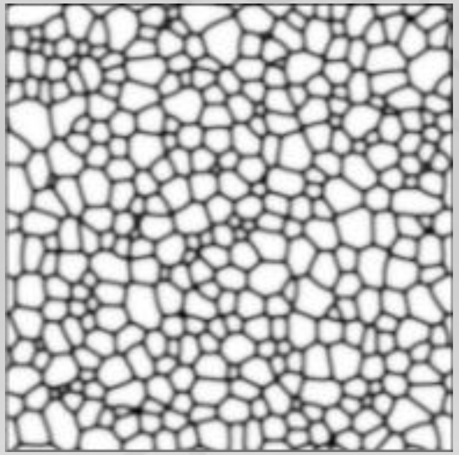
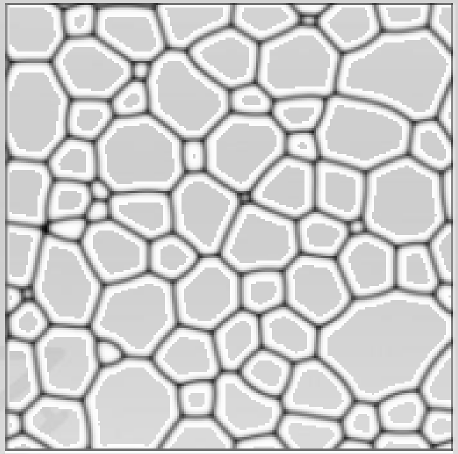
Single class grain growth model in MatCalc 6

(MatCalc 6.01.1000)

P. Warczok

Grain growth





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

Grain growth kinetics

MatCalc Engineering

- General idea: Mobility & Driving force

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

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

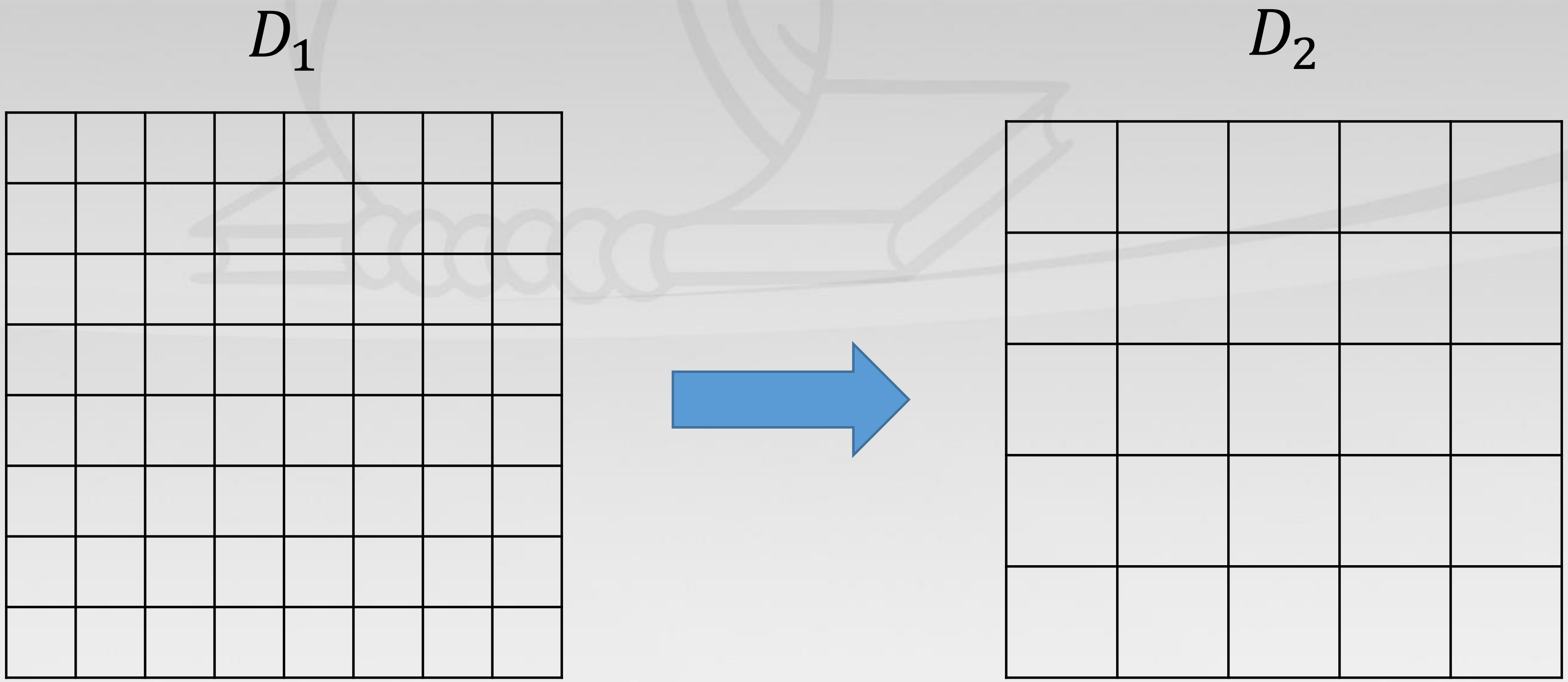
M - Grain boundary mobility

P_D - Driving force/pressure for grain growth

t - Time

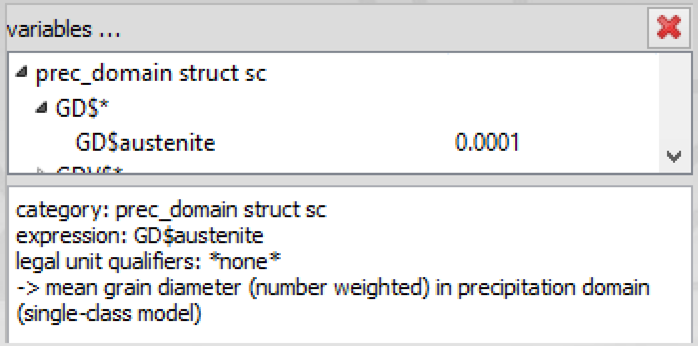
Single class grain growth

- Single quantity: Mean grain size



Single class grain growth

- Single quantity: Mean grain size



Growth driving pressure

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

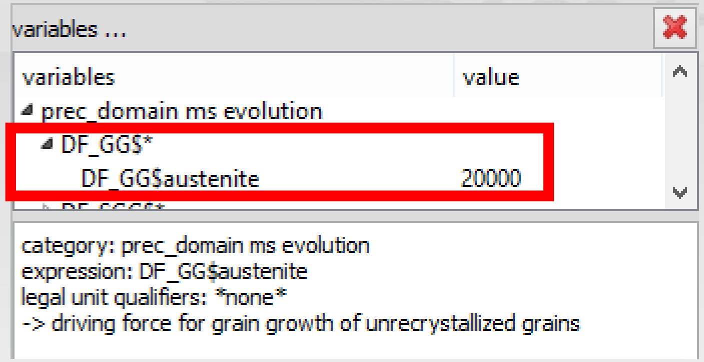
$$P_D \sim \frac{\gamma_{HA}}{D}$$

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

Growth driving pressure

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



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

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor

Growth driving pressure

MatCalc Engineering

- Driving pressure dependent on
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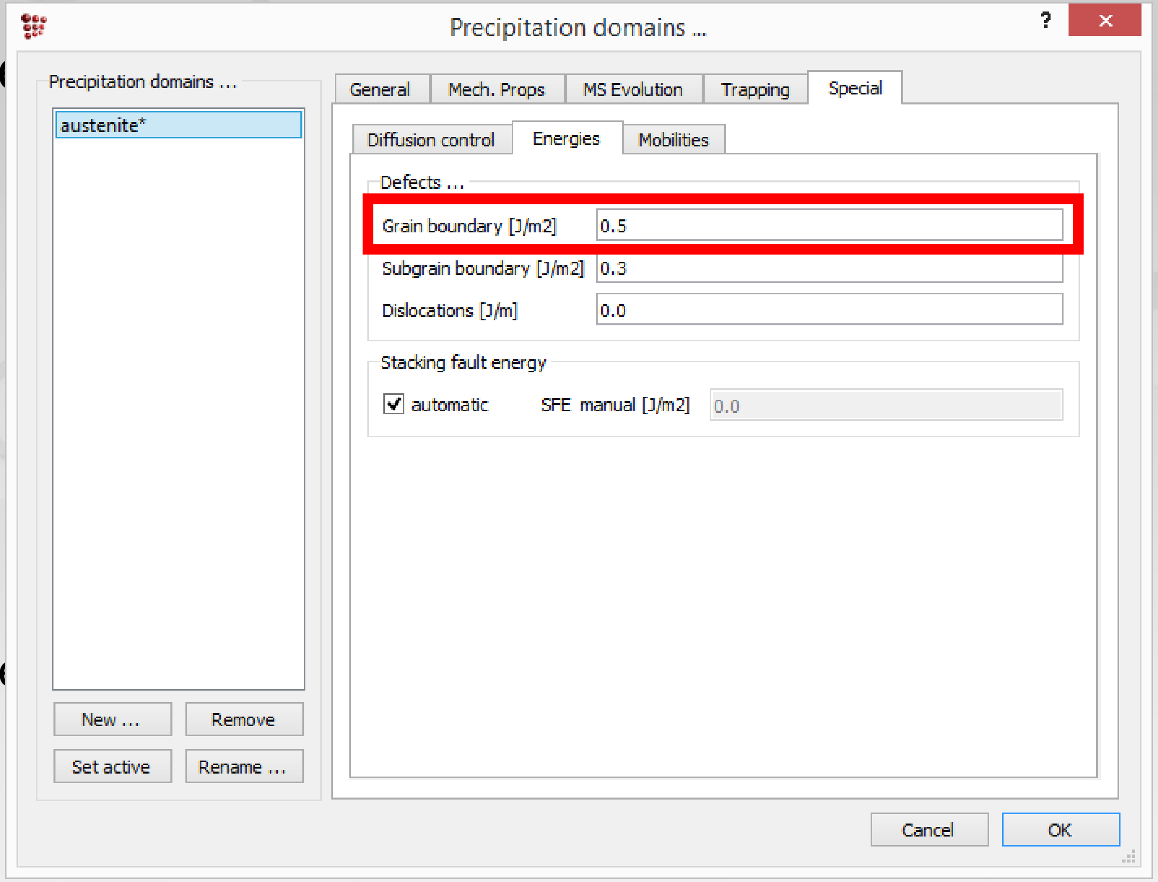

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Growth driving pressure

MatCalc Engineering

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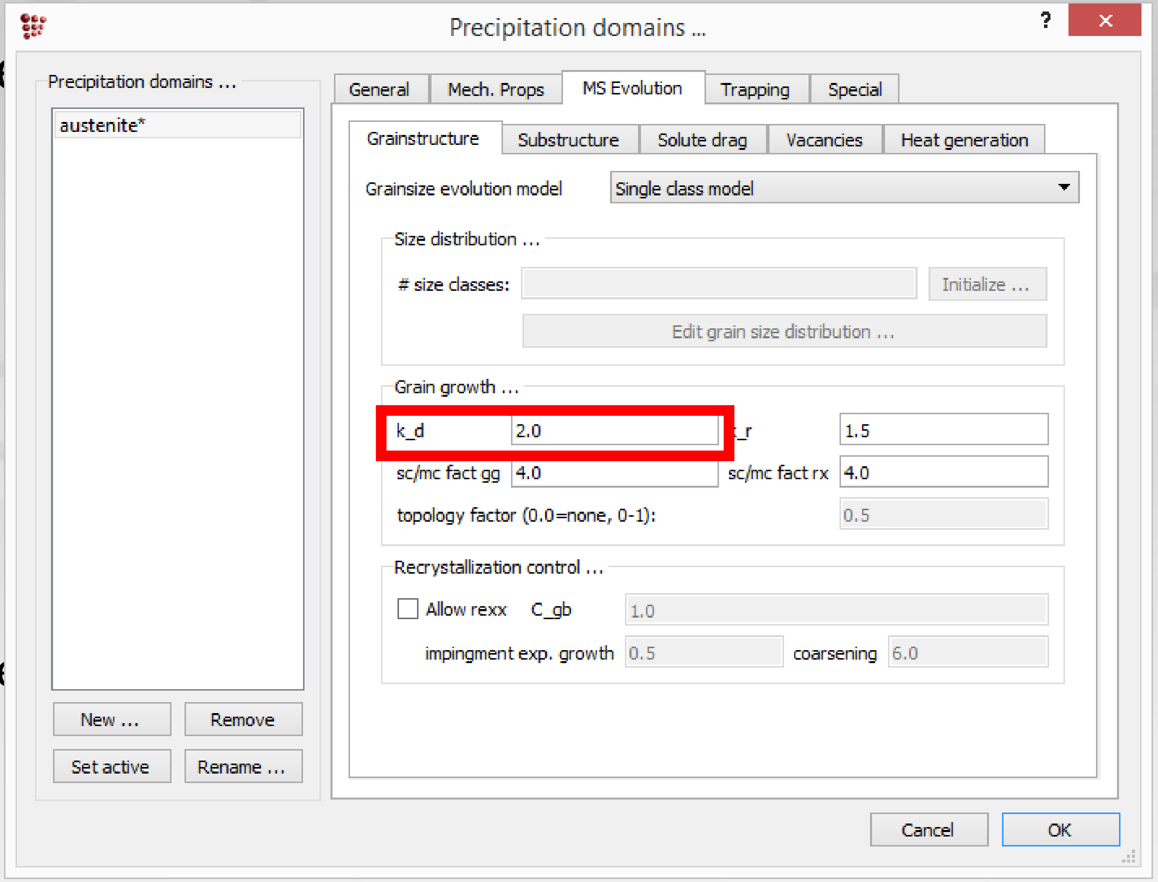

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

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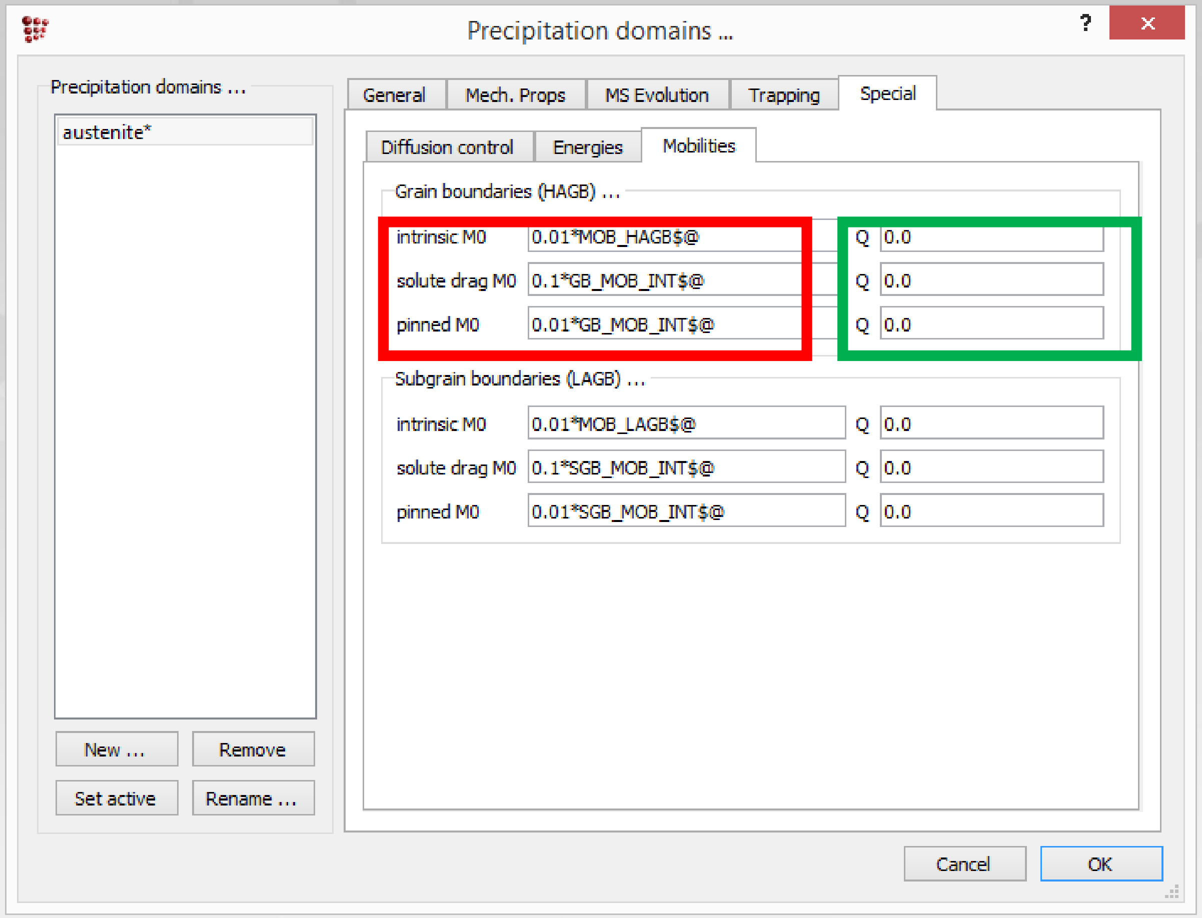
Mobility – general approach

- 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

Mobility – general approach

- General form $$M = M_0 exp(-Q/RT)$$

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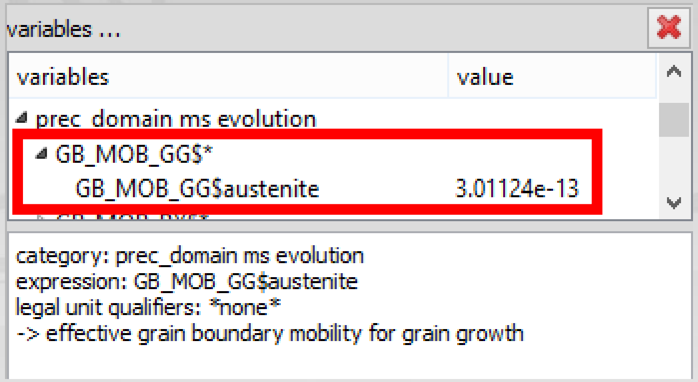

No obstacles

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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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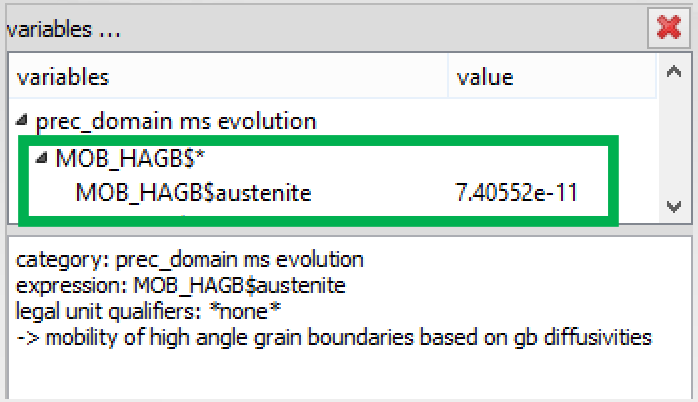

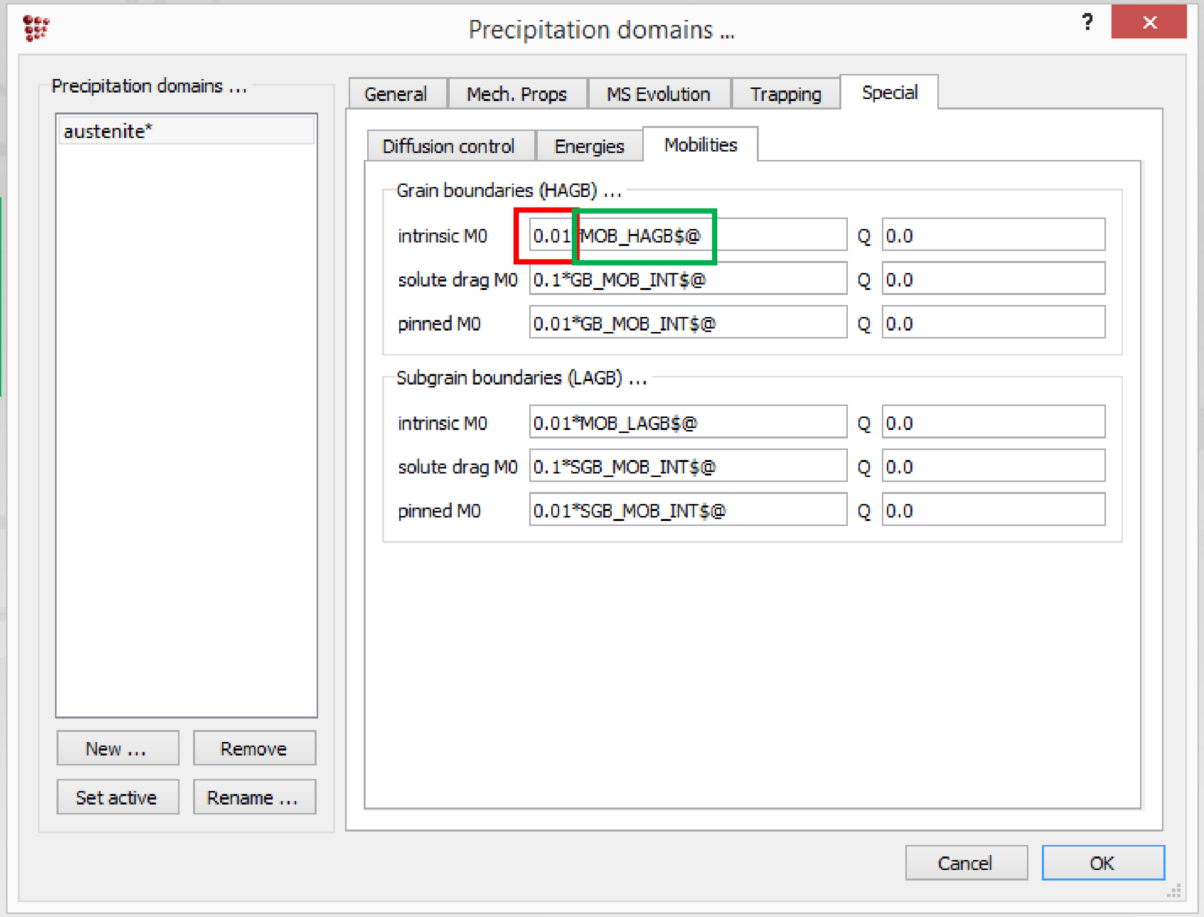

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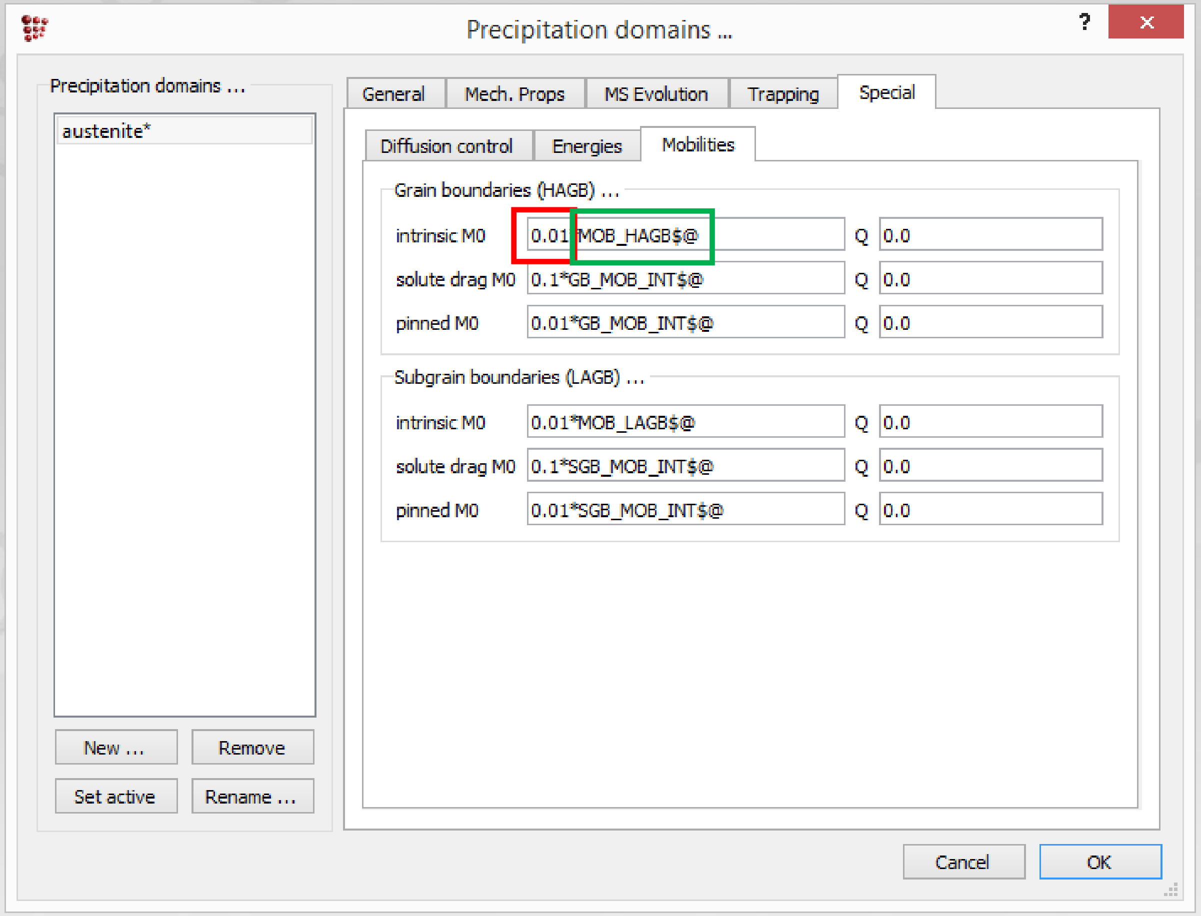
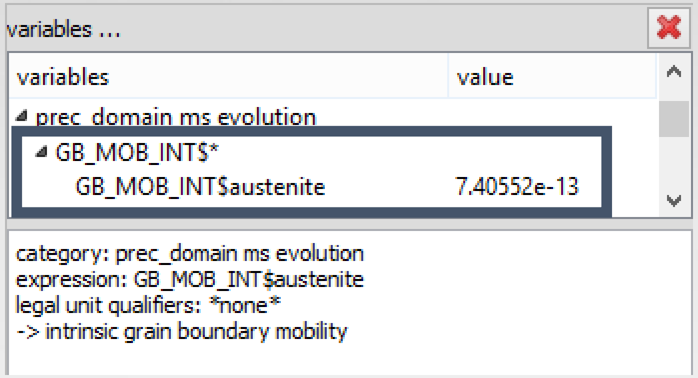




No obstacles

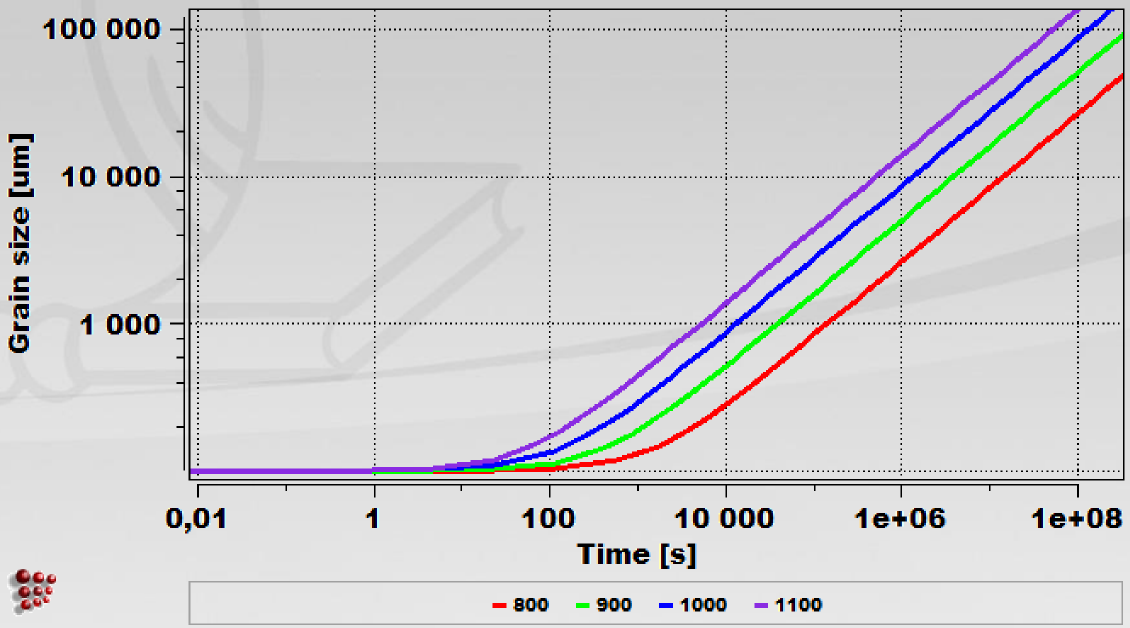
MatCalc Engineering

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

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

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

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



System with precipitates

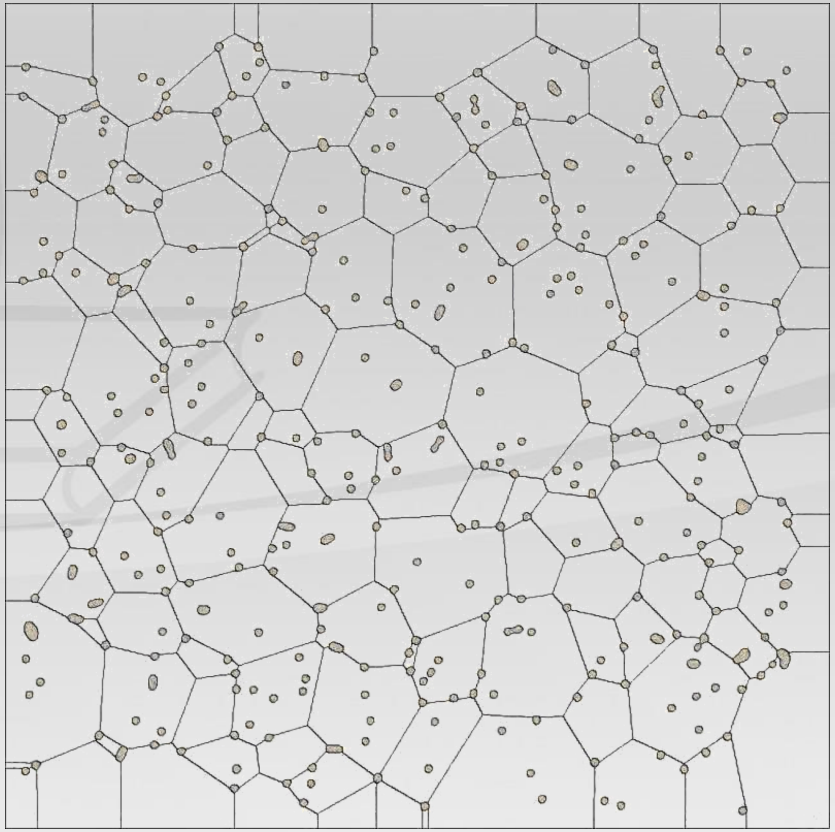
MatCalc Engineering

Grain boundary movement

Precipitates on the grain boundary

Reduction of grain boundary energy

Grain boundary pinning/slowdown

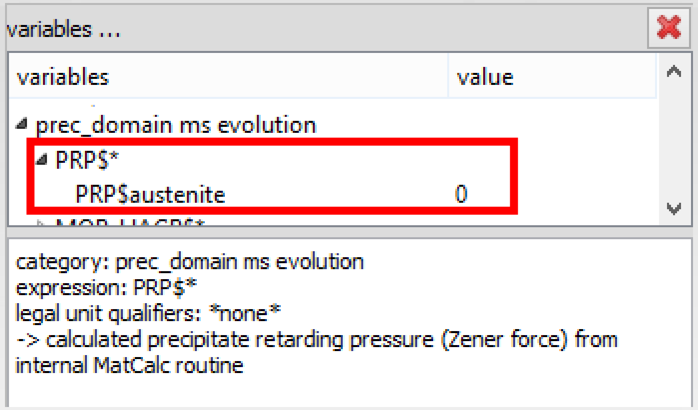


https://i.ytimg.com/vi/8EET_T6LIWY/maxresdefault.jpg

System with precipitates

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

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



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*

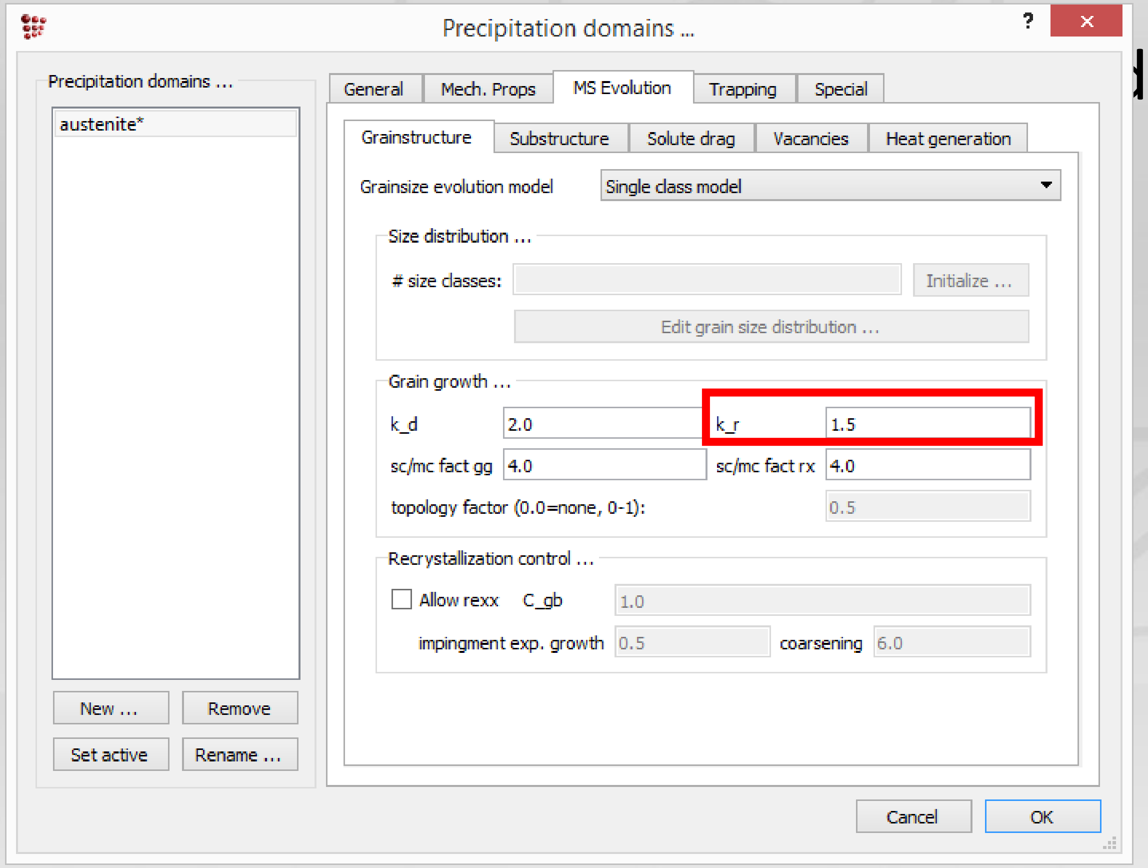
k_r - Scaling factor

α_i - Pinning factor of precipitate i

β_i - Pinning exponent of precipitate i

System with precipitates

MatCalc Engineering



dent on

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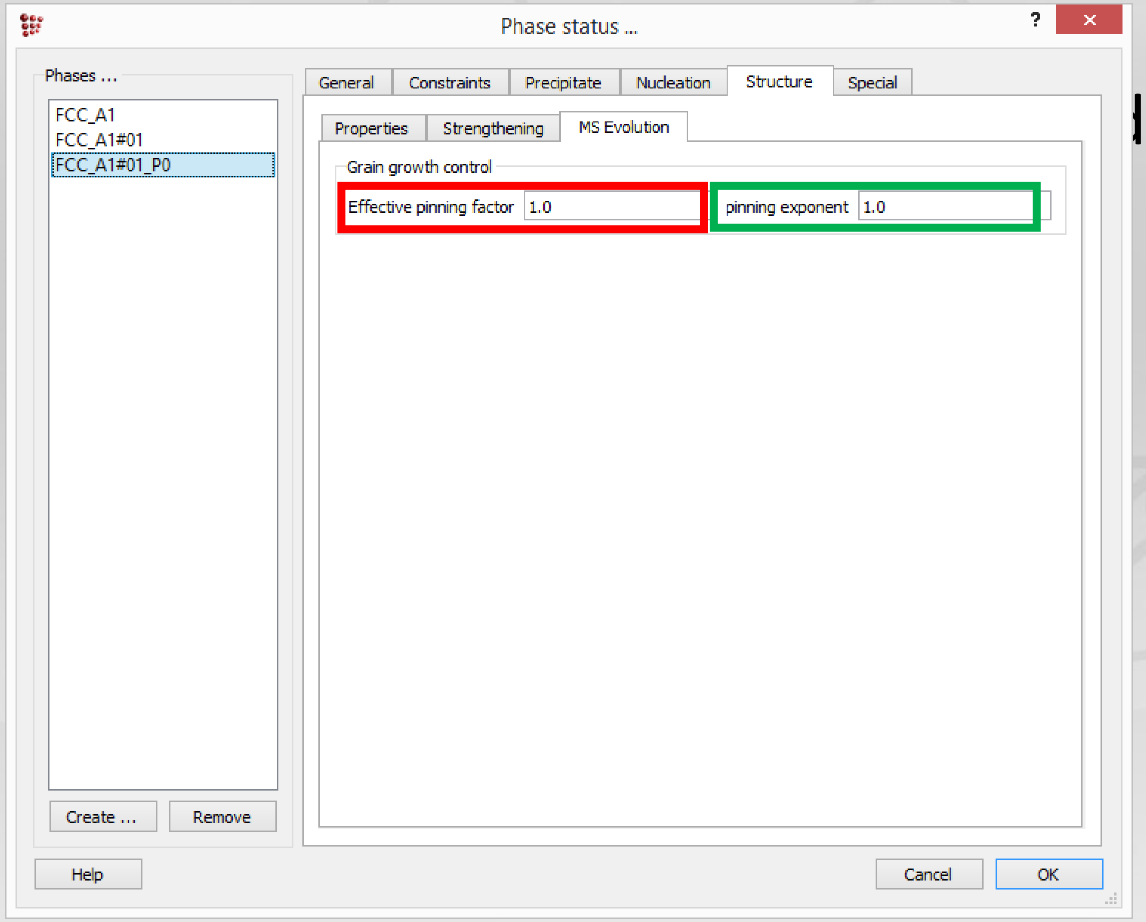
System with precipitates

MatCalc Engineering



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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

MatCalc Engineering

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

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

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

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

M_p - Grain boundary mobility for pinned interface

η_p - Scaling factor

System with precipitates

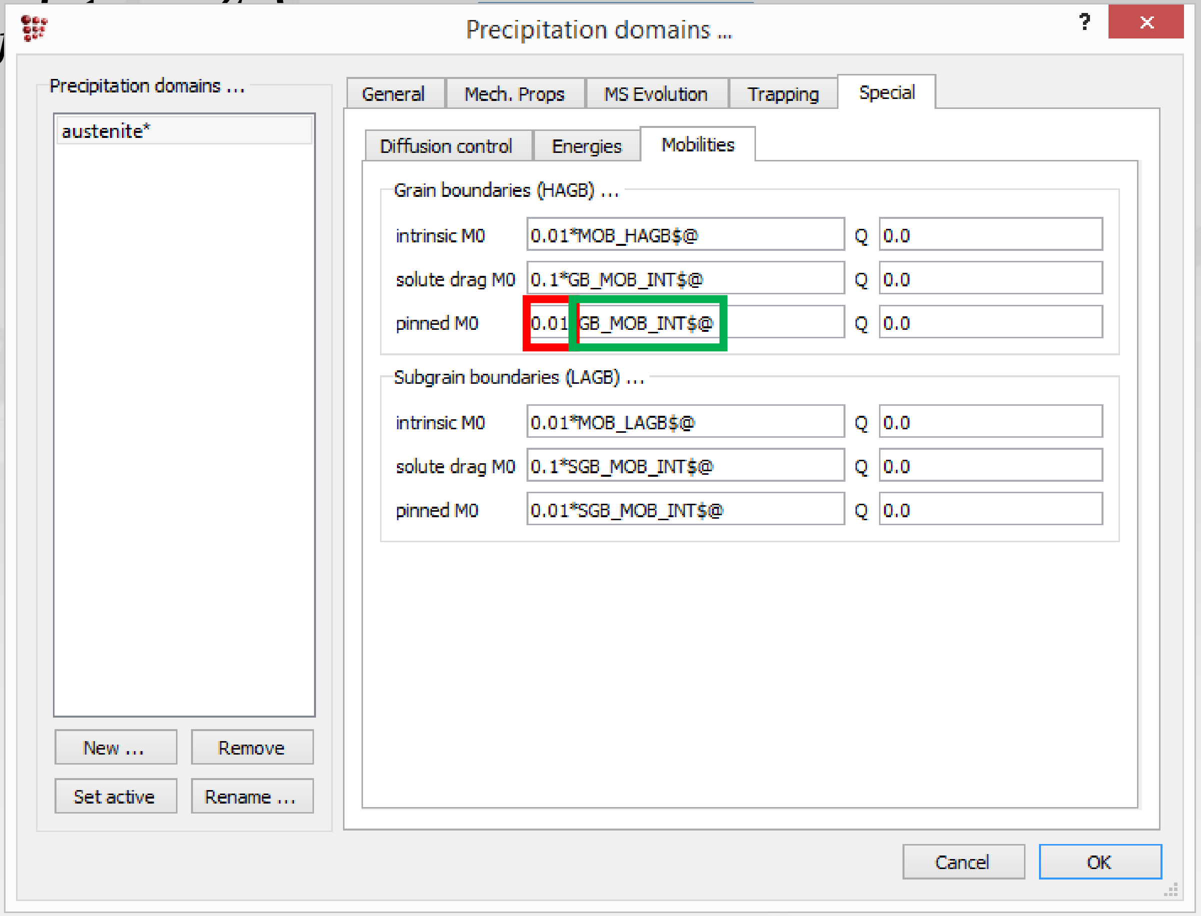
MatCalc Engineering

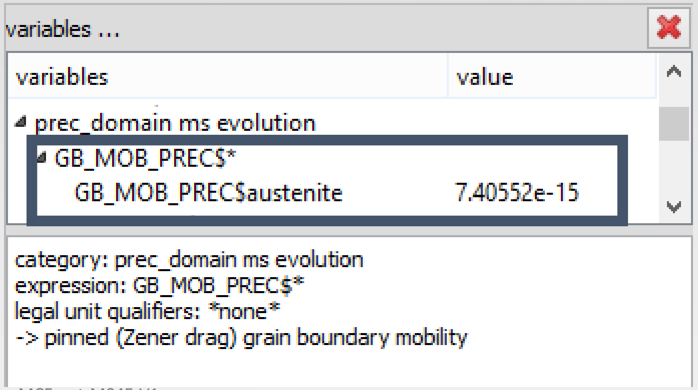
$$M_{prec} = \begin{cases} M_p \\ M_p \dfrac{P_Z}{P_D} + M_j \left(\ldots \dfrac{P_Z}{\ldots} \right) \end{cases}$$

$$P_Z \geq P_D$$

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

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





System with precipitates

MatCalc Engineering

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

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

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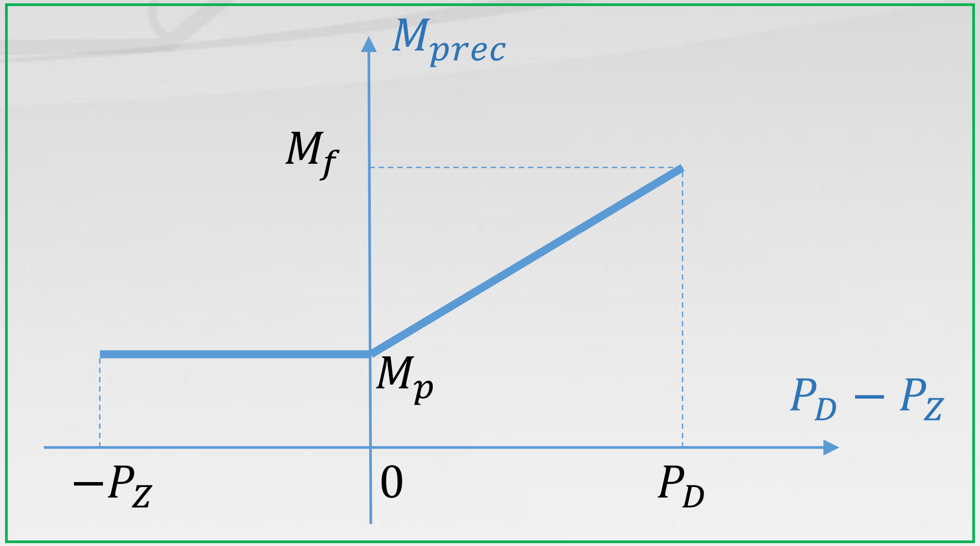

System with precipitates

MatCalc Engineering

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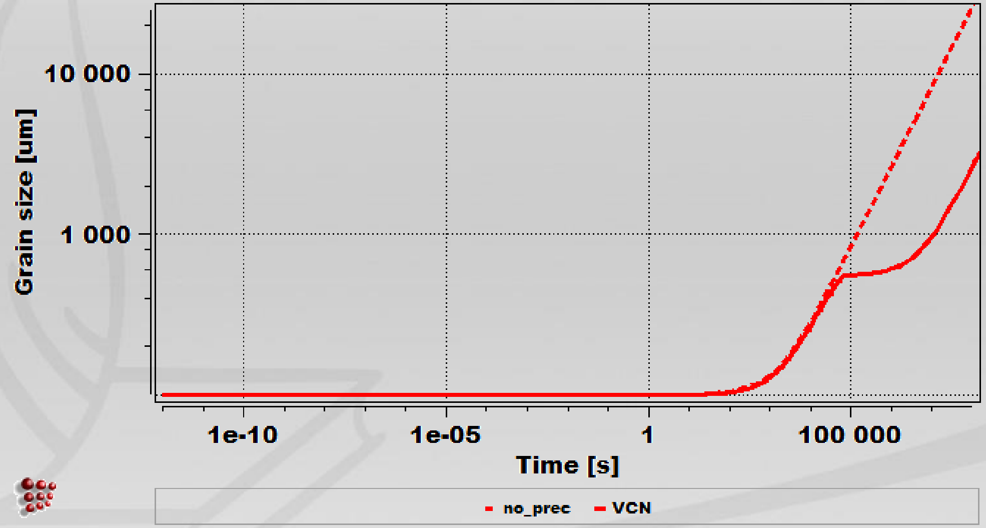
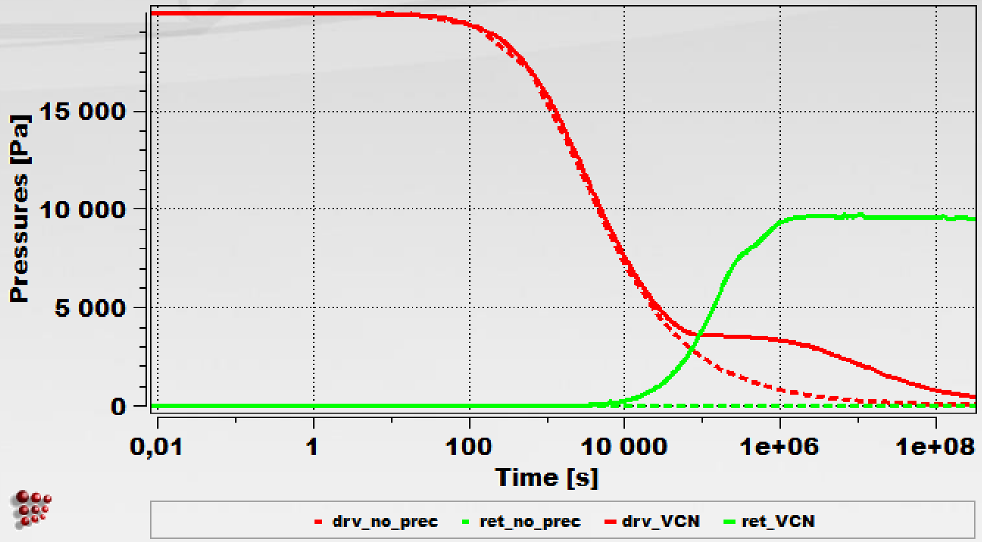


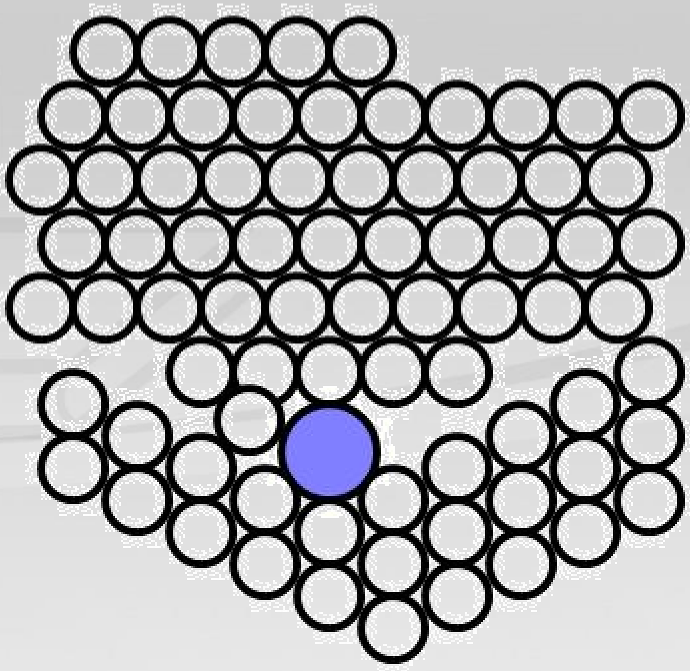


Case with solute drag

Solutes on the grain boundary

Reduction of grain boundary energy

Grain boundary pinning/slowdown



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

Case with solute drag

MatCalc Engineering

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

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

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

M_{eff} - Effective grain boundary mobility

M_{sd} - Grain boundary mobility with solute drag

Cahn impurity drag

MatCalc Engineering

- 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

MatCalc Engineering

- Evaluation of critical velo

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

- Comparison of current gr
  - $\dot{D} \geq v_{crit,i}$ - „fast branc
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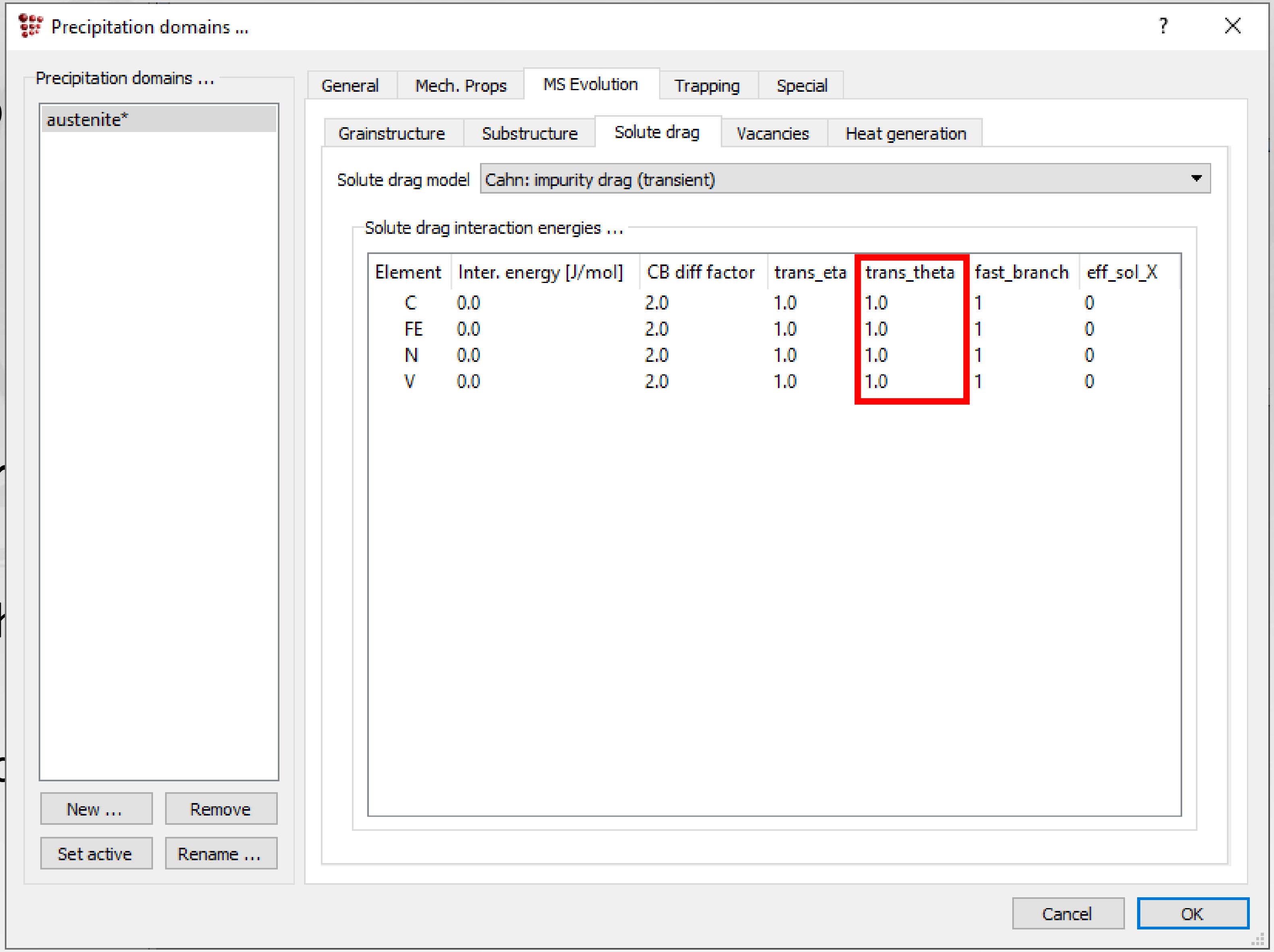


Cahn impurity drag

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

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

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

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

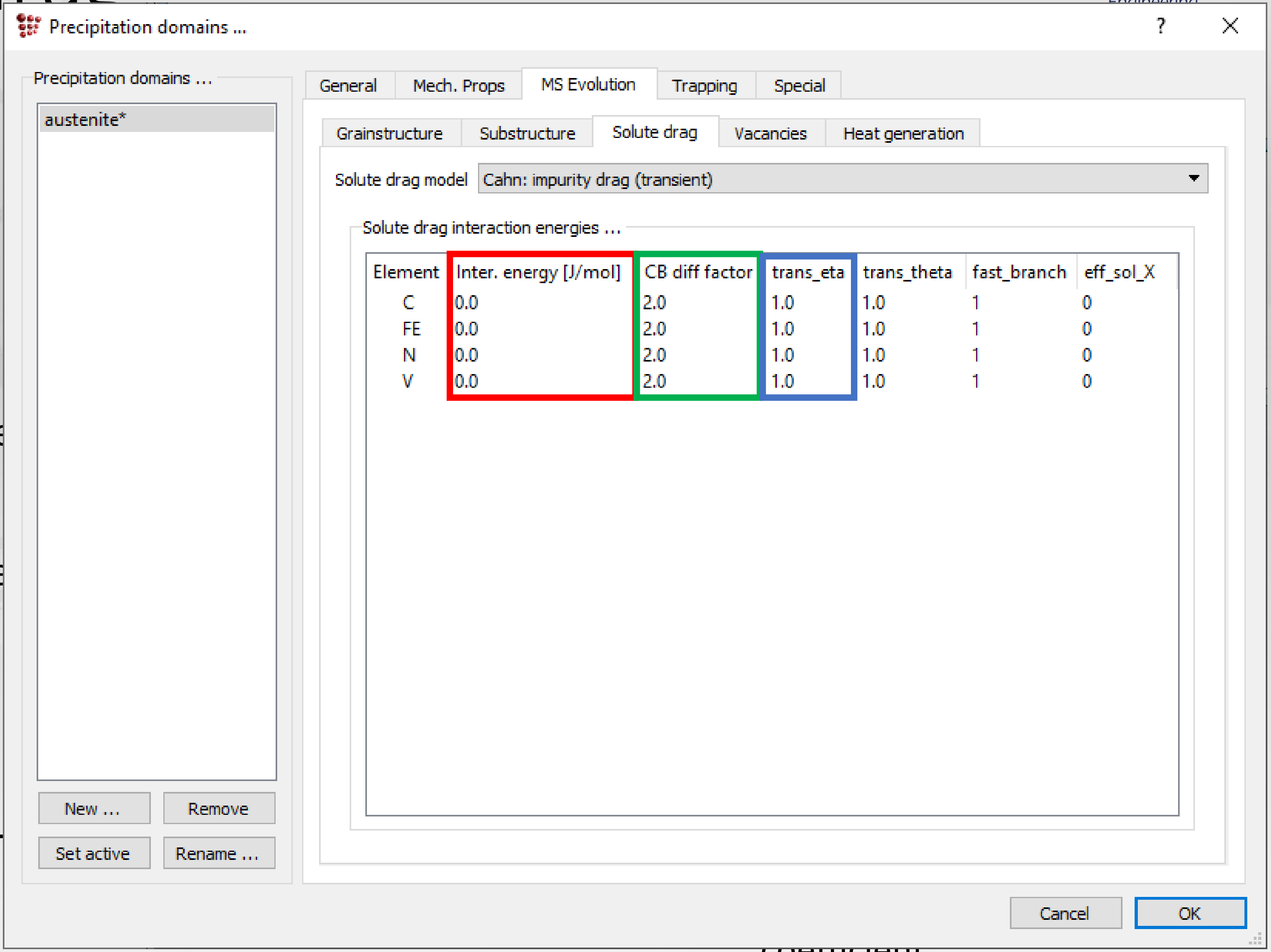
Cahn impurity drag

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

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

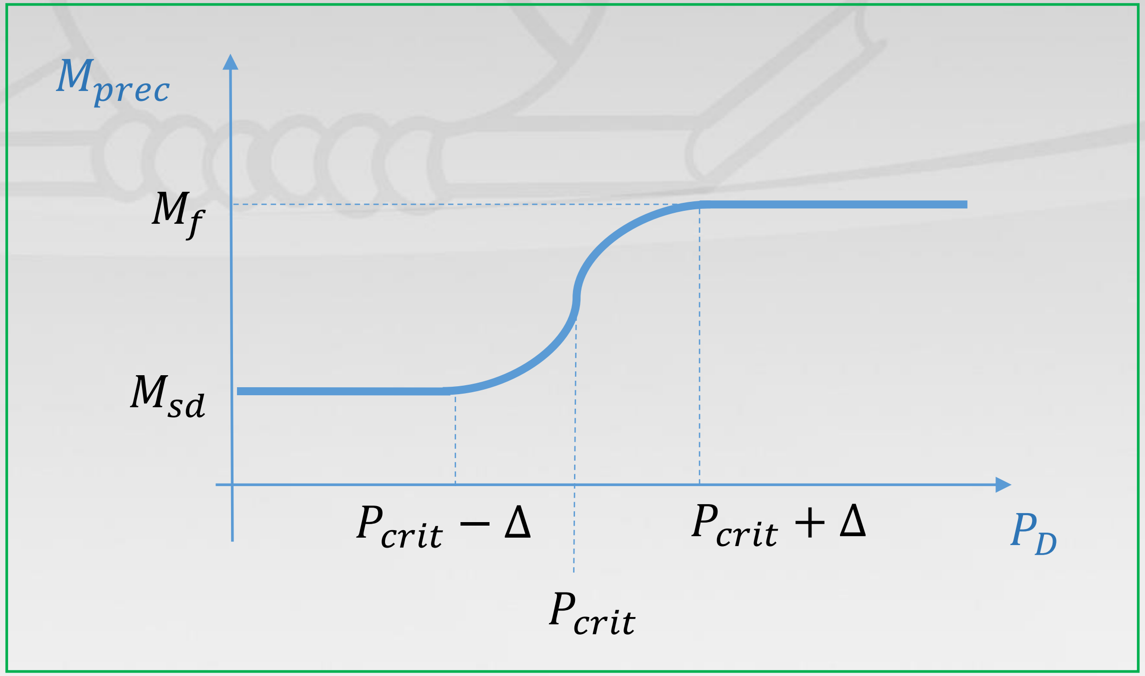
$$\alpha_i = \frac{\omega (RT)^2}{E_i D_{CB} V_m}\left(sinh\left(\frac{E_i}{RT}\right) - \ldots\right.$$

coefficient



Buken-Kozeschnik critical pressure

- Continuous mobility change dependent on the driving pressure.

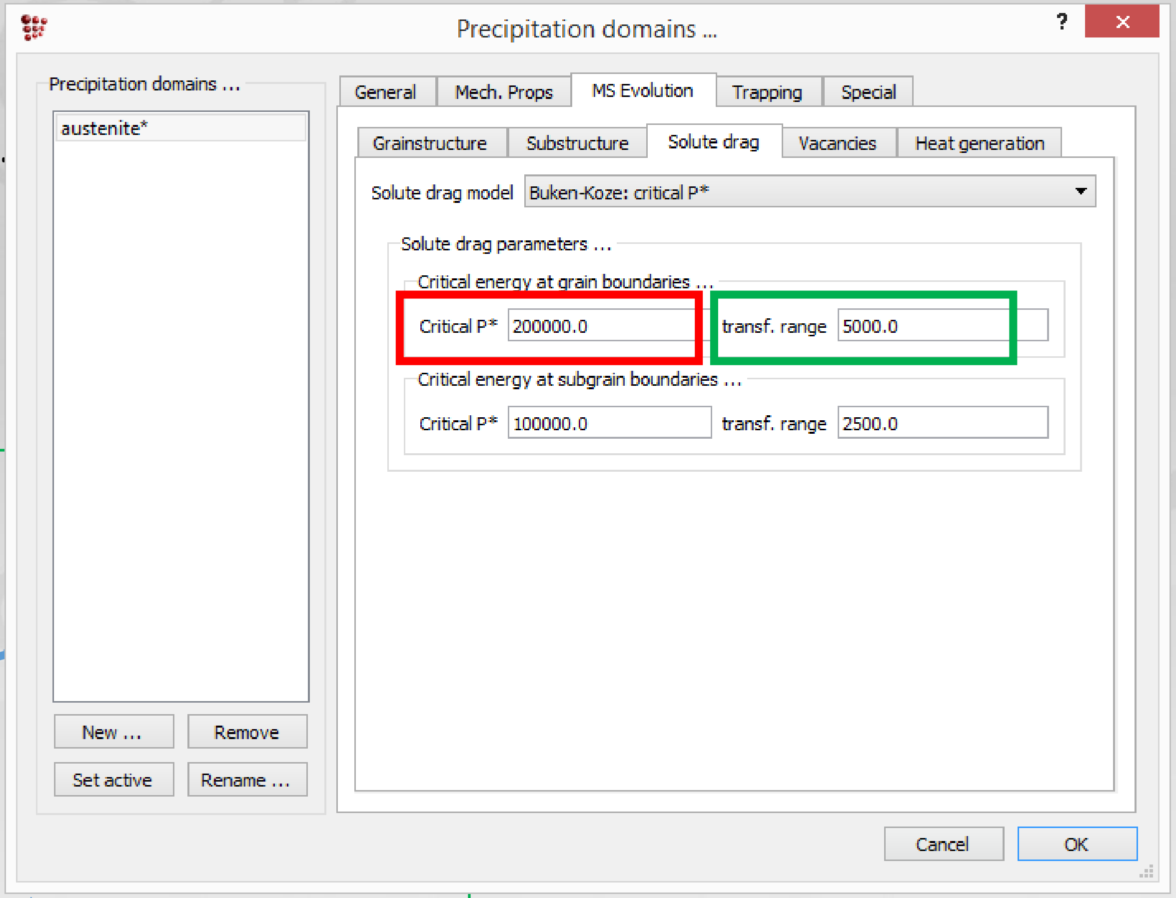


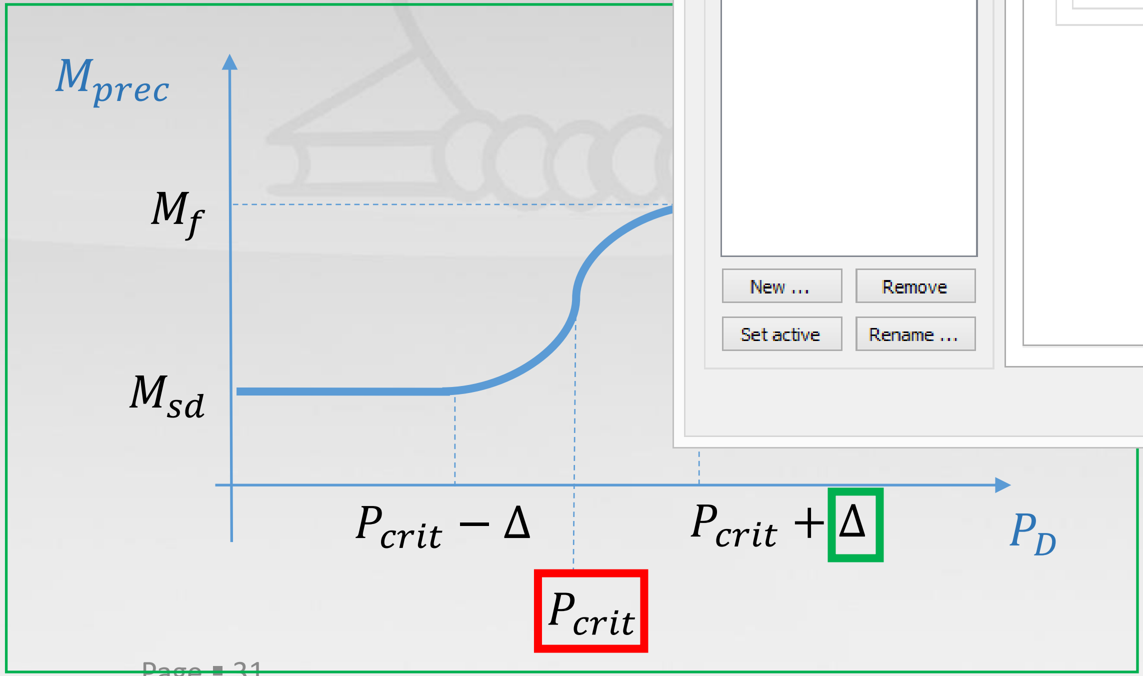
Buken-Kozeschnik critical pressure

MatCalc Engineering

- Continuous mobili

  pressure.





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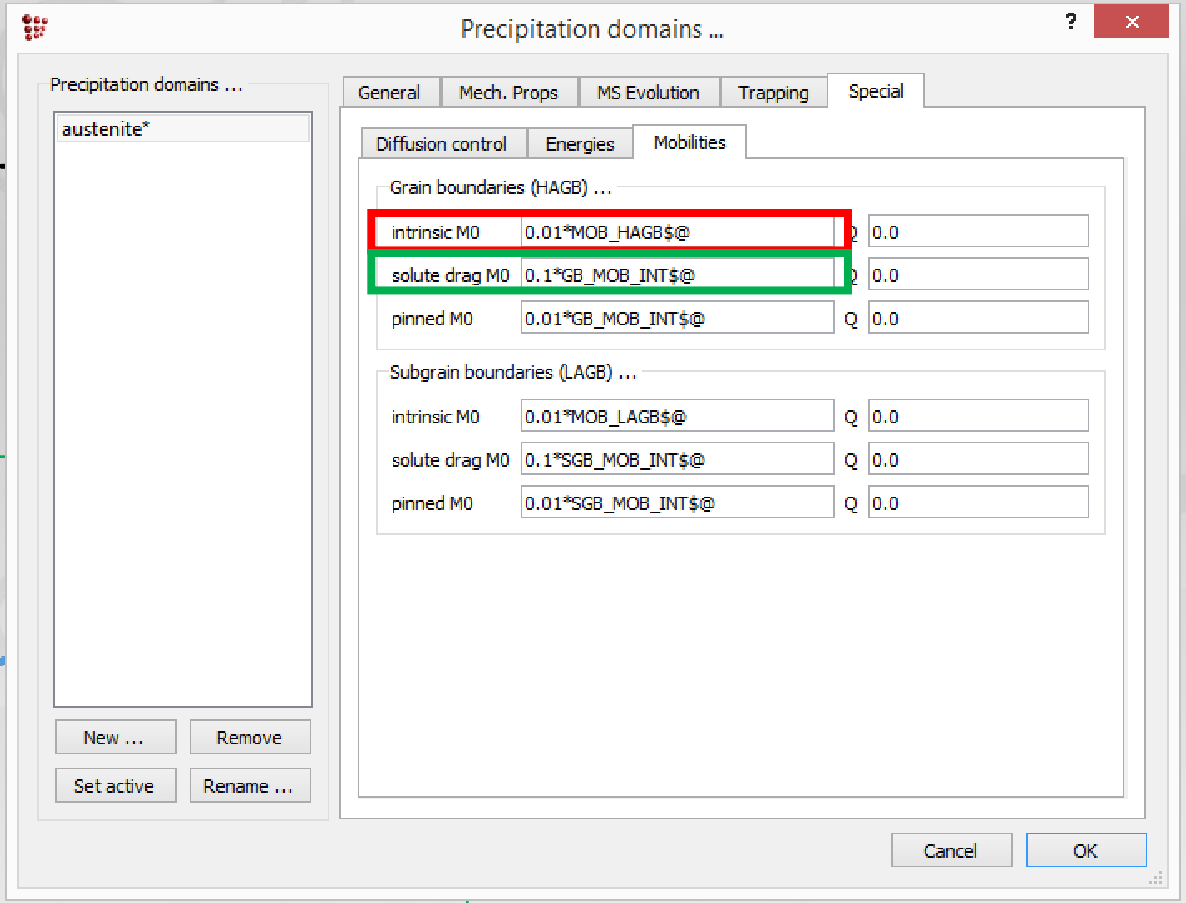
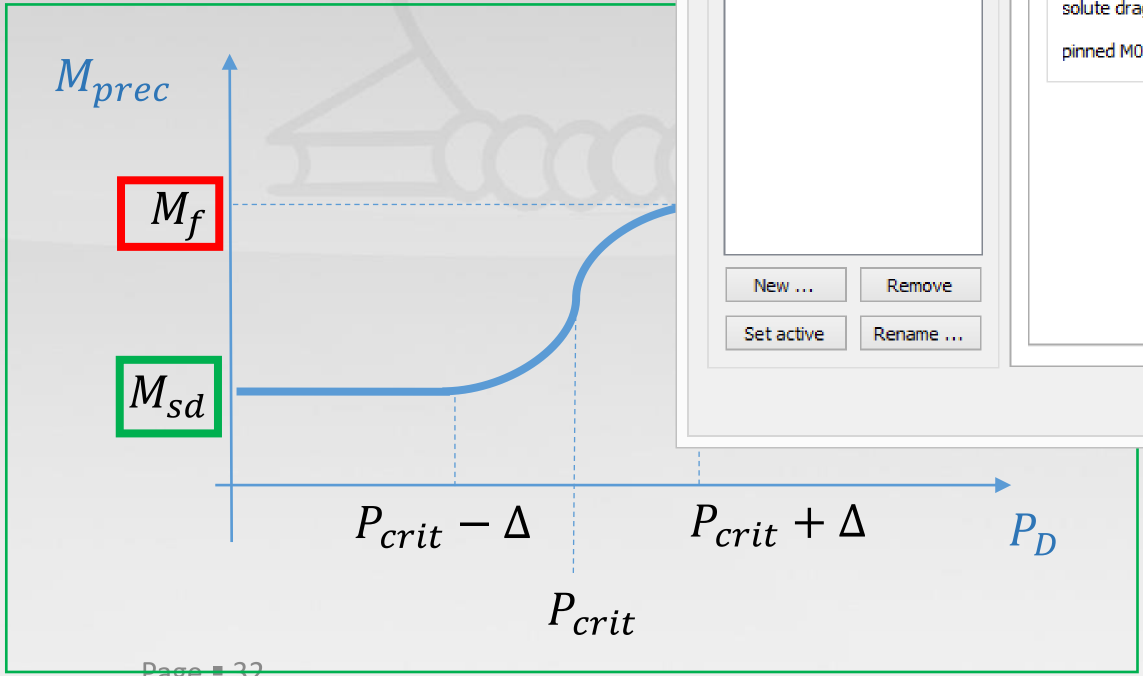




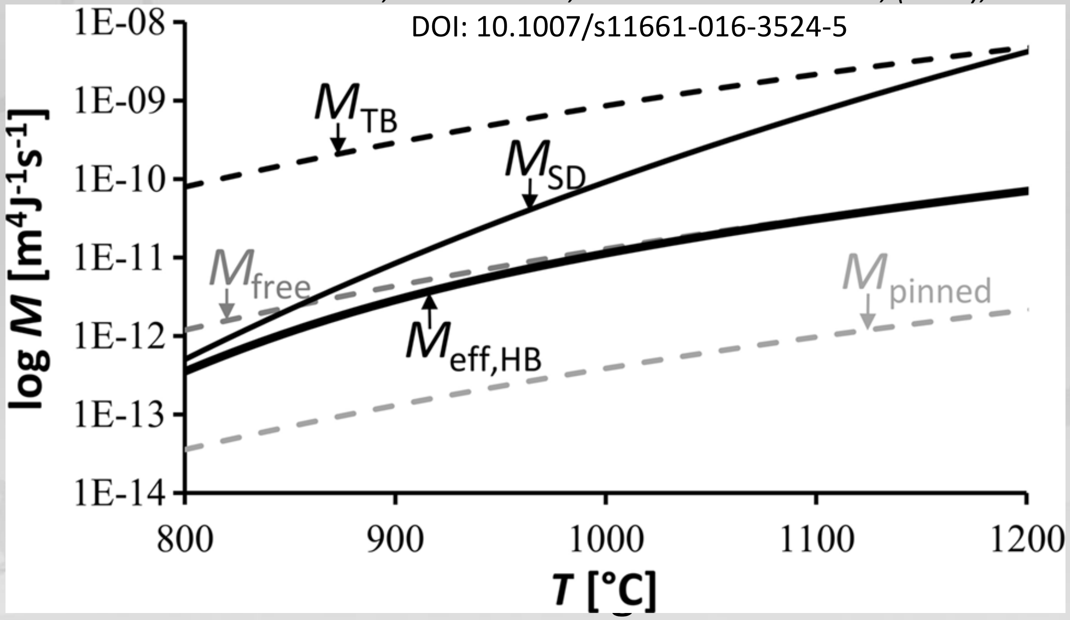
Case with solute drag

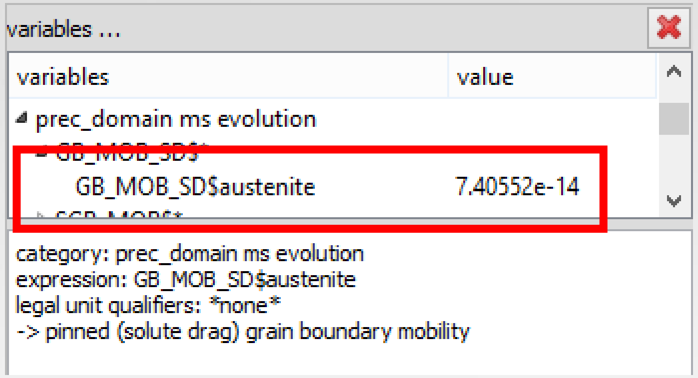
$$\dot{D} = M_{eff} P_D$$

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

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

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





Acknowledgments

MatCalc Engineering

- Heinrich Buken
- Philipp Retzl
- Yao Shan

MatCalc
Engineering