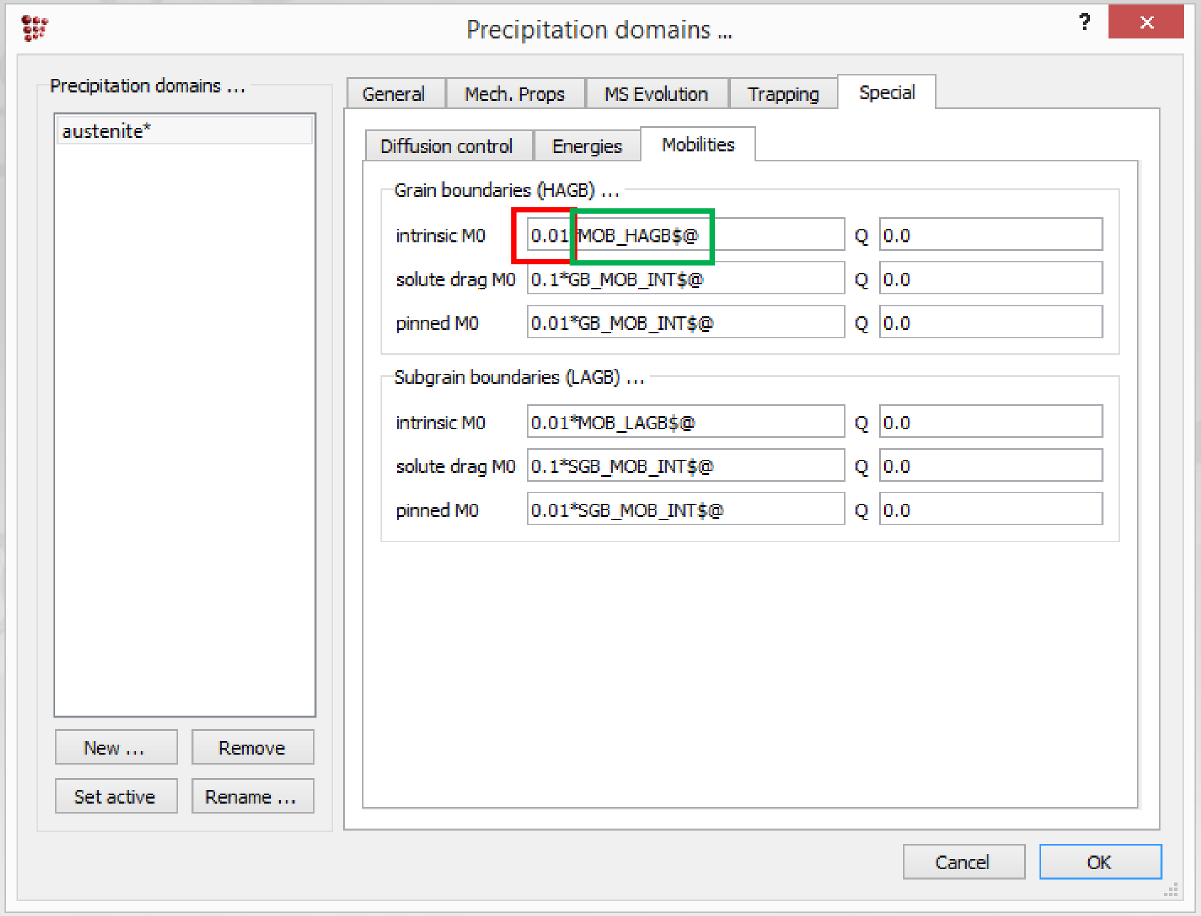

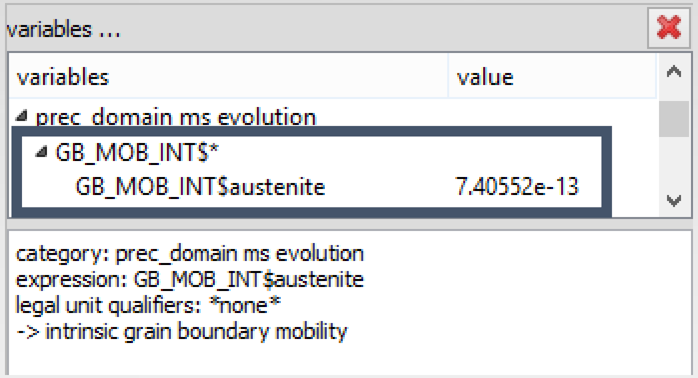

No obstacles

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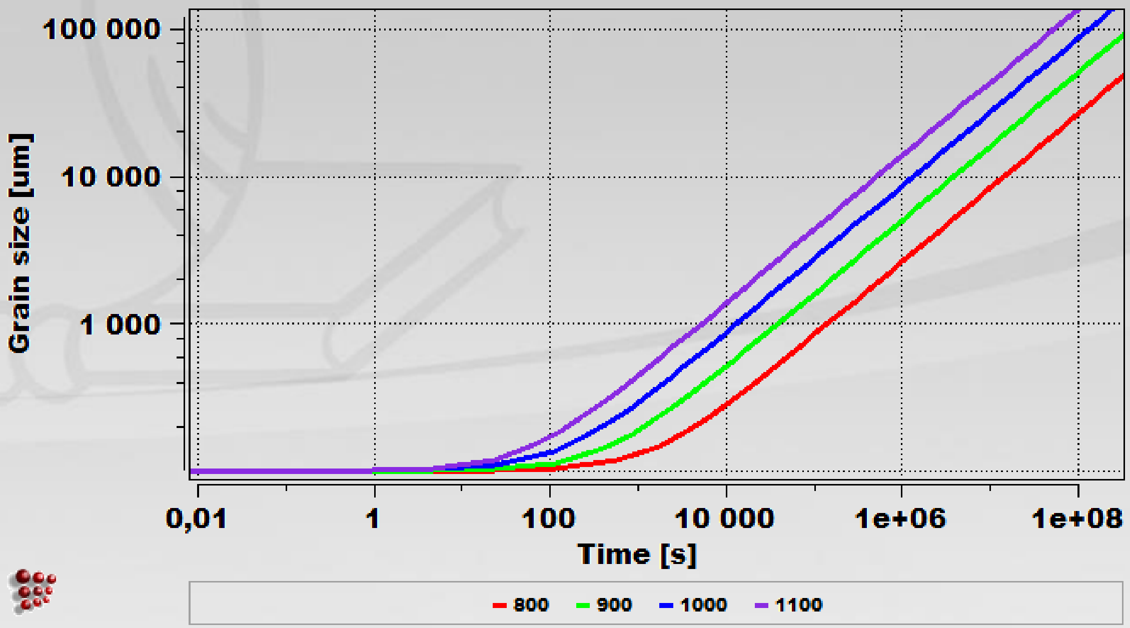
$$\dot{D} = M_f P_D$$

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

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

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



System with precipitates

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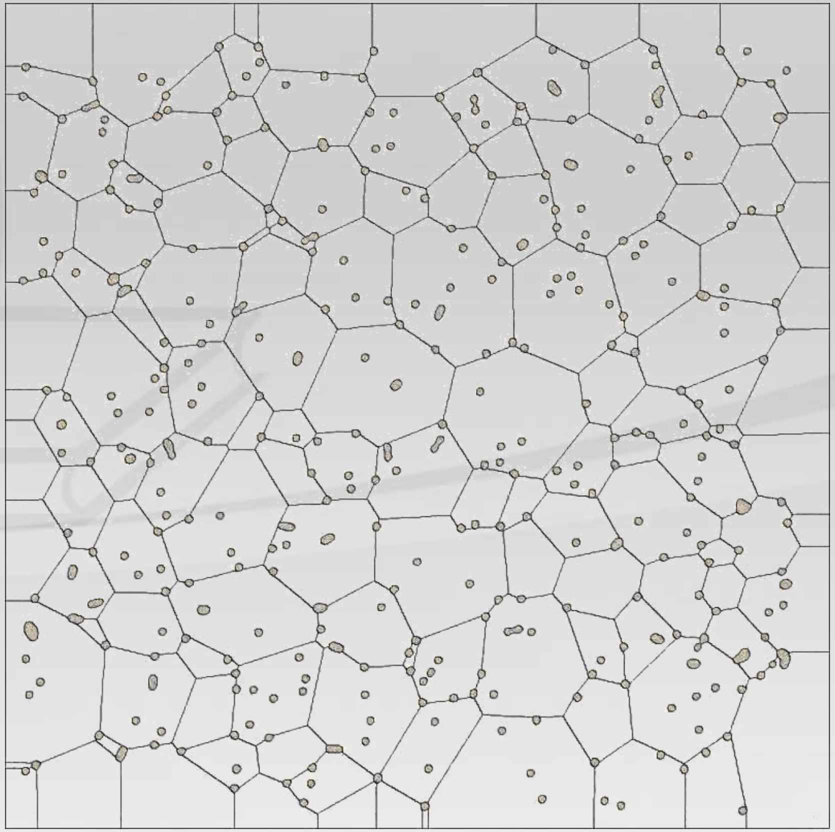
Grain boundary movement

Precipitates on the grain boundary

Reduction of grain boundary energy

Grain boundary pinning/slowdown



https://i.ytimg.com/vi/8EET_T6LIWY/maxresdefault.jpg

System with precipitates

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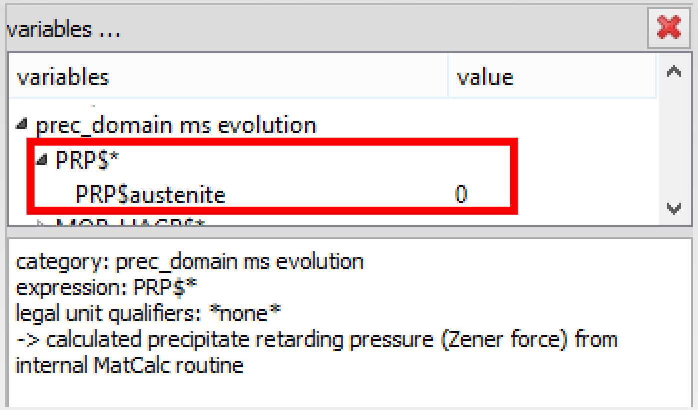
- Growth retarding pressure dependent on
  - Precipitate phase fraction
  - Precipitate radius

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



P_Z - Pinning force (Zener force)

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

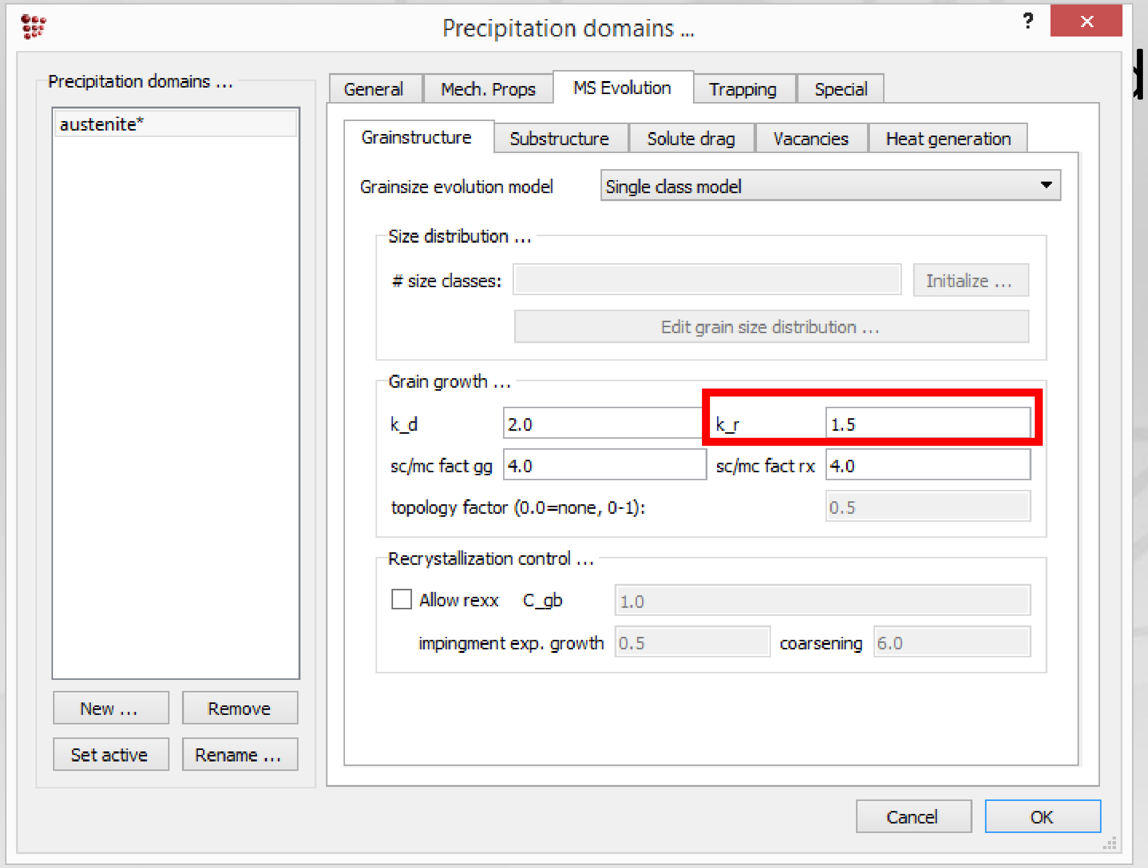
$r_{i,j}$ - Mean radius of class *j* of precipitate *i*

k_r - Scaling factor

α_i - Pinning factor of precipitate i

β_i - Pinning exponent of precipitate i

System with precipitates



dent on

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System with precipitates

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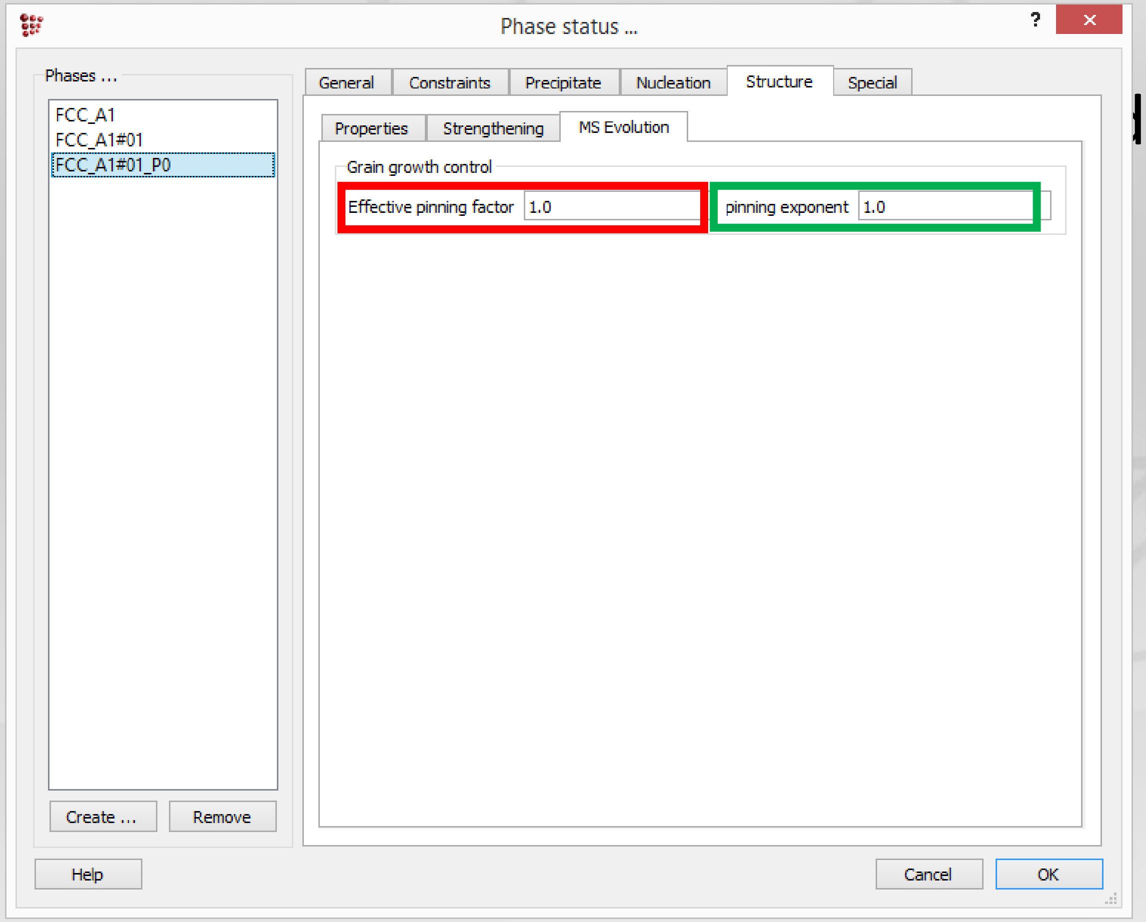
Engineering



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System with precipitates

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

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

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

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

M_p - Grain boundary mobility for pinned interface

η_p - Scaling factor

System with precipitates

MatCalc Engineering

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

$$\boxed{P_Z \geq P_D}$$

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

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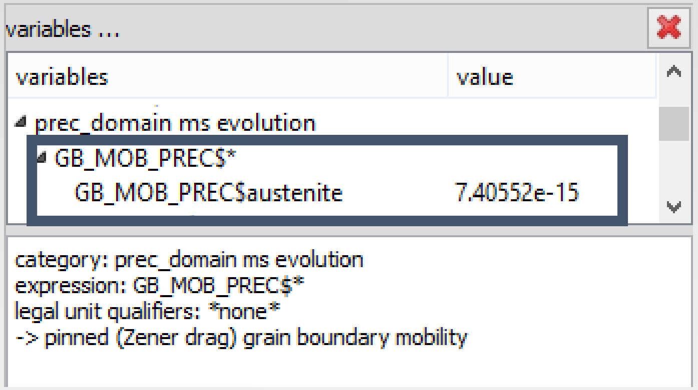

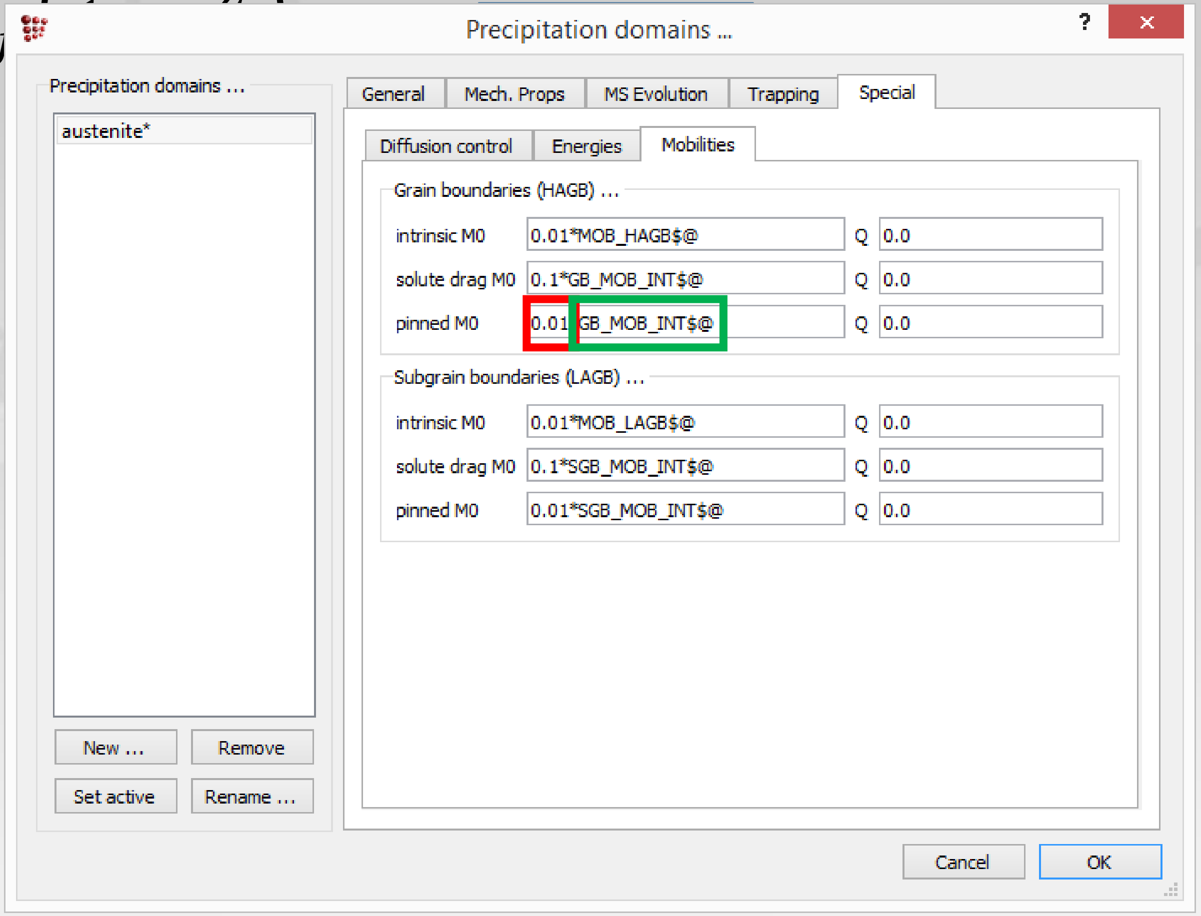

System with precipitates

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

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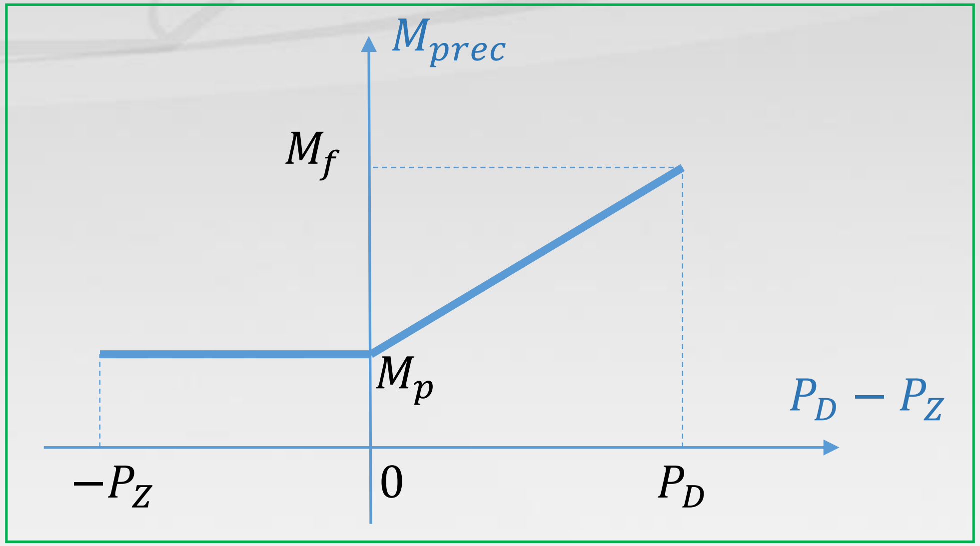

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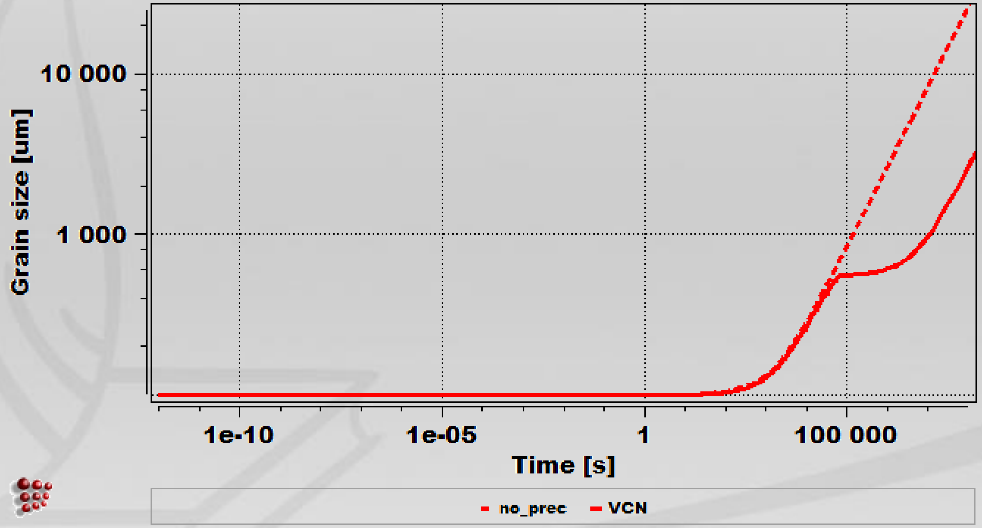

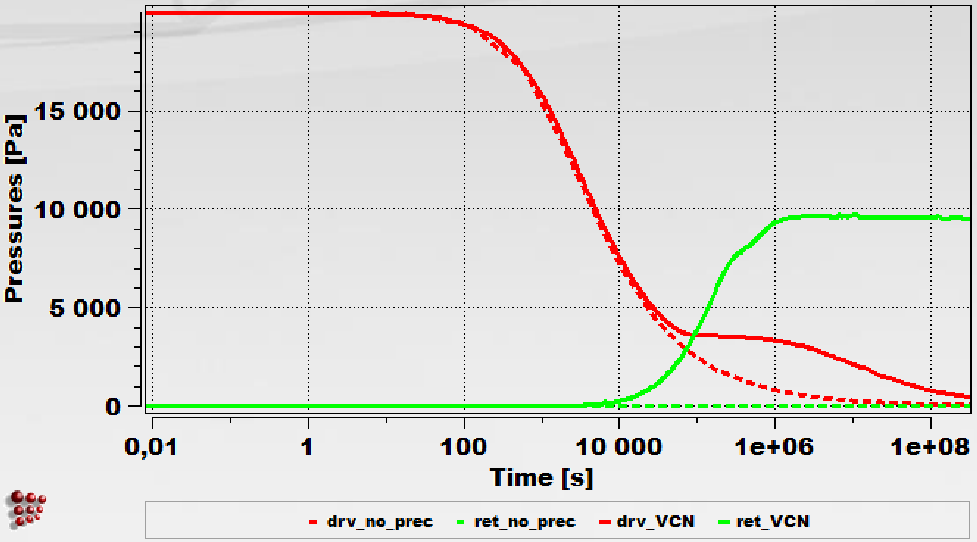

Case with solute drag

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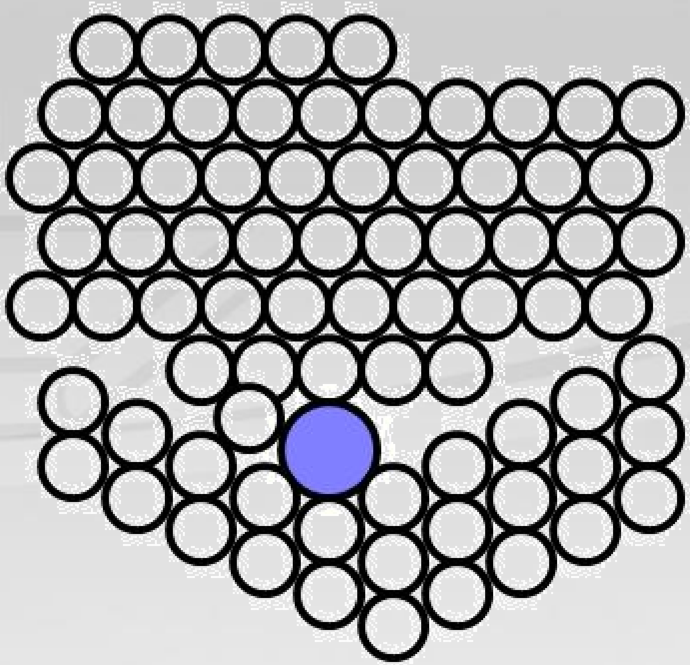
Solutes on the grain boundary

Reduction of grain boundary energy

Grain boundary pinning/slowdown



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

Case with solute drag

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

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

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

M_{eff} - Effective grain boundary mobility

M_{sd} - Grain boundary mobility with solute drag

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

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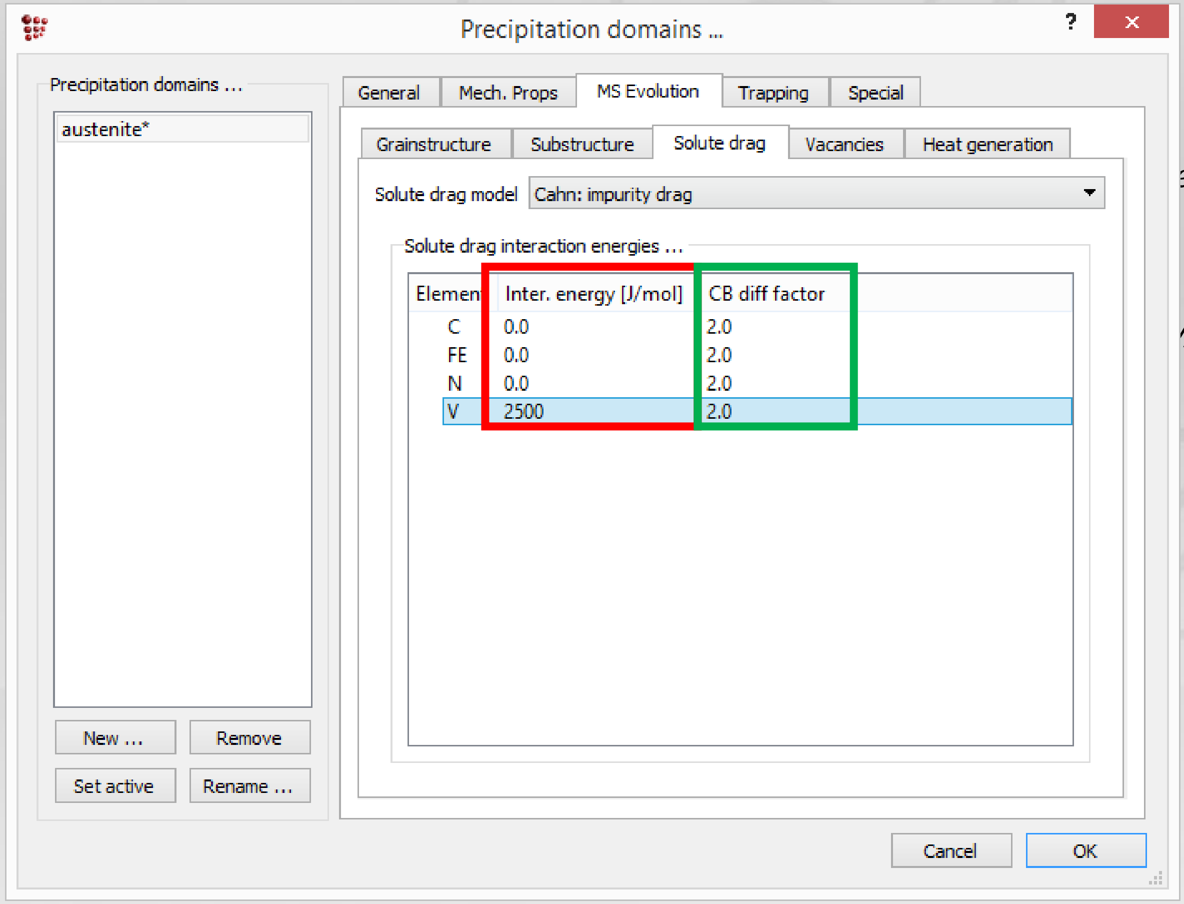

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$_{eff}$ - Effective grain boundary mobility

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

Buken-Kozeschnik critical pressure

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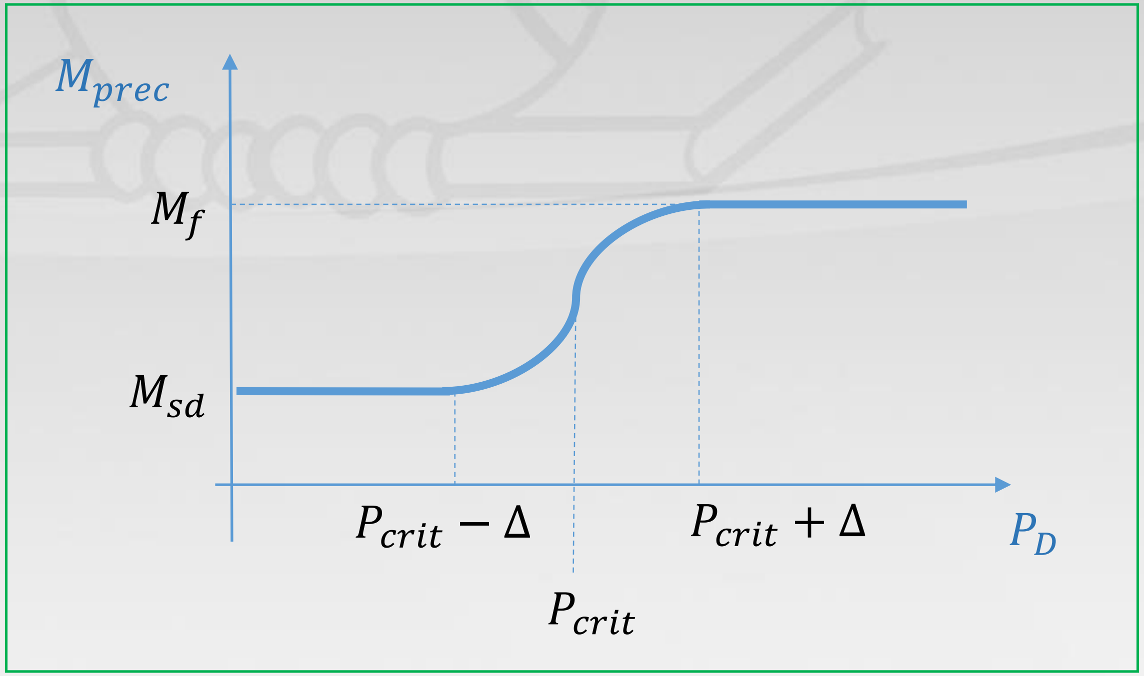
- Continuous mobility change dependent on the driving pressure.



Buken-Kozeschnik critical pressure

- Continuous mobili
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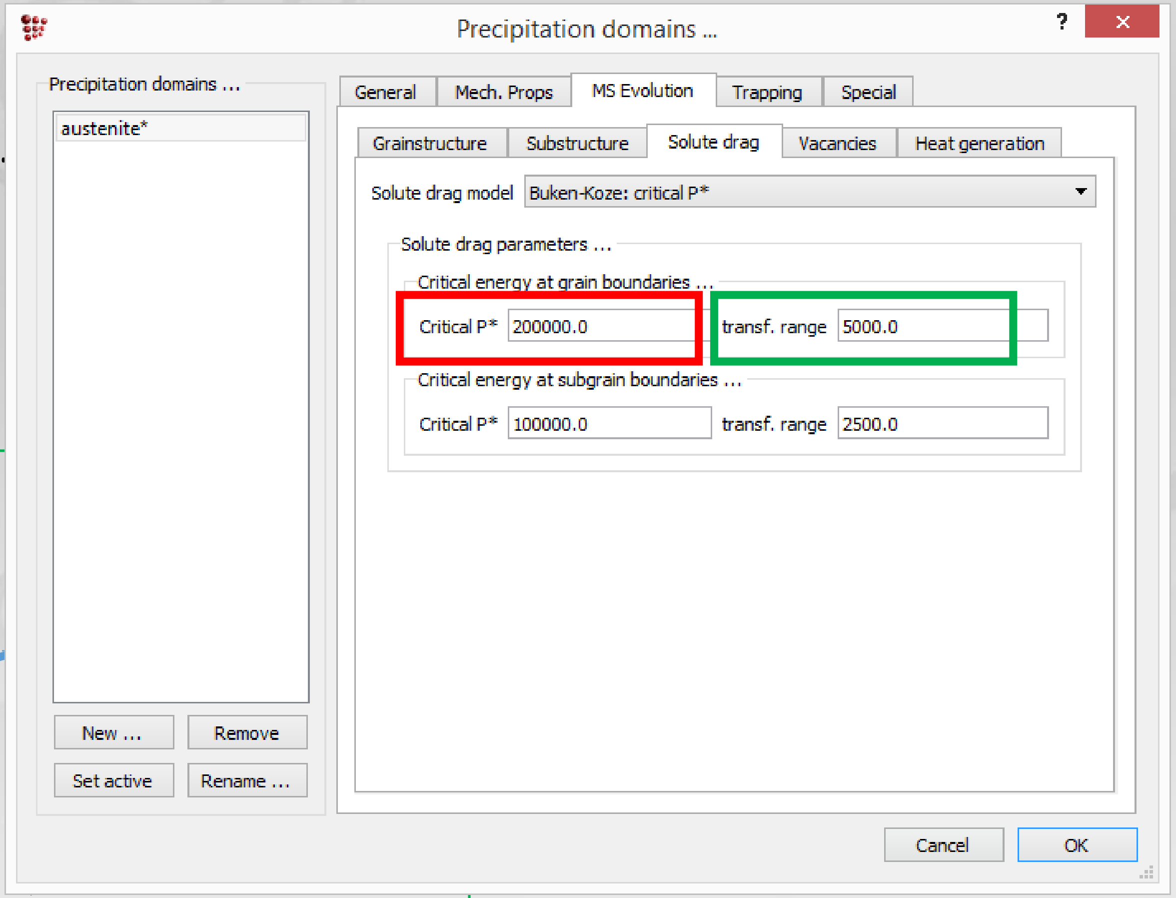

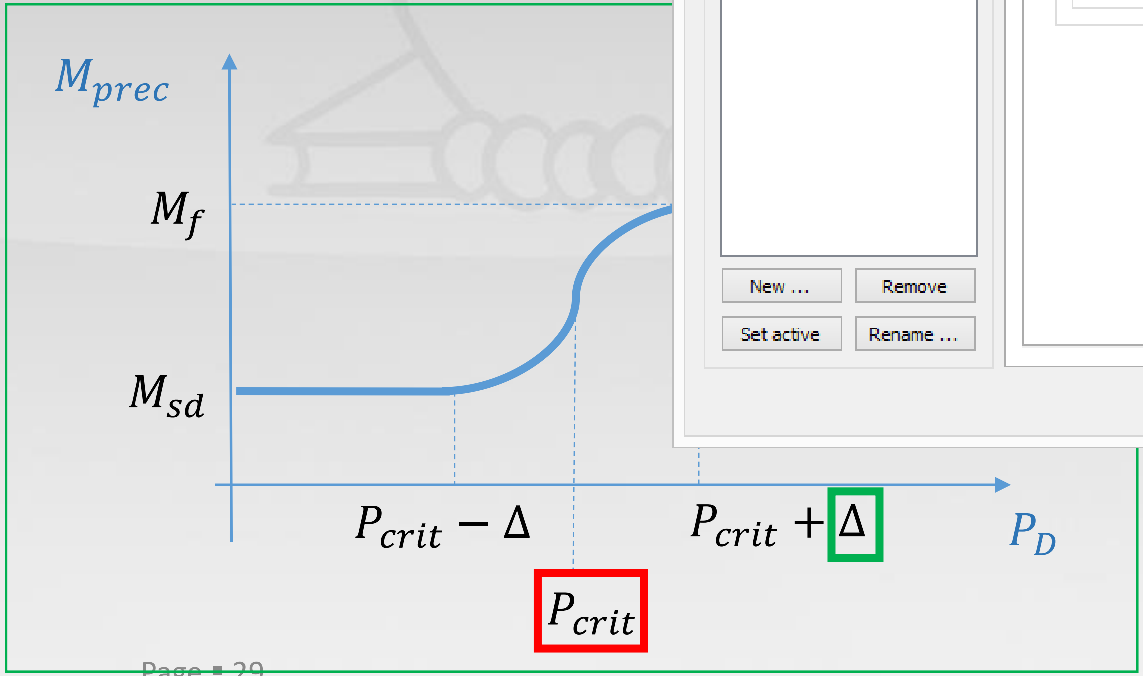

Buken-Kozeschnik critical pressure

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- Continuous mobili

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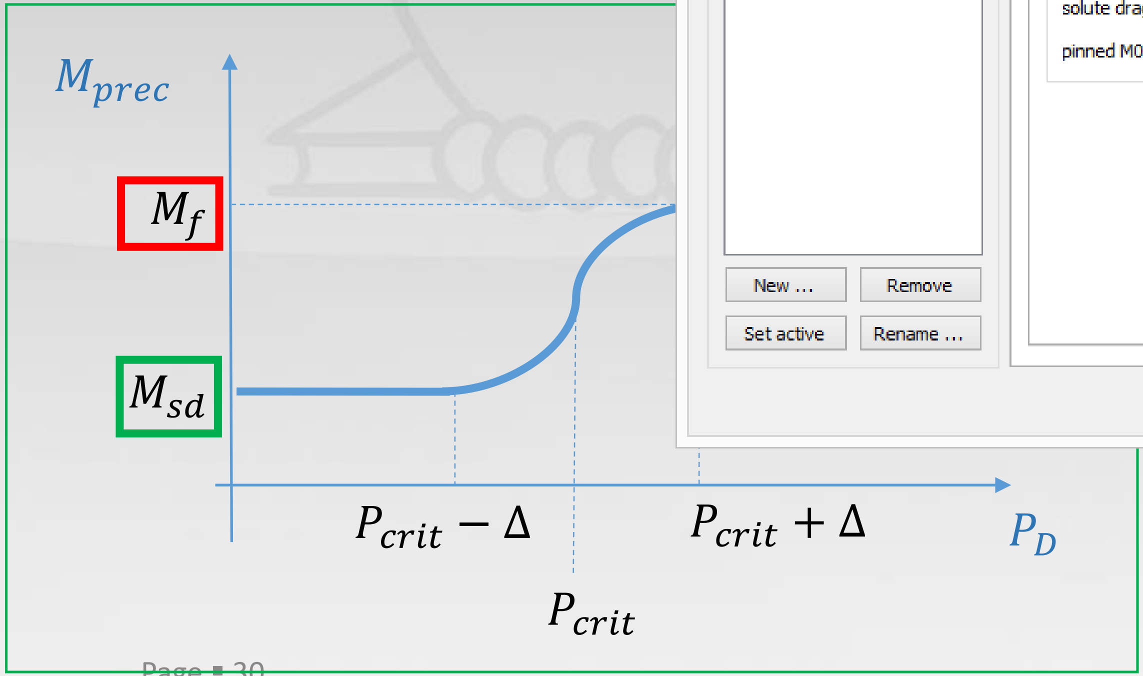
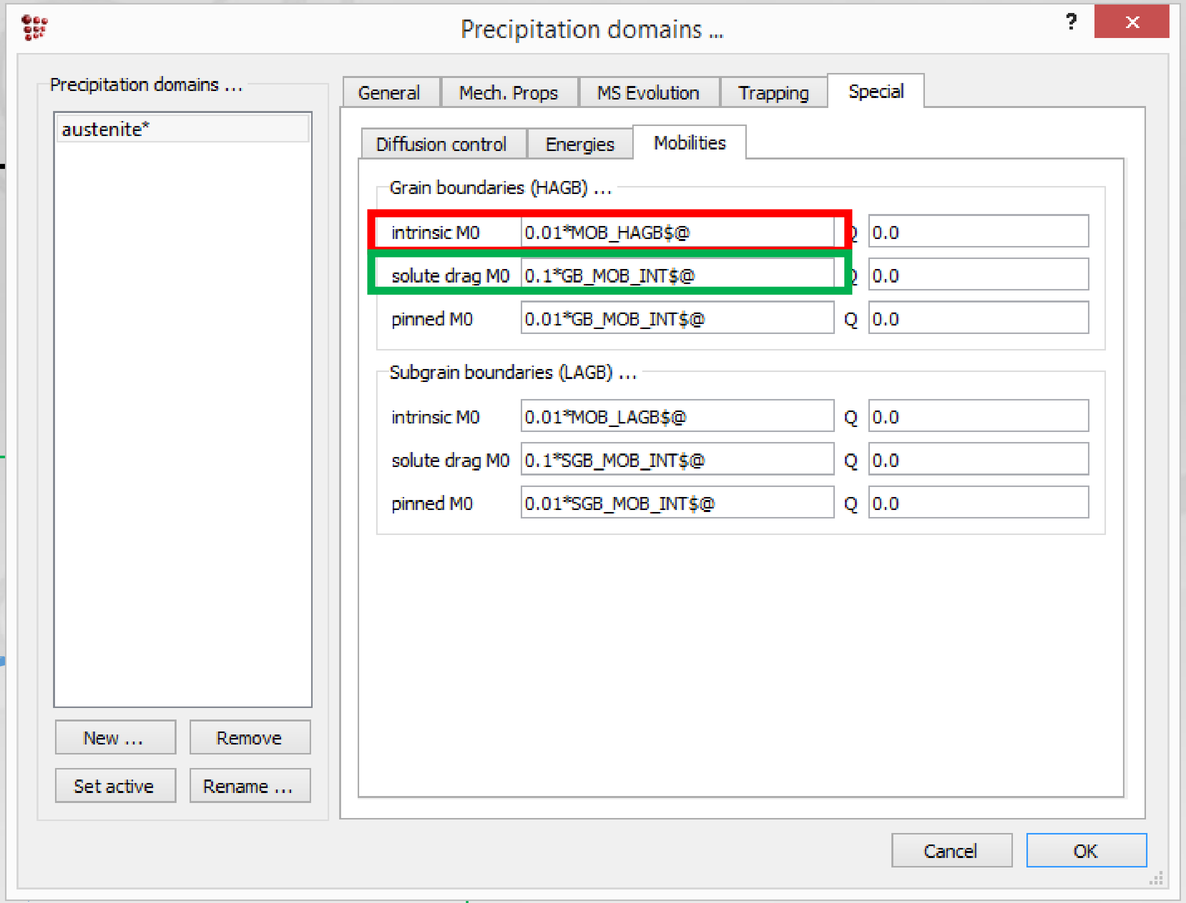




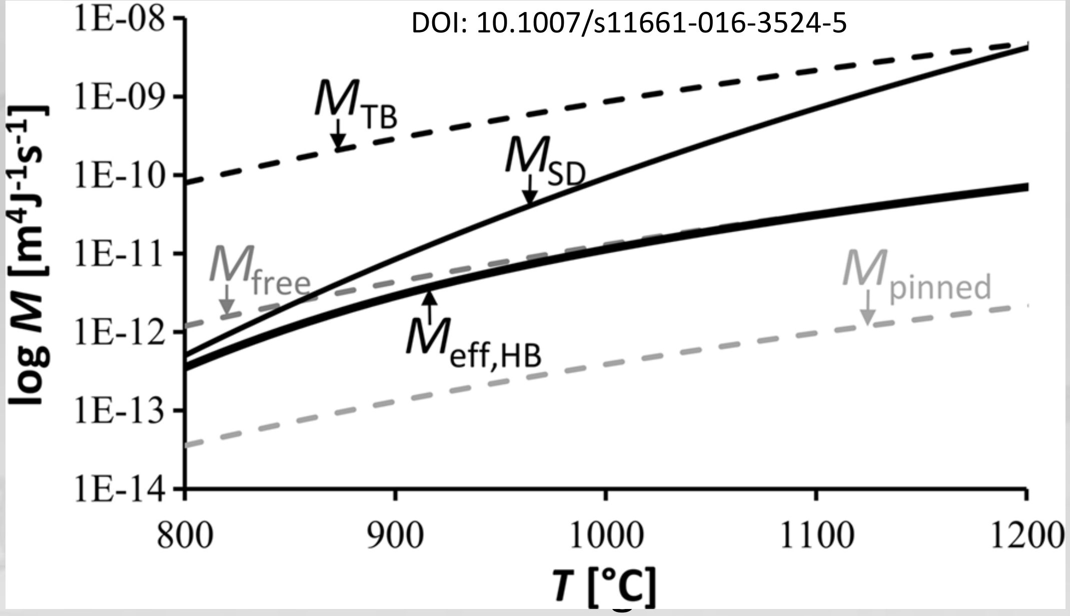
Case with solute drag

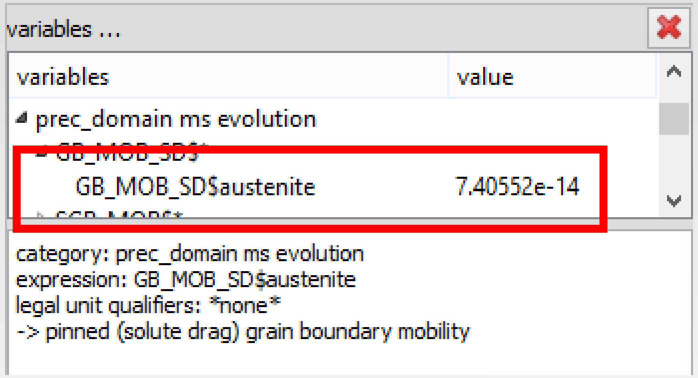
$$\dot{D} = M_{eff} P_D$$

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

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

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





Acknowledgments

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- Heinrich Buken
- Yao Shan