

MatCalc

Engineering

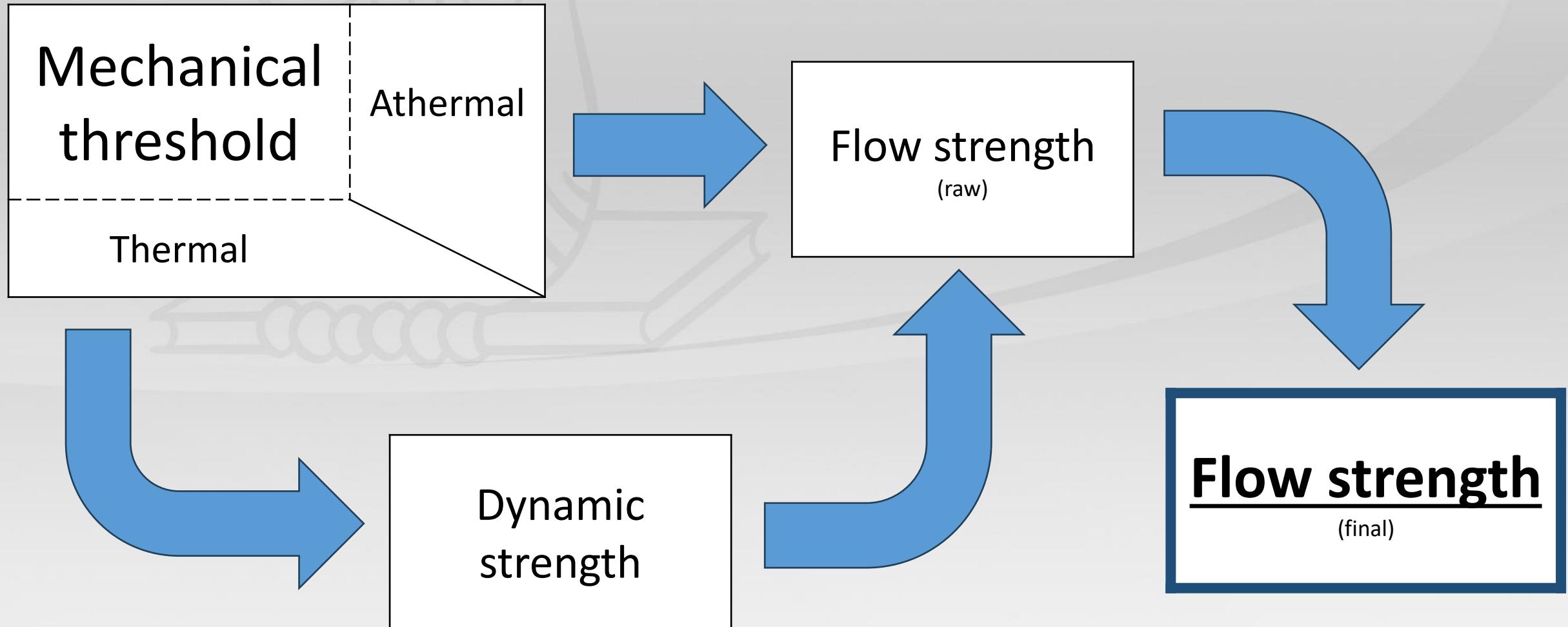
Flow curve calculation in MatCalc

MatCalc 6.04.1004

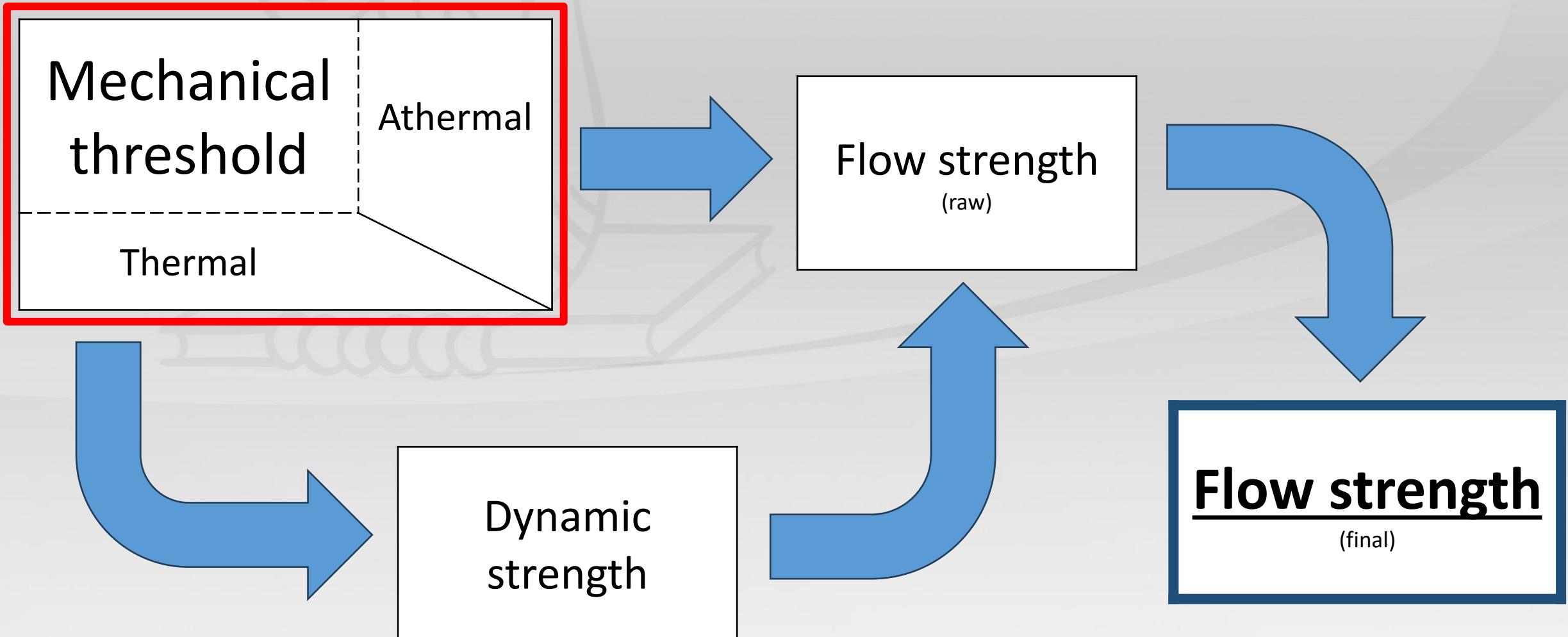
P. Warczok



Overview



Overview



Mechanical threshold

- Yield stress at temperature 0 K
- Microstructure dependent

$$\sigma_0 = f(\rho, d_g, d_{sg}, c_i^m, r_{pj}, N_{pj}, \dots)$$

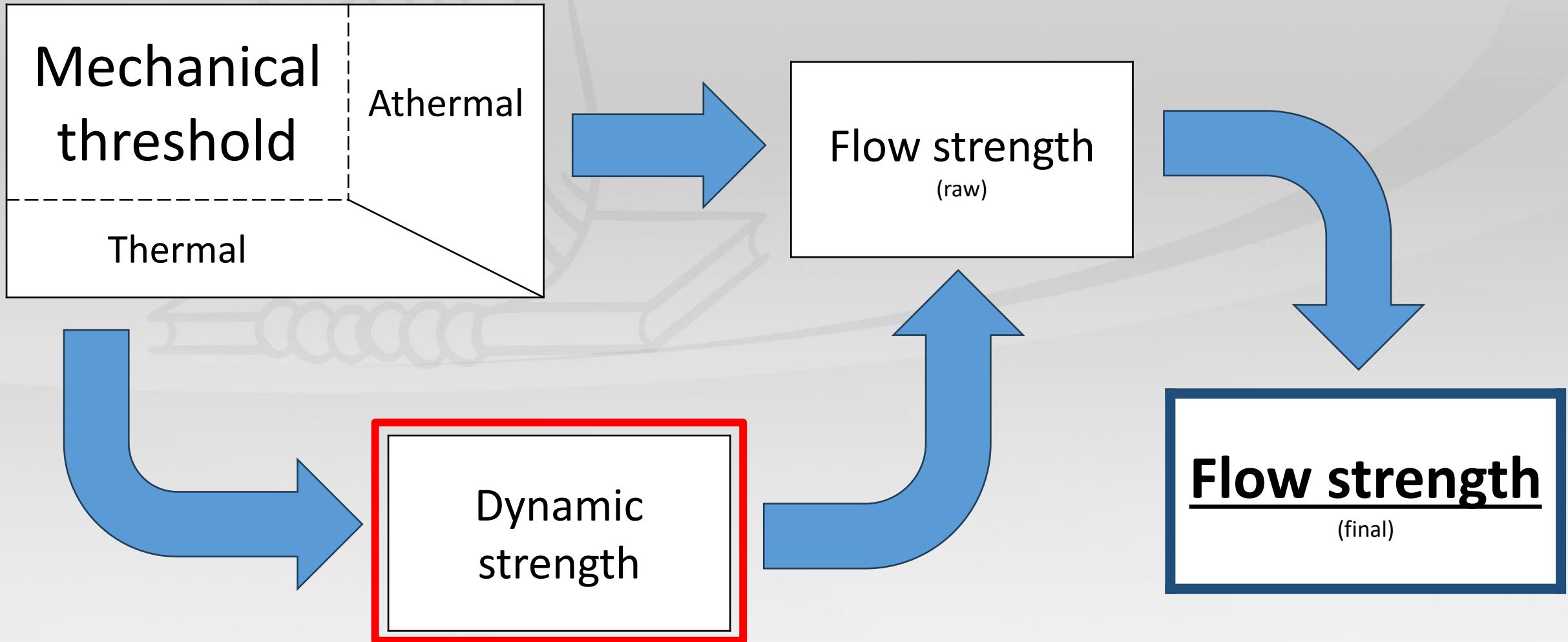
- Thermal & athermal contributions

$$\sigma_0 = \sigma_{ath} + \sigma_{th}$$

ρ - Dislocation density [m-2]
 d_g - Grain diameter [m]
 d_{sg} - Subgrain diameter [m]
 c_i^m - Concentration of i-element in matrix
 r_{pj} - Radius of precipitate j [m]
 N_{pj} - Number density of precipitate j [m⁻³]

σ_{ath} - Athermal contribution [Pa]
 σ_{th} - Thermal contribution [Pa]

Overview



Dynamic stress contribution

- Sum of various contributions

$$\sigma_d = (\sigma_{dyn,lt}^{-n_{dyn}} + \sigma_{dyn,ht}^{-n_{dyn}} + \sigma_{dyn,lt,pbd}^{-n_{dyn}} + \dots \\ \dots + \sigma_{dyn,ht,pbd}^{-n_{dyn}} + \sigma_{dyn,NHc}^{-n_{dyn}} + \sigma_{dyn,Cc}^{-n_{dyn}} + \dots \\ \dots + \sigma_{dyn,HDC}^{-n_{dyn}} + \sigma_{dyn,gbs,gb}^{-n_{dyn}} + \sigma_{dyn,gbs,eff}^{-n_{dyn}})^{-1/n_{dyn}}$$

$\sigma_{dyn,lt}$	– Low temperature regime	$\sigma_{dyn,lt,pbd}$	– Power law breakdown, low temperature regime
$\sigma_{dyn,ht}$	– High temperature regime	$\sigma_{dyn,ht,pbd}$	– Power law breakdown, high temperature regime
$\sigma_{dyn,NHc}$	– Nabarro-Herring creep	$\sigma_{dyn,gbs,gb}$	– Grain boundary sliding, lattice diffusion regime
$\sigma_{dyn,Cc}$	– Coble creep	$\sigma_{dyn,gbs,eff}$	– Grain boundary sliding, grain boundary diffusion regime
$\sigma_{dyn,HDC}$	– Harper-Dorn creep	n_{dyn}	– Exponent

Dynamic stress contribution

- Sum of various contributions

$$\sigma_d = (\sigma_{dyn,lt}^{-n_{dyn}} + \sigma_{dyn,ht}^{-n_{dyn}} + \sigma_{dyn,lt,pbd}^{-n_{dyn}} + \dots \\ \dots + \sigma_{dyn,ht,pbd}^{-n_{dyn}} + \sigma_{dyn,NHc}^{-n_{dyn}} + \sigma_{dyn,Cc}^{-n_{dyn}} + \dots \\ \dots + \sigma_{dyn,HDc}^{-n_{dyn}} + \sigma_{dyn,gbs,gb}^{-n_{dyn}} + \sigma_{dyn,gbs,eff}^{-n_{dyn}})^{-1/n_{dyn}}$$

- Strain rate absence $\rightarrow \sigma_d = 0$
- All but $\sigma_{dyn,lt}$ and $\sigma_{dyn,ht}$ contributions dependent on diffusivity in material

Dynamic stress contribution

- Sum of various contributions

$$\sigma_d = (\sigma_{dyn,lt}^{-n_{dyn}} + \sigma_{dyn,ht}^{-n_{dyn}} + \sigma_{dyn,lt,pbd}^{-n_{dyn}} + \dots \\ \dots + \sigma_{dyn,ht,pbd}^{-n_{dyn}} + \sigma_{dyn,NHc}^{-n_{dyn}} + \sigma_{dyn,Cc}^{-n_{dyn}} + \dots \\ \dots + \sigma_{dyn,HDC}^{-n_{dyn}} + \sigma_{dyn,gbs,gb}^{-n_{dyn}} + \sigma_{dyn,gbs,eff}^{-n_{dyn}})^{-1/n_{dyn}}$$

variable	value
prec_domain strength	
▼ TYS_DYN\$*	
TYS_DYN\$matrix	1,39036e+07

- Strain rate absence $\rightarrow \sigma_d = 0$
- All but $\sigma_{dyn,lt}$ and $\sigma_{dyn,ht}$ contributions dependent on diffusivity in material

Low temperature

$$\sigma_{dyn,lt} = \sigma_{th} \left(\frac{\dot{\varepsilon}}{A_{\varepsilon_0} b c_{snd} \rho_{eq}} \right)^{RT/\Delta F_{\sigma_0}^{lt}}$$

Minimal value limit
for $\dot{\varepsilon} \geq 10^{-18} \text{ s}^{-1}$

b – Burgers vector [m]

R – Gas constant [$\text{Jmol}^{-1}\text{K}^{-1}$]

T – Temperature [K]

c_{snd} – Speed of sound [ms^{-1}]

σ_{th} – Mechanical threshold, thermal contribution [Pa]

$\Delta F_{\sigma_0}^{lt}$ – Yield stress activation energy, low temperature [Jmol^{-1}]

ρ_{eq} – Equilibrium dislocation density [m^{-2}]

A_{ε_0} – Scaling factor for strain rate limit

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

Low temperature

$$\sigma_{dyn,lt} = \sigma_{th} \left(\frac{\dot{\varepsilon}}{A_{\varepsilon_0} b c_{snd} \rho_{eq}} \right)^{RT/\Delta F_{\sigma_0}^{lt}}$$

Minimal value limit
for $\dot{\varepsilon} \geq 10^{-18} \text{ s}^{-1}$

variable	value
prec_domain strength	
TYS_DYN_LT\$*	
TYS_DYN_LT\$matrix	1,47412e+07

b – Burgers vector [m]

R – Gas constant [$\text{Jmol}^{-1}\text{K}^{-1}$]

T – Temperature [K]

c_{snd} – Speed of sound [ms^{-1}]

σ_{th} – Mechanical threshold, thermal contribution [Pa]

$\Delta F_{\sigma_0}^{lt}$ – Yield stress activation energy, low temperature [Jmol^{-1}]

ρ_{eq} – Equilibrium dislocation density [m^{-2}]

A_{ε_0} – Scaling factor for strain rate limit

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

High temperature

$$\sigma_{dyn,ht} = \left[\sigma_{th} \frac{bRT(\alpha_{int} M_T G)^2}{2c_{snd}\Delta F_{\sigma_0}^{ht}} \exp\left(\frac{\Delta F_{\sigma_0}^{ht}}{RT}\right) \dot{\varepsilon}^{n_{eps_dot}} \right]^{n_{ht}}$$

Minimal value limit
for $\dot{\varepsilon} \geq 10^{-18} \text{ s}^{-1}$

G – Shear modulus [Pa]

M_T – Taylor factor

b – Burgers vector [m]

R – Gas constant [$\text{Jmol}^{-1}\text{K}^{-1}$]

T – Temperature [K]

c_{snd} – Speed of sound [ms^{-1}]

σ_{th} – Mechanical threshold, thermal contribution [Pa]

$\Delta F_{\sigma_0}^{ht}$ – Yield stress activation energy, high temperature [Jmol^{-1}]

α_{int} – Strengthening coefficient for internal dislocations

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

n_{eps_dot} – Strain rate exponent

n_{ht} – Exponent

High temperature

$$\sigma_{dyn,ht} = \left[\sigma_{th} \frac{bRT(\alpha_{int} M_T G)^2}{2c_{snd}\Delta F_{\sigma_0}^{ht}} \exp\left(\frac{\Delta F_{\sigma_0}^{ht}}{RT}\right) \dot{\varepsilon}^{n_{eps_dot}} \right]^{n_{ht}}$$

Minimal value limit
for $\dot{\varepsilon} \geq 10^{-18} \text{ s}^{-1}$

variable	value
prec_domain strength	
TYS_DYNHTS*	TYS_DYNHTSmatrix 2,64128e+08

G – Shear modulus [Pa]

M_T – Taylor factor

b – Burgers vector [m]

R – Gas constant [$\text{Jmol}^{-1}\text{K}^{-1}$]

T – Temperature [K]

c_{snd} – Speed of sound [ms^{-1}]

σ_{th} – Mechanical threshold, thermal contribution [Pa]

$\Delta F_{\sigma_0}^{ht}$ – Yield stress activation energy, high temperature [Jmol^{-1}]

α_{int} – Strengthening coefficient for internal dislocations

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

n_{eps_dot} – Strain rate exponent

n_{ht} – Exponent

Low temperature, power law breakdown

$$\sigma_{dyn,lt,plb} = G A_{lt,plb,1} \operatorname{arsinh} \left[\left(A_{lt,plb,2} \frac{M_T k_B T}{G D_{disl} f_{pipe} b} \dot{\varepsilon} \right)^{n_{lt,plb}} \right]$$

$A_{lt,plb,1}$ – Scaling factor (10^{-3} ; hardcoded)

$A_{lt,plb,2}$ – Scaling factor (10^{128} ; hardcoded)

G – Shear modulus [Pa]

M_T – Taylor factor

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

D_{disl} – Diffusion coefficient along dislocations

(reference element) [m^2s^{-1}]

f_{pipe} – Correction factor for pipe diffusion

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

$n_{lt,plb}$ – Exponent (5; hardcoded)

Low temperature, power law breakdown

$$\sigma_{dyn,lt,plb} = G A_{lt,plb,1} \operatorname{arsinh} \left[\left(A_{lt,plb,2} \frac{M_T k_B T}{G D_{disl} f_{pipe} b} \dot{\varepsilon} \right)^{n_{lt,plb}} \right]$$

variable	value
prec_domain strength	
TYS_DYN_POW_LT_BDS*	
TYS_DYN_POW_LT_BDSmatrix	inf

$A_{lt,plb,1}$ – Scaling factor (10^{-3} ; hardcoded)

$A_{lt,plb,2}$ – Scaling factor (10^{128} ; hardcoded)

G – Shear modulus [Pa]

M_T – Taylor factor

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

D_{disl} – Diffusion coefficient along dislocations

(reference element) [m^2s^{-1}]

f_{pipe} – Correction factor for pipe diffusion

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

$n_{lt,plb}$ – Exponent (5; hardcoded)

High temperature, power law breakdown

$$\sigma_{dyn,ht,plb} = G A_{ht,plb,1} \operatorname{arsinh} \left[\left(A_{ht,plb,2} \frac{M_T k_B T}{G D_{eff} b} \dot{\varepsilon} \right)^{n_{ht,plb}} \right]$$

$A_{ht,plb,1}$ – Scaling factor (10^{-3} ; hardcoded)

$A_{ht,plb,2}$ – Scaling factor (10^{16} ; hardcoded)

G – Shear modulus [Pa]

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

M_T – Taylor factor

D_{eff} – Effective diffusion coefficient (reference element) [m^2s^{-1}]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

$n_{ht,plb}$ – Exponent (3; hardcoded)

High temperature, power law breakdown

$$\sigma_{dyn,ht,plb} = G A_{ht,plb,1} \operatorname{arsinh} \left[\left(A_{ht,plb,2} \frac{M_T k_B T}{G D_{eff} b} \dot{\varepsilon} \right)^{n_{ht,plb}} \right]$$

variable	value
prec_domain strength	
TYS_DYN_POW_HT_BDS*	TYS_DYN_POW_HT_BD\$matrix 3,32355e+09

$A_{ht,plb,1}$ – Scaling factor (10^{-3} ; hardcoded)

$A_{ht,plb,2}$ – Scaling factor (10^{16} ; hardcoded)

G – Shear modulus [Pa]

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

M_T – Taylor factor

D_{eff} – Effective diffusion coefficient (reference element) [m^2s^{-1}]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

$n_{ht,plb}$ – Exponent (3; hardcoded)

Nabarro-Herring creep

$$\sigma_{dyn,NHc} = \frac{M_T k_B T d_g^2}{42 D_{eff} b^3} \dot{\varepsilon}$$

M_T – Taylor factor

k_B – Boltzmann constant [JK⁻¹]

T – Temperature [K]

d_g – Grain diameter [m]

D_{eff} Effective diffusion coefficient (reference element) [m²s⁻¹]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s⁻¹]

Nabarro-Herring creep

$$\sigma_{dyn,NHc} = \frac{M_T k_B T d_g^2}{42 D_{eff} b^3} \dot{\varepsilon}$$

variable	value
prec_domain strength	
TYS_DYN_NHCS*	
TYS_DYN_NHC\$matrix	4,81362e+14

M_T – Taylor factor

k_B – Boltzmann constant [JK⁻¹]

T – Temperature [K]

d_g – Grain diameter [m]

D_{eff} Effective diffusion coefficient (reference element) [m²s⁻¹]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s⁻¹]

Coble creep

$$\sigma_{dyn,Cc} = \frac{M_T k_B T d_g^3}{42\pi \delta_{gb} D_{gb} b^3} \dot{\varepsilon}$$

M_T – Taylor factor

k_B – Boltzmann constant [JK⁻¹]

T – Temperature [K]

d_g – Grain diameter [m]

δ_{gb} – Grain boundary thickness (10^{-9} ; hardcoded) [m]

D_{gb} – Diffusion coefficient along grain boundaries
(reference element) [m²s⁻¹]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s⁻¹]

Coble creep

$$\sigma_{dyn,Cc} = \frac{M_T k_B T d_g^3}{42\pi \delta_{gb} D_{gb} b^3} \dot{\varepsilon}$$

variable	value
prec_domain strength	
TYS_DYN_COCS*	
TYS_DYN_COCS\$matrix	5,63809e+13

M_T – Taylor factor

k_B – Boltzmann constant [JK⁻¹]

T – Temperature [K]

d_g – Grain diameter [m]

δ_{gb} – Grain boundary thickness (10⁻⁹; hardcoded) [m]

D_{gb} – Diffusion coefficient along grain boundaries
(reference element) [m²s⁻¹]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s⁻¹]

Harper-Dorn creep

$$\sigma_{dyn,HDC} = G \left(A_{HDC} \frac{M_T k_B T}{D_{eff} b} \dot{\varepsilon} \right)^{n_{HDC}}$$

A_{HDC} – Scaling factor (10^{64} ; hardcoded)

G – Shear modulus [Pa]

M_T – Taylor factor

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

D_{eff} – Effective diffusion coefficient (reference element) [m^2s^{-1}]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

n_{HDC} – Exponent (1; hardcoded)

Harper-Dorn creep

$$\sigma_{dyn,HDC} = G \left(A_{HDC} \frac{M_T k_B T}{D_{eff} b} \dot{\varepsilon} \right)^{n_{HDC}}$$

variable	value
prec_domain strength	
TYS_DYN_HDC\$*	
TYS_DYN_HDC\$matrix	1,03742e+69

A_{HDC} – Scaling factor (10^{64} ; hardcoded)

G – Shear modulus [Pa]

M_T – Taylor factor

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

D_{eff} – Effective diffusion coefficient (reference element) [m^2s^{-1}]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

n_{HDC} – Exponent (1; hardcoded)

Grain boundary sliding, grain boundary diffusion regime

$$\sigma_{dyn,gbs,gb} = G \left(A_{gbs,gb} \frac{k_B T d_g^3}{G D_{gb} b^4} \dot{\varepsilon} \right)^{n_{gbs,gb}}$$

$A_{gbs,gb}$ – Scaling factor (10^{64} ; hardcoded)

G – Shear modulus [Pa]

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

d_g – Grain diameter [m]

D_{gb} – Diffusion coefficient along grain boundaries

(reference element) [m^2s^{-1}]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

$n_{gbs,gb}$ – Exponent (1/2; hardcoded)

Grain boundary sliding, grain boundary diffusion regime

$$\sigma_{dyn,gbs,gb} = G \left(A_{gbs,gb} \frac{k_B T d_g^3}{G D_{gb} b^4} \dot{\varepsilon} \right)^{n_{gbs,gb}}$$

variable	value
prec_domain strength	
TYS_DYN_GBS_GBS*	
TYS_DYN_GBS_GB\$matrix	2,22256e+45

$A_{gbs,gb}$ – Scaling factor (10^{64} ; hardcoded)

D_{gb} – Diffusion coefficient along grain boundaries

G – Shear modulus [Pa]

(reference element) [m^2s^{-1}]

k_B – Boltzmann constant [JK^{-1}]

b – Burgers vector [m]

T – Temperature [K]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

d_g – Grain diameter [m]

$n_{gbs,gb}$ – Exponent (1/2; hardcoded)

Grain boundary sliding, lattice diffusion regime

$$\sigma_{dyn,gbs,eff} = G \left(A_{gbs,d} \frac{k_B T d_g^2}{G D_{eff} b^3} \dot{\varepsilon} \right)^{n_{gbs,eff}}$$

$A_{gbs,d}$ – Scaling factor (10^{64} ; hardcoded)

G – Shear modulus [Pa]

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

d_g – Grain diameter [m]

D_{eff} – Effective diffusion coefficient (reference element) [m^2s^{-1}]

b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

$n_{gbs,eff}$ – Exponent (1/2; hardcoded)

Grain boundary sliding, lattice diffusion regime

$$\sigma_{dyn,gbs,eff} = G \left(A_{gbs,d} \frac{k_B T d_g^2}{G D_{eff} b^3} \dot{\varepsilon} \right)^{n_{gbs,eff}}$$

variable	value
prec_domain strength	
TYS_DYN_GBS_DISL\$*	TYS_DYN_GBS_DISL\$matrix 1,74384e+45

$A_{gbs,d}$ – Scaling factor (10^{64} ; hardcoded)

G – Shear modulus [Pa]

k_B – Boltzmann constant [JK^{-1}]

T – Temperature [K]

d_g – Grain diameter [m]

D_{eff} – Effective diffusion coefficient (reference element) [m^2s^{-1}]

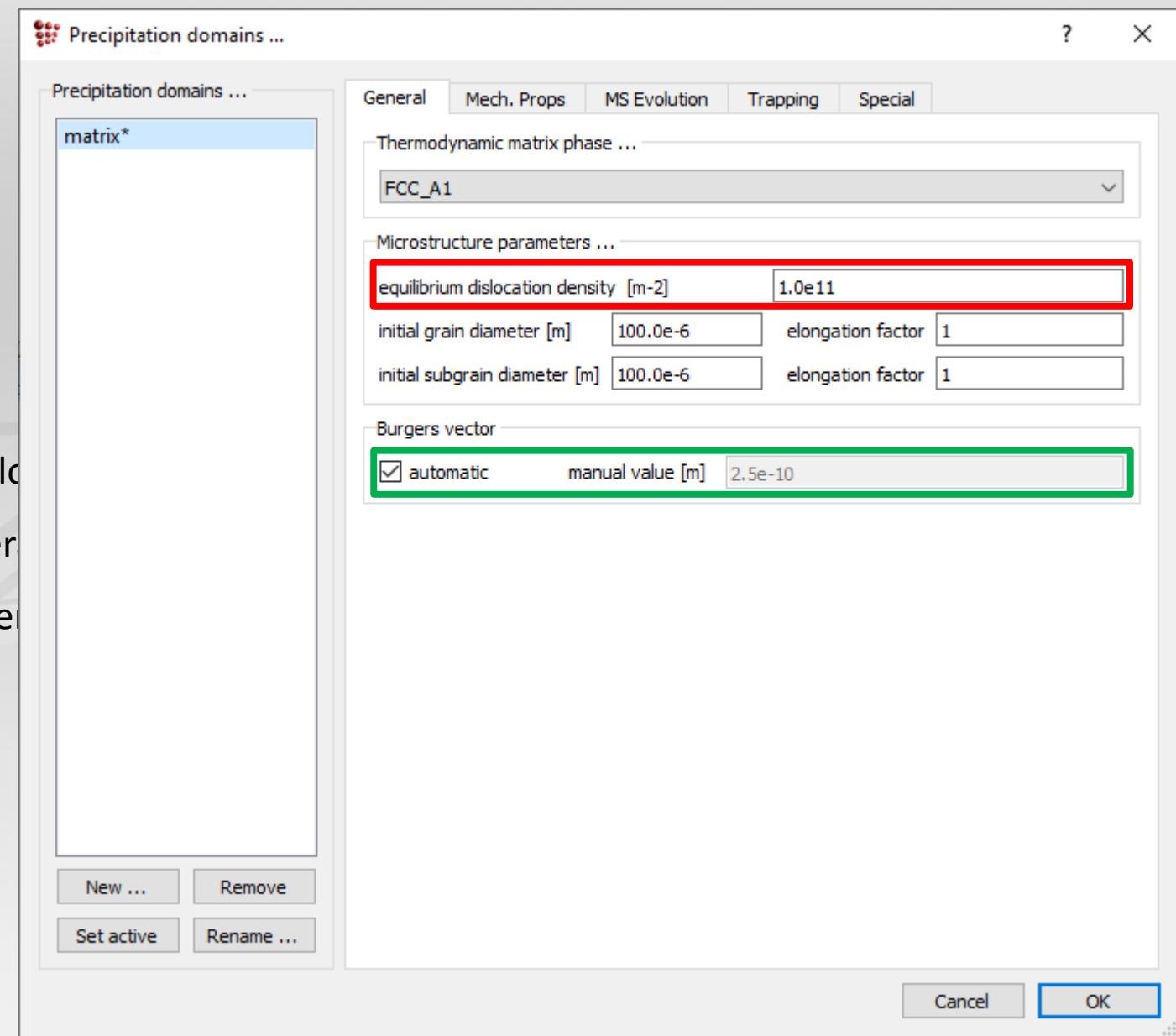
b – Burgers vector [m]

$\dot{\varepsilon}$ – Strain rate [s^{-1}]

$n_{gbs,eff}$ – Exponent (1/2; hardcoded)

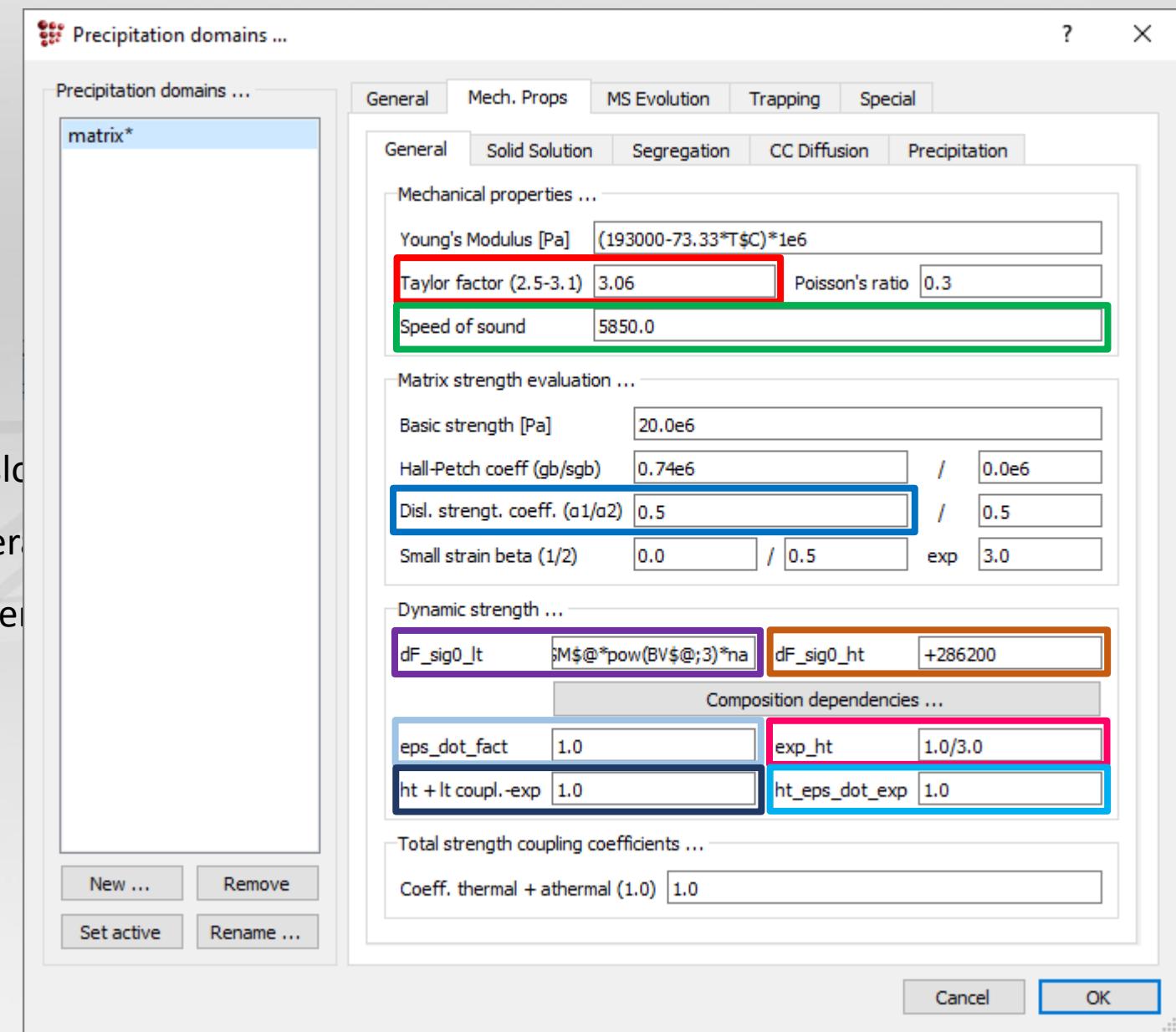
Some input values

- ρ_{eq} – Equilibrium dislocation density [m^{-2}]
- b – Burgers vector [m]
- M_T – Taylor factor
- c_{snd} – Speed of sound [ms^{-1}]
- α_{int} – Strengthening coefficient for internal dislocation
- $\Delta F_{\sigma_0}^{lt}$ – Yield stress activation energy, low temperature
- $\Delta F_{\sigma_0}^{ht}$ – Yield stress activation energy, high temperature
- A_{ε_0} – Scaling factor for strain rate limit
- n_{ht} – Exponent, high temperature
- n_{dyn} – Exponent, coupling
- n_{eps_dot} – Strain rate exponent

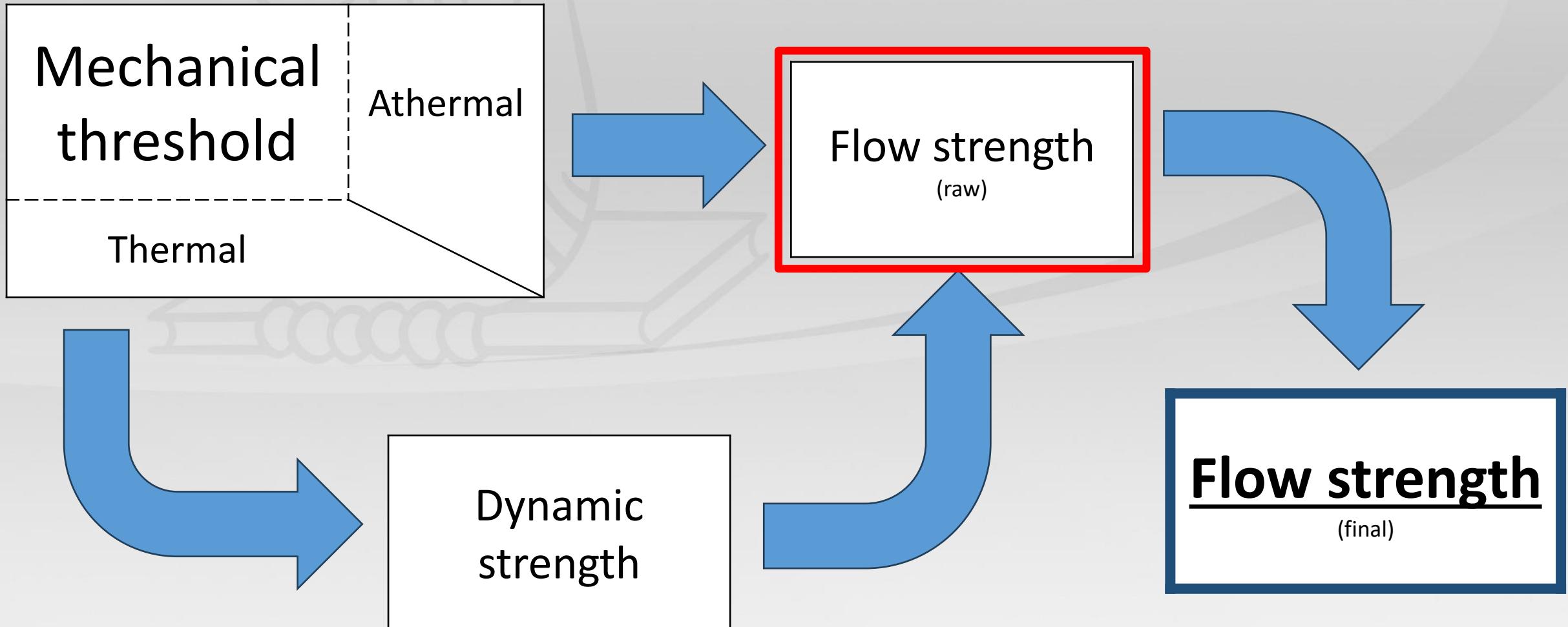


Some input values

- ρ_{eq} – Equilibrium dislocation density [m^{-2}]
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- α_{int} – Strengthening coefficient for internal dislocation
- $\Delta F_{\sigma_0}^{lt}$ – Yield stress activation energy, low temperature
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- n_{ht} – Exponent, high temperature
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- n_{eps_dot} – Strain rate exponent



Overview



Flow stress (raw)

- Sum of the athermal and dynamic contributions

$$\sigma = \sigma_{ath} + \sigma_{dyn}$$

- Strain rate absence $\rightarrow \sigma = 0$
- Values for small strains most likely overestimated - might need correction

Flow stress (raw)

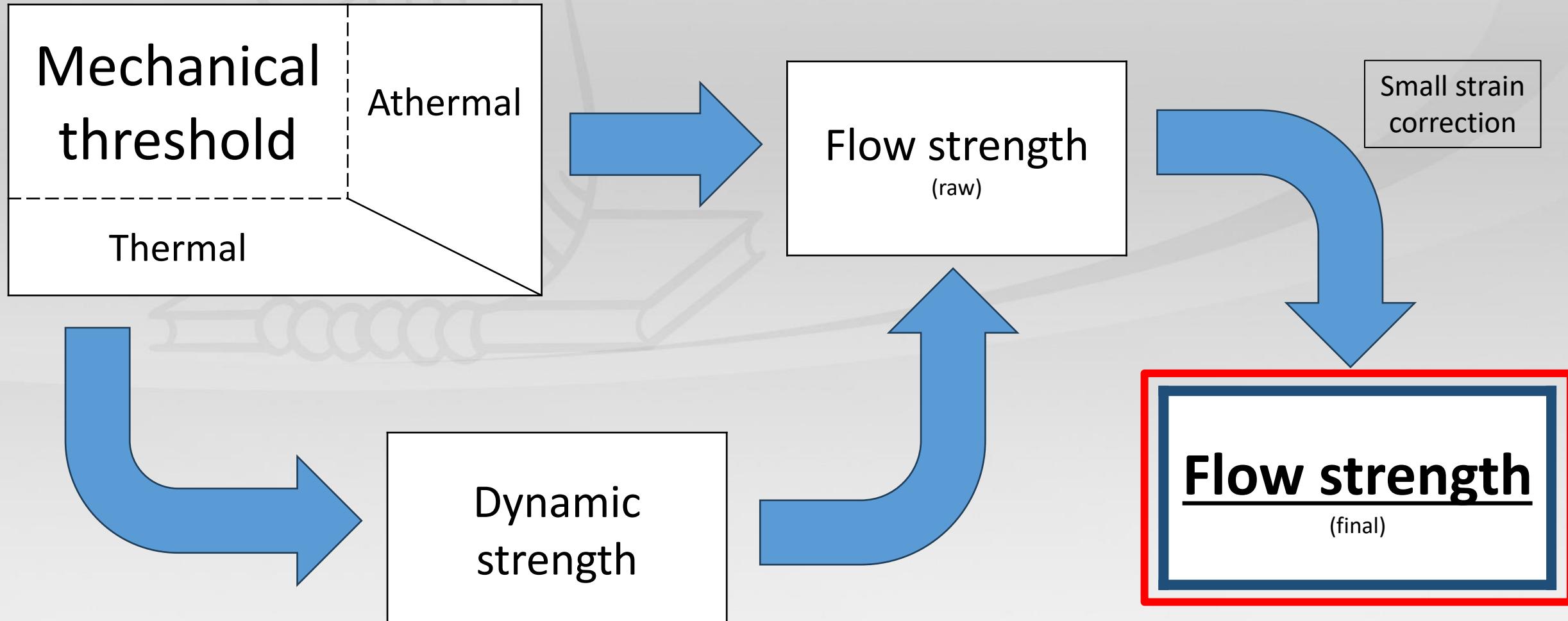
- Sum of the athermal and dynamic contributions

$$\boxed{\sigma} = \sigma_{ath} + \sigma_{dyn}$$

variable	value
prec_domain strength	
▼ TYS_NBS*	
TYS_NB\$matrix	2,40202e+08

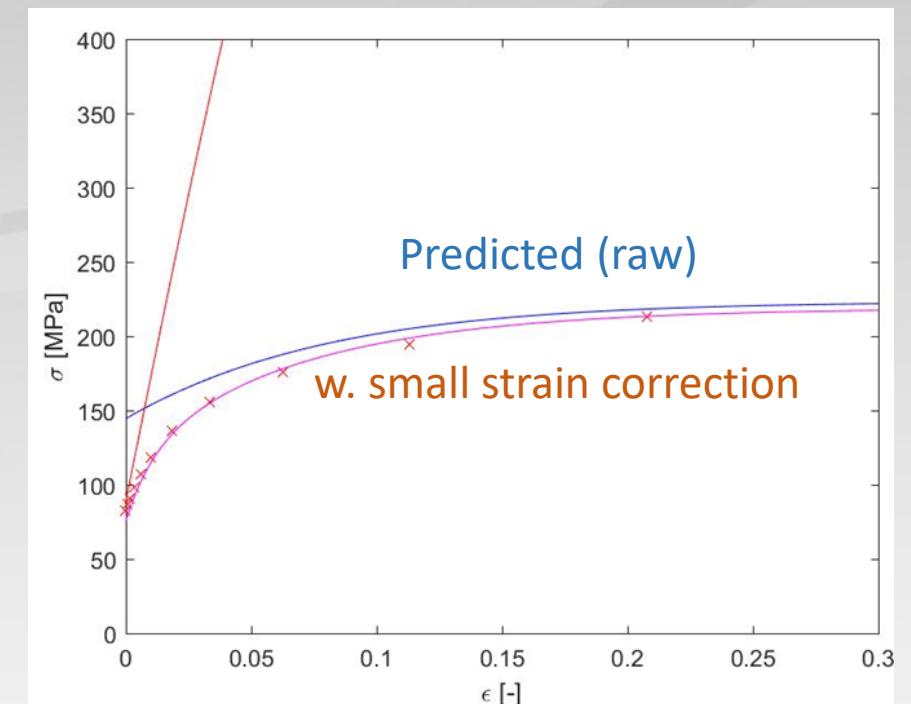
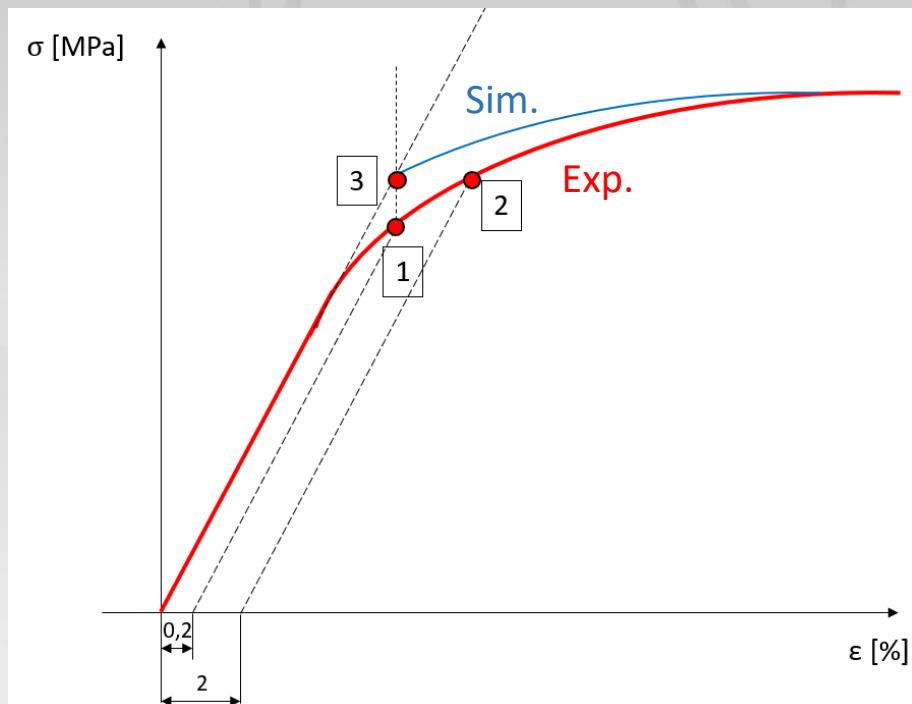
- Strain rate absence $\rightarrow \sigma = 0$
- Values for small strains most likely overestimated - might need correction

Overview



„Small strain“ correction

- Models are strictly valid for a fixed microstructure (fixed dislocation density)
- In practice → Relevant for materials with strain > 2%



„Small strain“ correction

- Models are strictly valid for a fixed microstructure (fixed dislocation density)
- In practice → Relevant for materials with strain > 2%
- Correction for small strains with a dislocation density saturation function β

$$\beta = \sqrt{\beta_1 \frac{\rho}{\rho_{sat}} + \beta_2}$$

$$\sigma_\beta^{-n} = \sigma^{-n} + (\beta\sigma)^{-n}$$

$$\sigma_\beta = \sigma(1 + \beta^{-n})^{-1/n}$$

ρ - Current dislocation density

ρ_{sat} - Saturated dislocation density

β_1, β_2 - Coefficients

n - Exponent

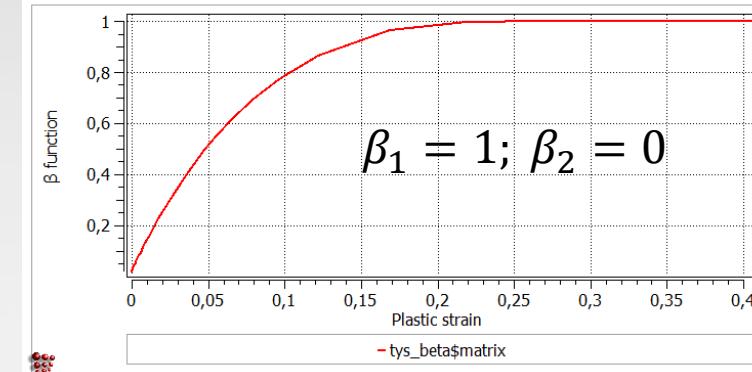
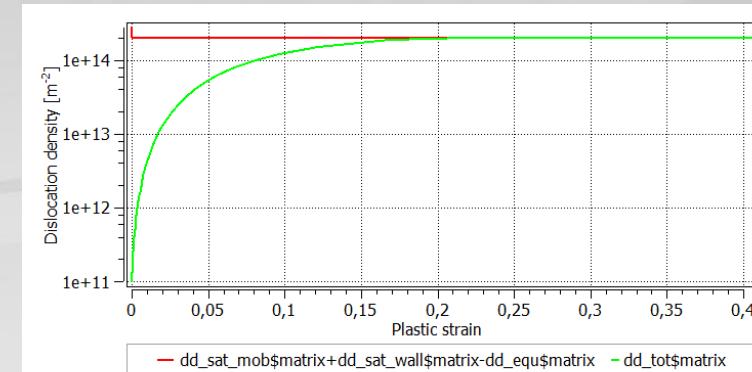
„Small strain“ correction

- Models are strictly valid for a fixed microstructure (fixed dislocation density)
- Relevant for materials with strain > 2%
- Correction for small strains with a dislocation density saturation function β

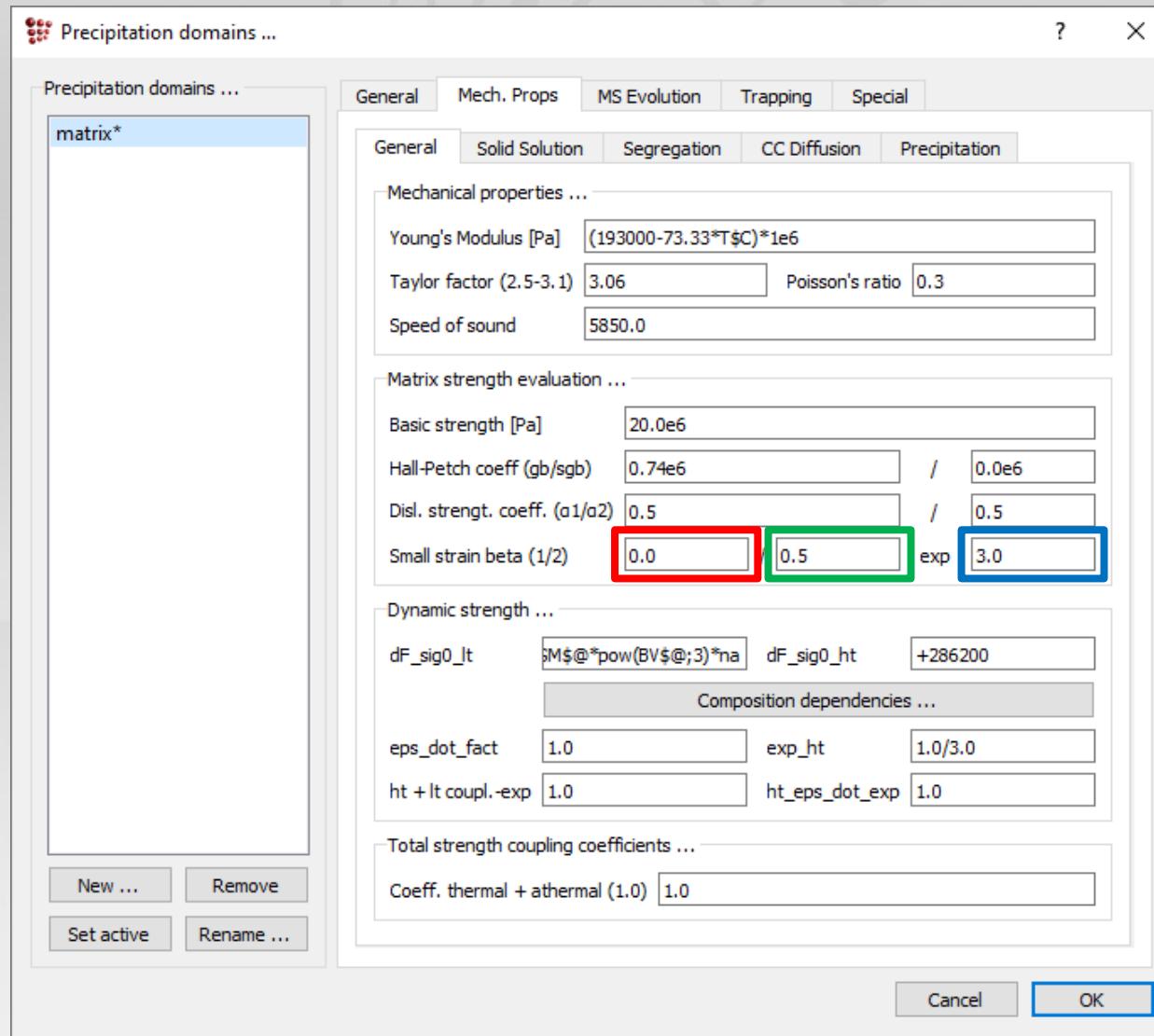
$$\beta = \sqrt{\beta_1 \frac{\rho}{\rho_{sat}} + \beta_2}$$

$$\sigma_\beta^{-n} = \sigma^{-n} + (\beta\sigma)^{-n}$$

$$\sigma_\beta = \sigma(1 + \beta^{-n})^{-1/n}$$



„Small strain“ correction



Microstructure (fixed dislocation density)

dislocation density saturation function β

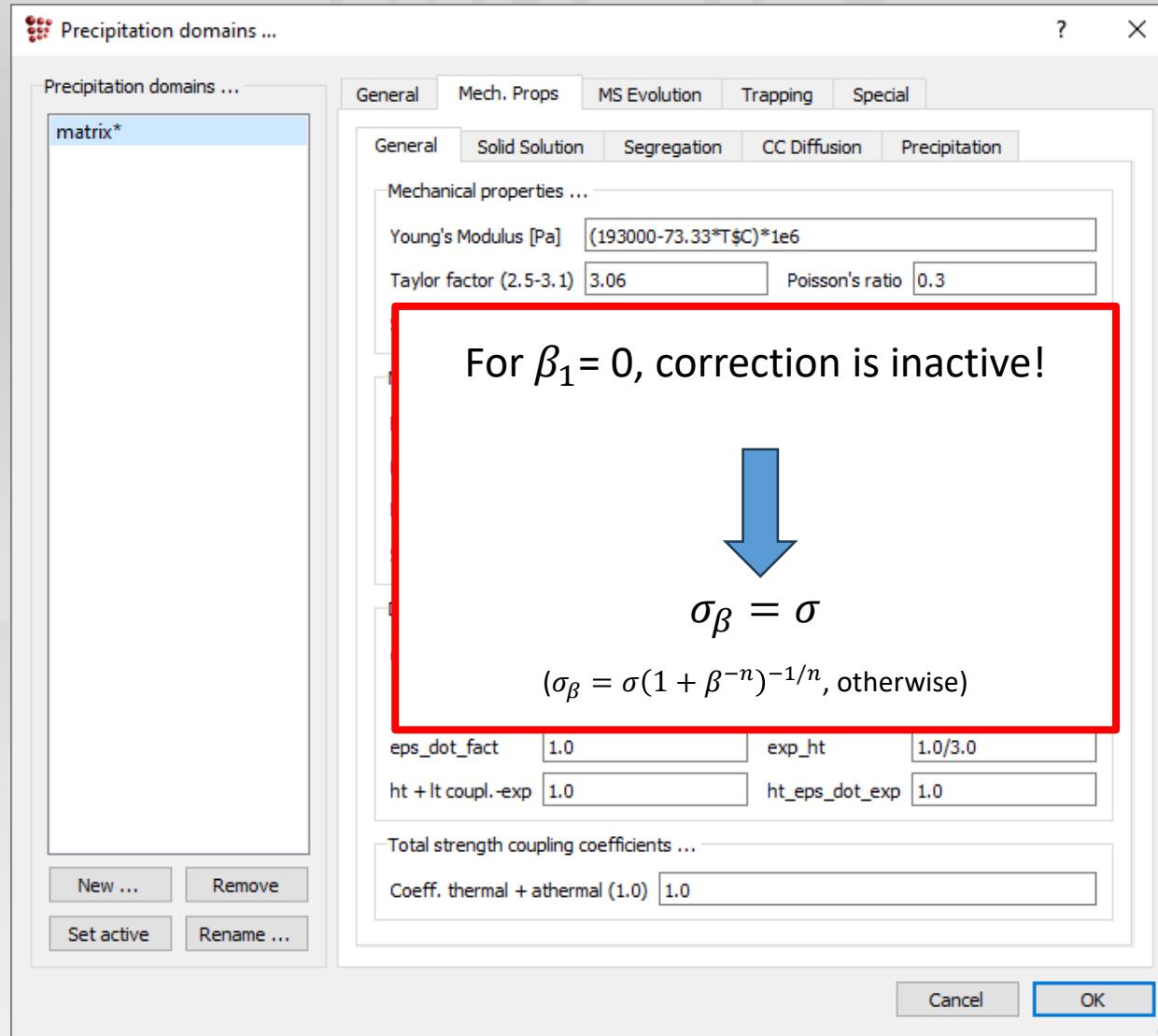
ρ - Current dislocation density

ρ_{sat} - Saturated dislocation density

β_1, β_2 - Coefficients

n - Exponent

„Small strain“ correction



Microstructure (fixed dislocation density)

dislocation density saturation function β

ρ - Current dislocation density

ρ_{sat} - Saturated dislocation density

β_1, β_2 - Coefficients

n - Exponent

„Small strain“ correction

- Models are strictly valid for a fixed microstructure (fixed dislocation density)
- Relevant for materials with strain > 2%
- Correction for small strains with a dislocation density saturation function β

$$\beta = \sqrt{\beta_1 \frac{\rho}{\rho_{sat}} + \beta_2}$$

$$\sigma_\beta^{-n} = \sigma^{-n} + (\beta\sigma)^{-n}$$

$$\boxed{\sigma_\beta} = \sigma(1 + \boxed{\beta}^{-n})^{-1/n}$$

variable	value
prec_domain strength	
TYSS*	
TYSS\$matrix	1,90543e+08
TYS_BETA\$*	
TYS_BETA\$matrix	1,00025

Acknowledgments

- Johannes Kreyca
- Bernhard Viernstein
- Yao Shan



MatCalc

Engineering

Thank you for
your attention!

