MatCalc Engineering

Evaluation of mechanical threshold for alloys with MatCalc
(rel. 6.04.1004)

P. Warczok

Mechanical threshold

- Yield stress at temperature 0 K
- Microstructure dependent

$$\sigma_0 = f\left(\rho, d_g, d_{sg}, c_i^m, r_{p_j}, N_{p_j}, \ldots\right)$$

- 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_{p_j} - Radius of precipitate j [m]

N_{p_j} - Number density of precipitate j [m^{-3}]

σ_{ath} - Athermal contribution [Pa]

σ_{th} - Thermal contribution [Pa]

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Model overview

- Contributions to mechanical threshold, σ_0
  - Intrinsic strength, σ_i
  - Work hardening, σ_{disl}
  - Grain/subgrain boundary strengthening, σ_{gb} , σ_{sgb}
  - Solid solution strengthening, σ_{ss}
  - Precipitation strenghtening, σ_{prec}

$$\sigma_0 = f(\sigma_i, \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \sigma_{ss}, \sigma_{prec})$$

Model overview

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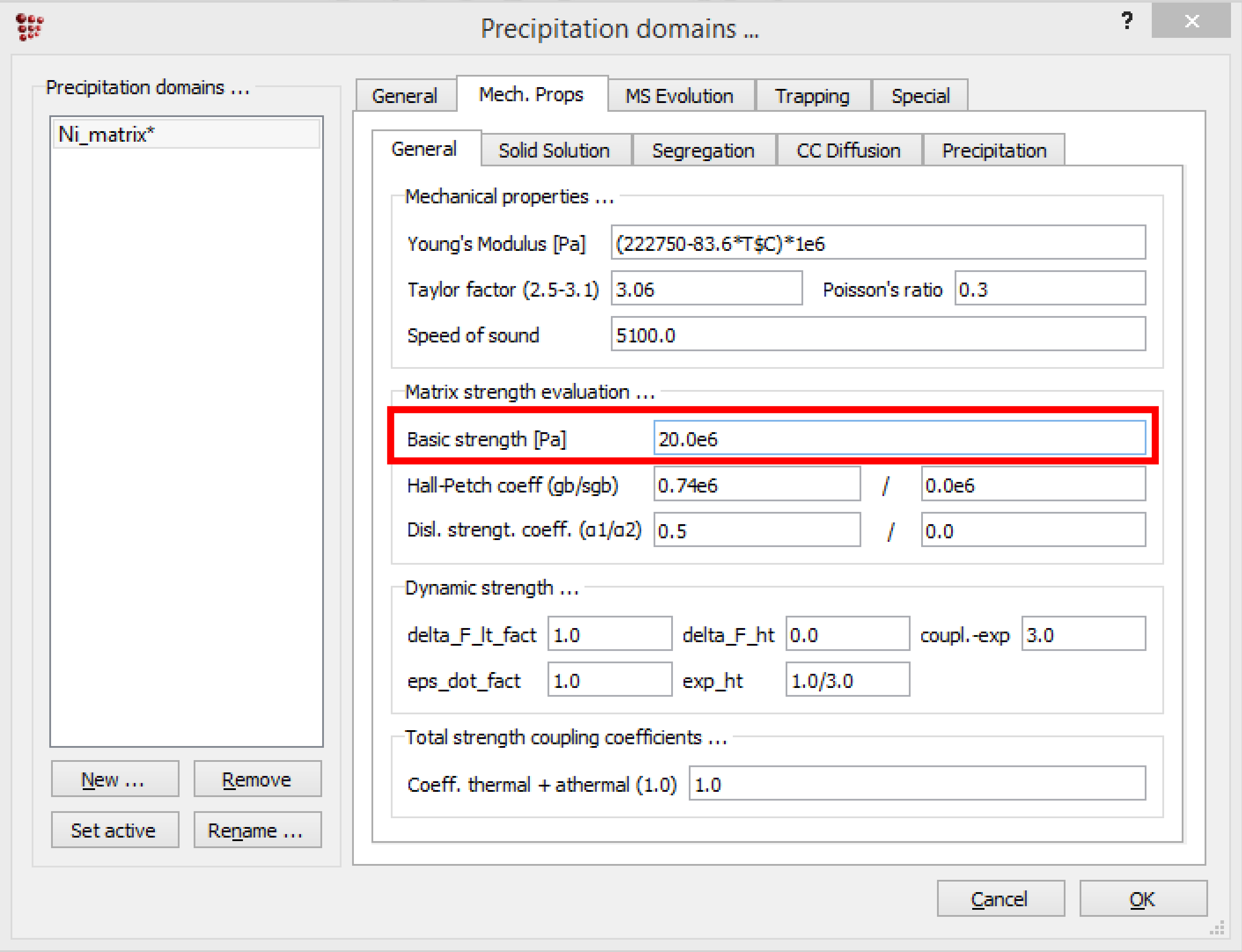
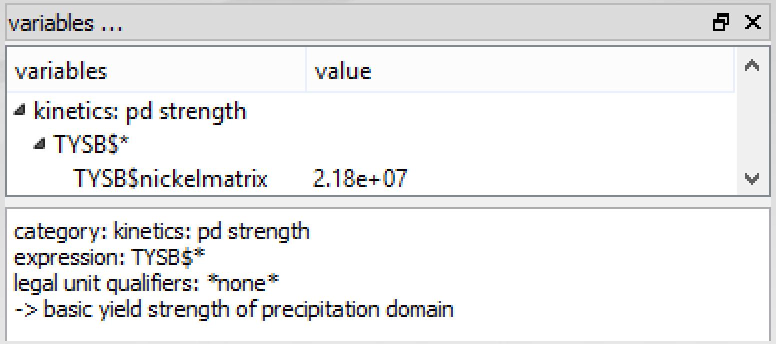
Intrinsic strength, σ_i





Model overview

- Contributions to yield strength, σ_{YS}
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  - Work hardening, σ_{disl}
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$$\sigma_0 = f(\sigma_i, \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \sigma_{ss}, \sigma_{prec})$$

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Work hardening, σ_{disl}

- Taylor equation

$$\sigma_{disl} = \alpha M G b \sqrt{\rho}$$

M - Taylor factor

G - Shear modulus

b - Burger's vector

ρ - Dislocation density

α - Strengthening coefficient

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Work hardening, σ_{disl}

- Taylor equation

$$\sigma_{disl} = \alpha M G b \sqrt{\rho}$$

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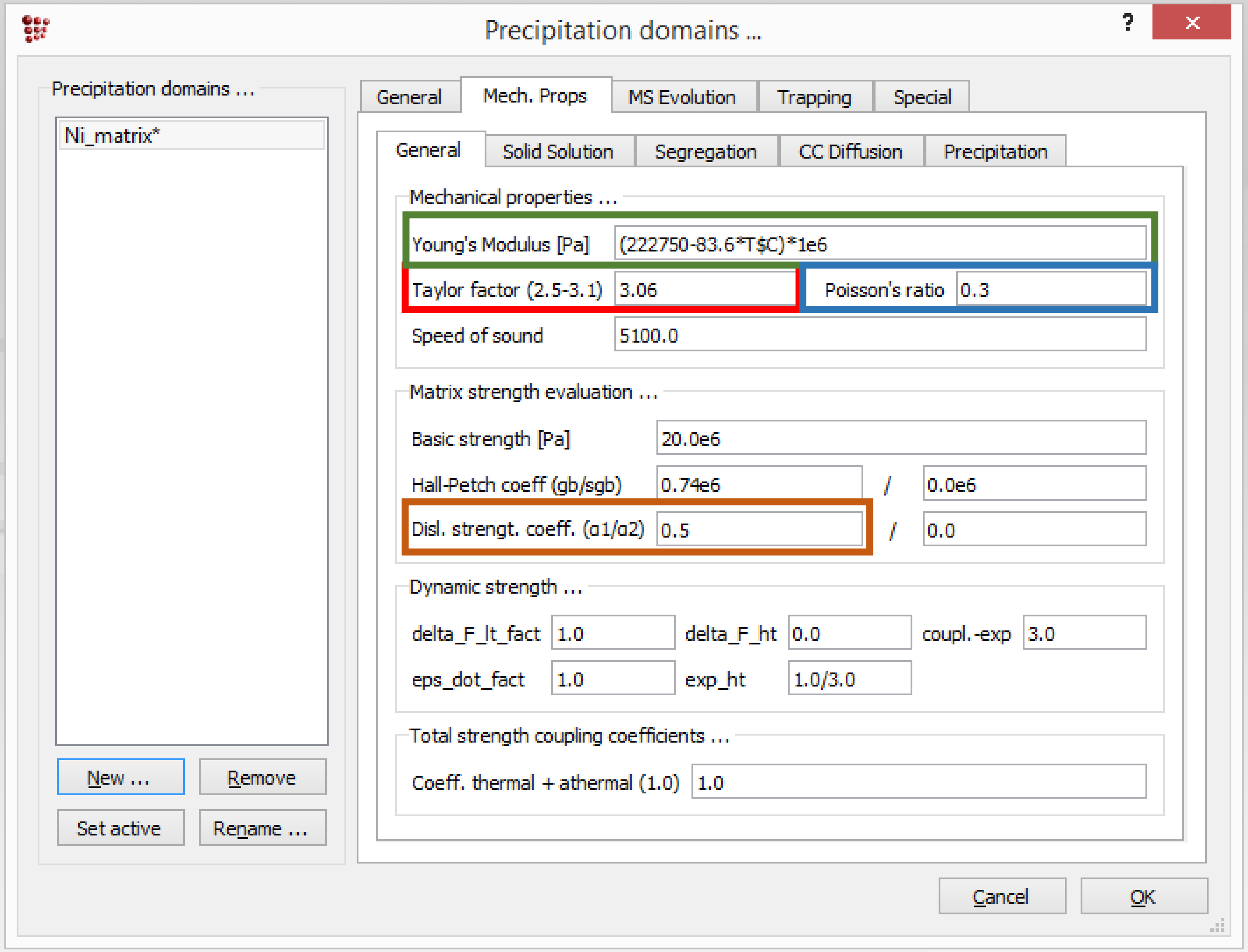
α - Strengthening coefficient

$$G = \frac{E}{2(1-\upsilon)}$$



Work hardening, σ_{disl}

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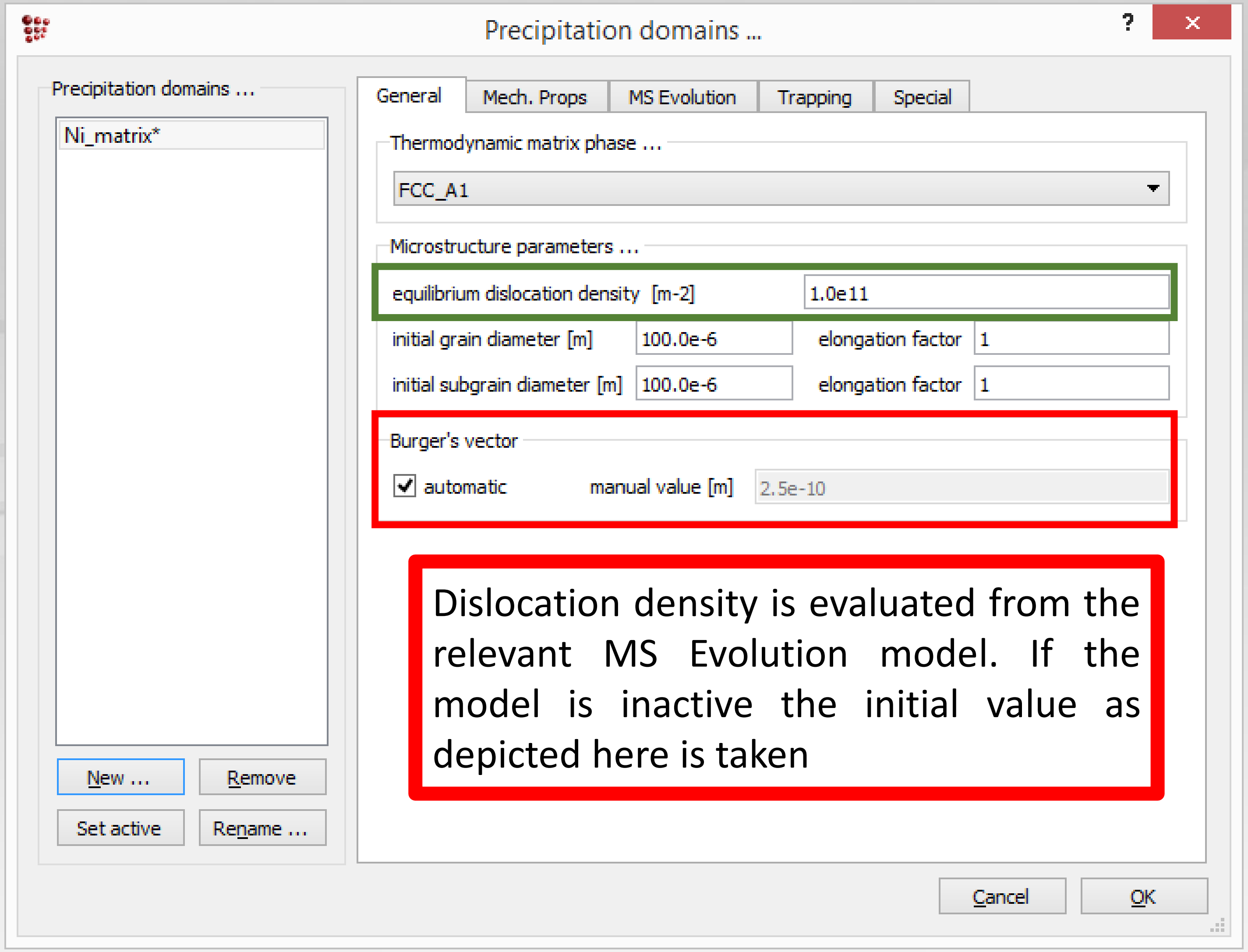


Dislocation density is evaluated from the relevant MS Evolution model. If the model is inactive the initial value as depicted here is taken

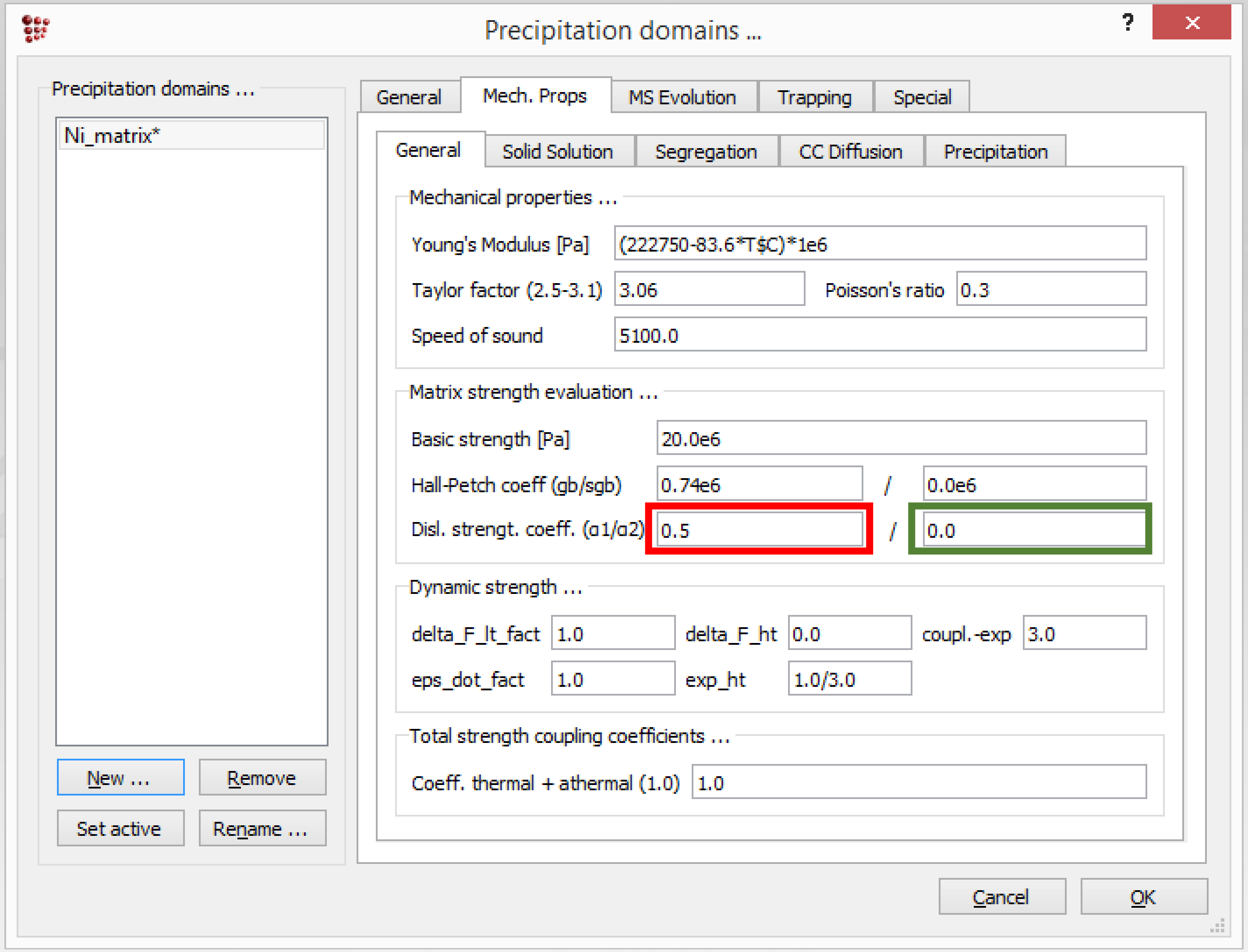
Work hardening, σ_{disl}

- Taylor equation
  - Two parameter model

$$\sigma_{disl} = \alpha_1 MGb\sqrt{\rho_1} + \alpha_2 MGb\sqrt{\rho_2}$$

ρ_1 - Internal dislocation density

ρ_2 - Wall dislocation density



Work hardening, σ_{disl}

- Taylor equation
  - Two parameter model

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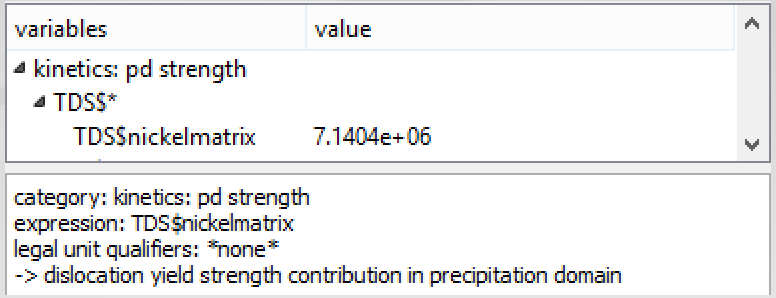

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- Contributions to yield strength, σ_{YS}
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$$\sigma_0 = f(\sigma_i, \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \sigma_{ss}, \sigma_{prec})$$

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Grain/subgrain boundary strengthening, σ_{gb} , σ_{sgb}

- Hall-Petch equation

$$\sigma_{gb} = \frac{k_{gb}}{\sqrt{D}} \qquad \sigma_{sgb} = \frac{k_{sgb}}{\sqrt{\delta}}$$

D - Grain diameter

δ - Subgrain diameter

k_n - Constant

Grain/subgrain boundary strengthening, σ_{gb}, σ_{sgb}

- Hall-Petch equation

$$\sigma_{gb} = \frac{k_{gb}}{\sqrt{D}} \qquad \sigma_{sgb} = \frac{k_{sgb}}{\sqrt{\delta}}$$

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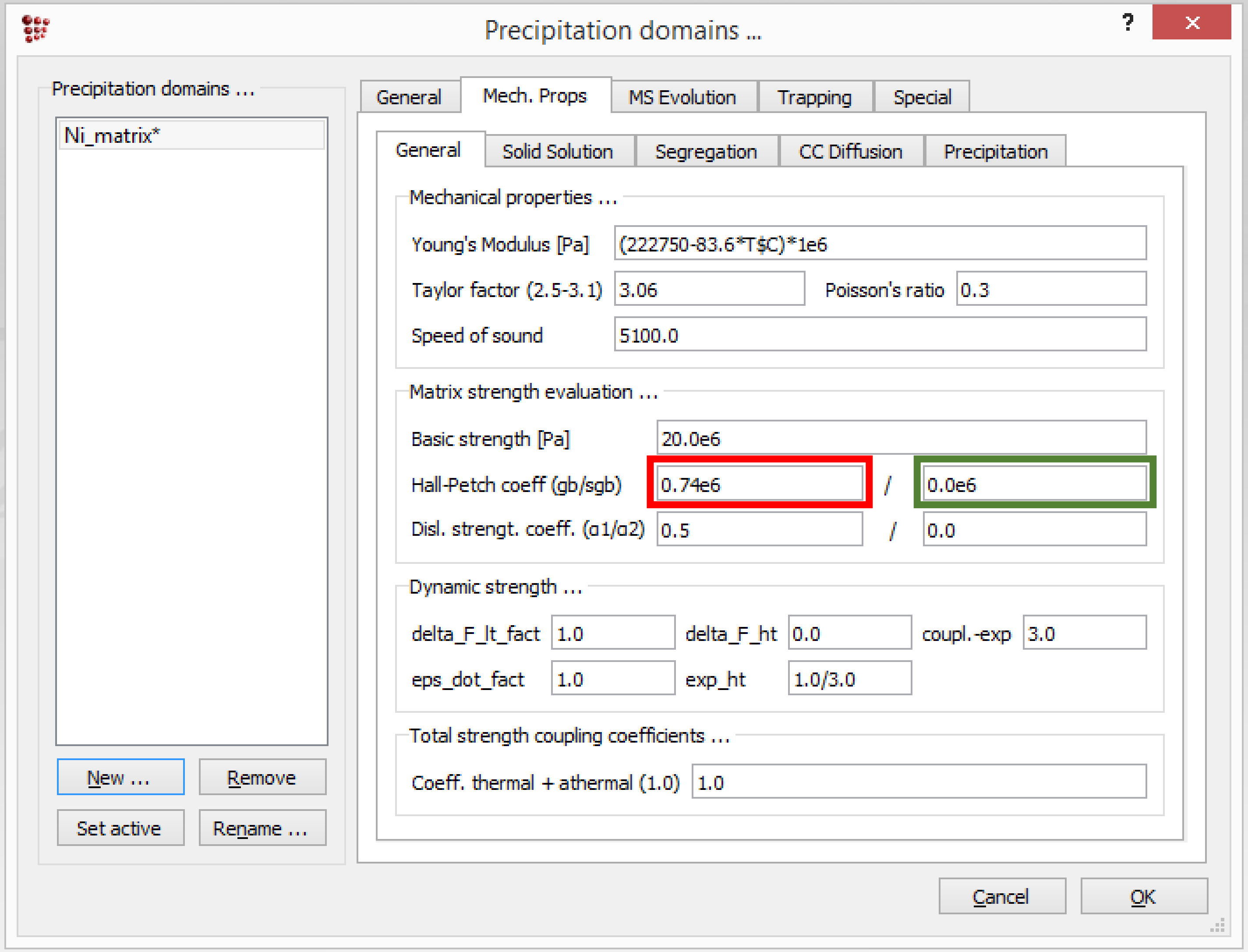

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Grain/subgrain boundary strengthening, σ_{gb} , σ_{sgb}

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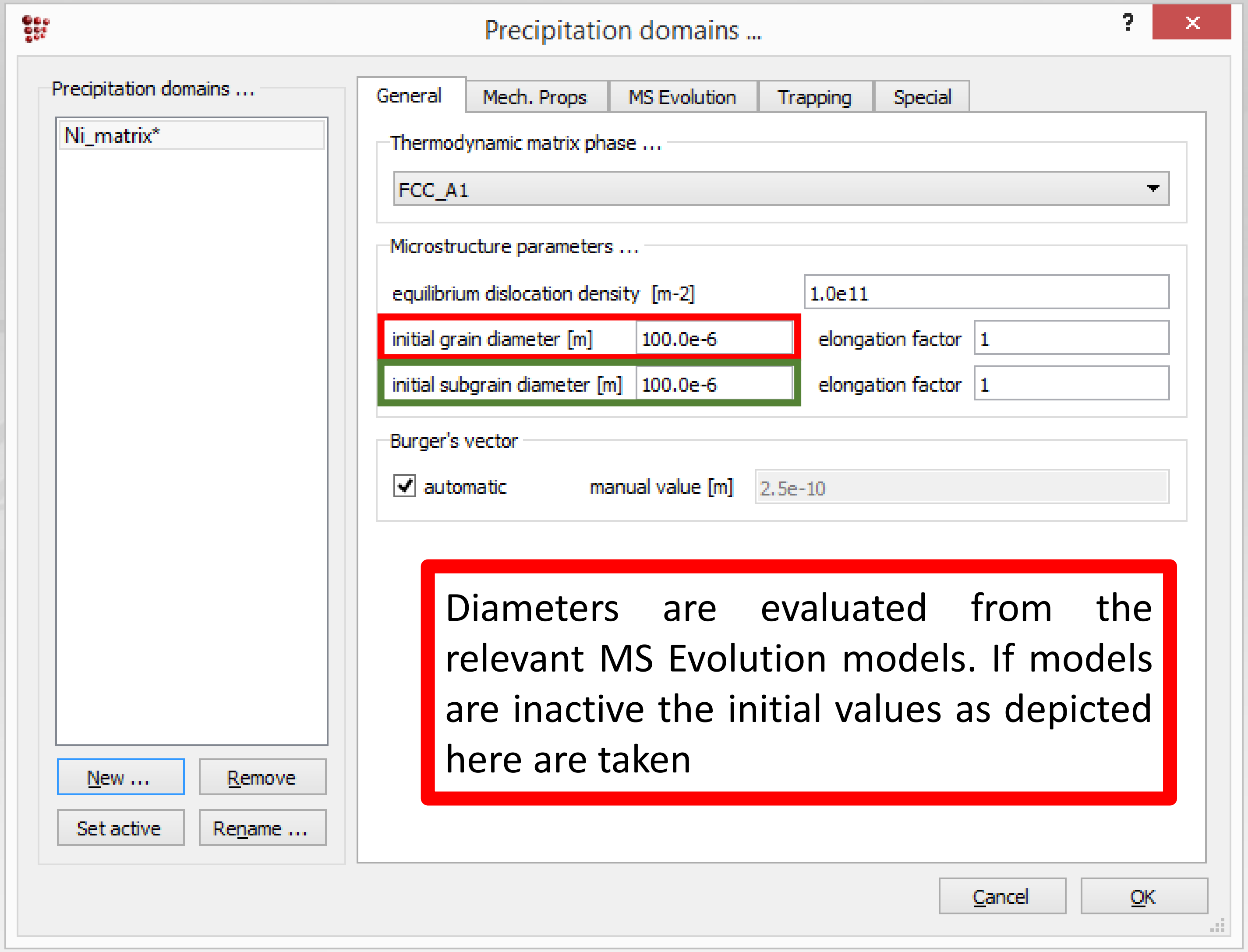

Grain/subgrain boundary strengthening, σ_{gb} , σ_{sgb}

- Hall-Petch equation

$$\sigma_{gb} = \frac{k_{gb}}{\sqrt{D}} \qquad \sigma_{sgb} = \frac{k_{sgb}}{\sqrt{\delta}}$$

D - Grain diameter

δ - Subgrain diameter

k_n - Constant

variables	value
◢ kinetics: pd strength	
◢ TGS$*	
TGS$nickelmatrix	3.57771e+07

category: kinetics: pd strength
expression: TGS$*
legal unit qualifiers: *none*
-> fine grain yield strength contribution in precipitation domain

variables	value
◢ kinetics: pd strength	
◢ TSGS$*	
TSGS$nickelmatrix	0

category: kinetics: pd strength
expression: TSGS$nickelmatrix
legal unit qualifiers: *none*
-> subgrain yield strength contribution in precipitation domain

Model overview

- Contributions to yield strength, σ_{YS}
  - Intrinsic strength, σ_i
  - Work hardening, σ_{disl}
  - Grain/subgrain boundary strengthening, σ_{gb} , σ_{sgb}
  - Solid solution strengthening, σ_{ss}
  - Precipitation strenghtening, σ_{prec}

$$\sigma_0 = f\left(\sigma_i, \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \sigma_{ss}, \sigma_{prec}\right)$$

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Solid solution strengthening, σ_{ss}

$$\sigma_{ss} = \left[\left(\sum_i \left(k_i c_i^{n_i} \right)^{m_{sub}} \right)_{sub}^{\frac{m_{tot}}{m_{sub}}} + \left(\sum_i \left(k_i c_i^{n} \right)^{m_{int}} \right)_{int}^{\frac{m_{tot}}{m_{int}}} \right]^{\frac{1}{m_{tot}}}$$

k_i - Coefficient for element i

c_i - Element i content in the prec. Domain (mole fraction)

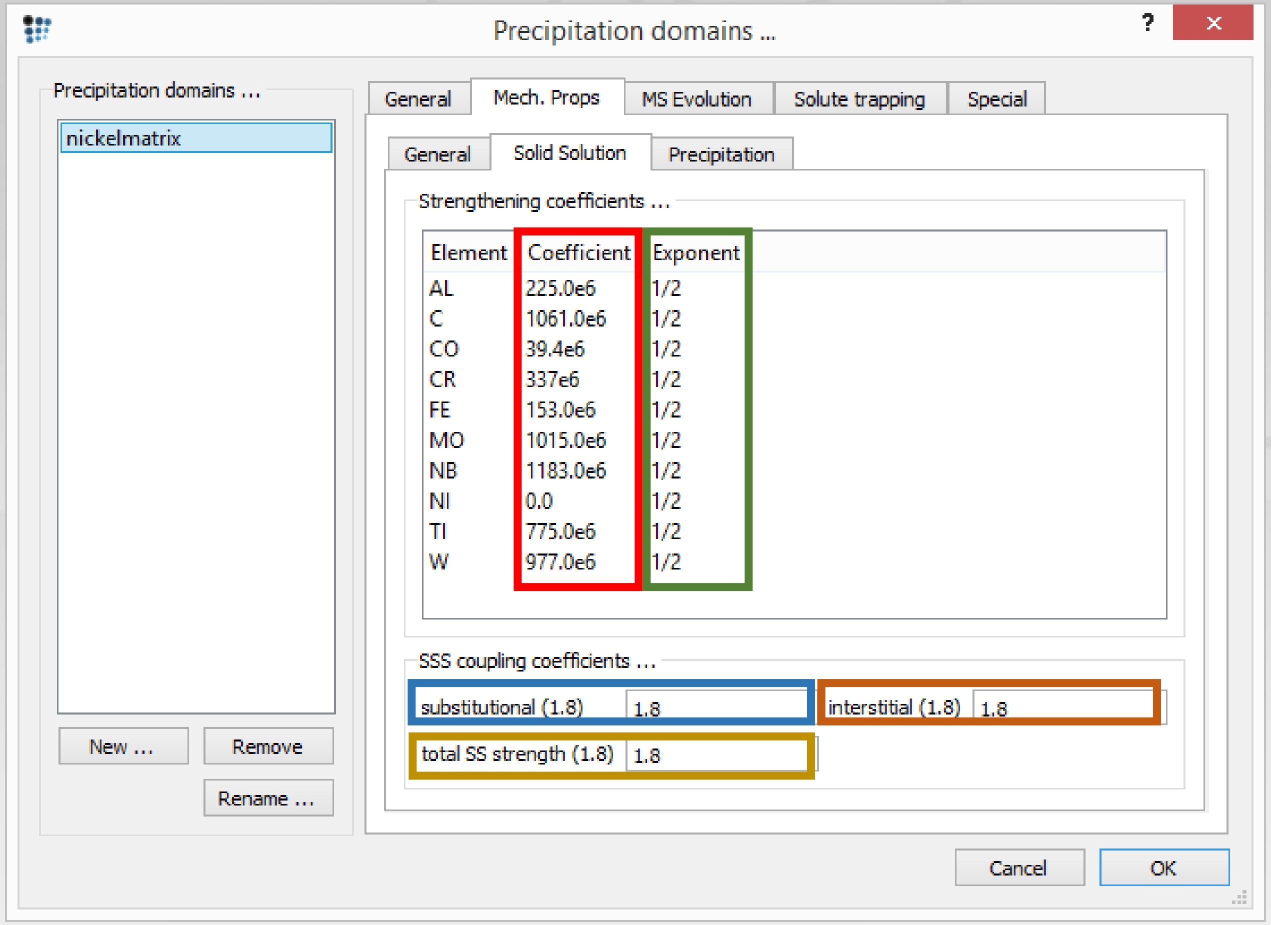
n_i - Exponent for element i

m_{sub} - Exponent for substitutional elements

m_{int} - Exponent for interstitial elements

m_{tot} - Global exponent

Solid solution strengthening, σ_{ss}



$$\sigma_{ss} = \left[\left(\sum_i \left(k_i c_i^{n_i} \right)^{m_{sub}} \right)_{sub}^{\frac{m_{tot}}{m_{sub}}} + \left(\sum_i \left(k_i c_i^{n} \right)^{m_{int}} \right)_{int}^{\frac{m_{tot}}{m_{int}}} \right]^{\frac{1}{m_{tot}}}$$

k_i - Coefficient for element *i*

c_i - Element i content in the prec. domain

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Solid solution strengthening, σ_{ss}

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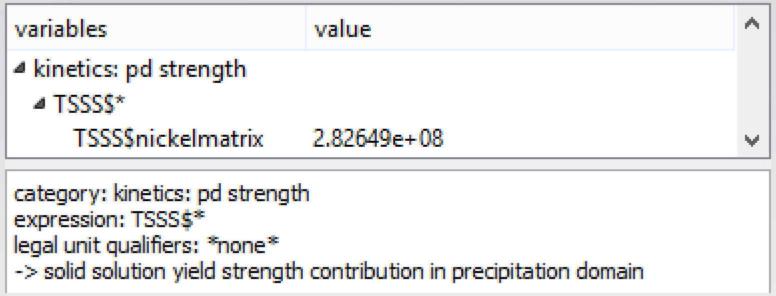

Solid solution strengthening, σ_{ss}

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$$\sigma_{ss} = \left[\left(\sum_i \left(k_i c_i^{n_i} \right)^{m_{sub}} \right)_{sub}^{\frac{m_{tot}}{m_{sub}}} + \left(\sum_i \left(k_i c_i^{n} \right)^{m_{int}} \right)_{int}^{\frac{m_{tot}}{m_{int}}} \right]^{\frac{1}{m_{tot}}}$$

variables	value
kinetics: pd strength	
TSSS_EL$*$*	
TSSS_EL$nickelmatrix$*	
TSSS_EL$nickelmatrix$VA	0
TSSS_EL$nickelmatrix$AL	2.78874e+07
TSSS_EL$nickelmatrix$C	4.56667e+07
TSSS_EL$nickelmatrix$CO	1.27085e+07
TSSS_EL$nickelmatrix$CR	1.70234e+08
TSSS_EL$nickelmatrix$FE	5.49895e+07
TSSS_EL$nickelmatrix$MO	1.47716e+08
TSSS_EL$nickelmatrix$NB	8.44694e+07
TSSS_EL$nickelmatrix$NI	0
TSSS_EL$nickelmatrix$TI	1.95807e+07
TSSS_EL$nickelmatrix$W	5.71824e+07

category: kinetics: pd strength
expression: TSSS_EL$*$W
legal unit qualifiers: *none*
-> solid solution yield strength contribution of element in precipitation domain

Model overview

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  - Intrinsic strength, σ_i
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$$\sigma_0 = f\left(\sigma_i, \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \sigma_{ss}, \sigma_{prec}\right)$$

Precipitation strengthening, σ_{prec}

- 2 alternative models available
  - Size distribution dependent strengthening
  - Co-cluster strengthening

- $\tau_{prec} \rightarrow \sigma_{prec}$

τ_{prec} - Critical shear stress for a dislocation to cut/by-pass a particle

Precipitation strengthening, σ_{prec}

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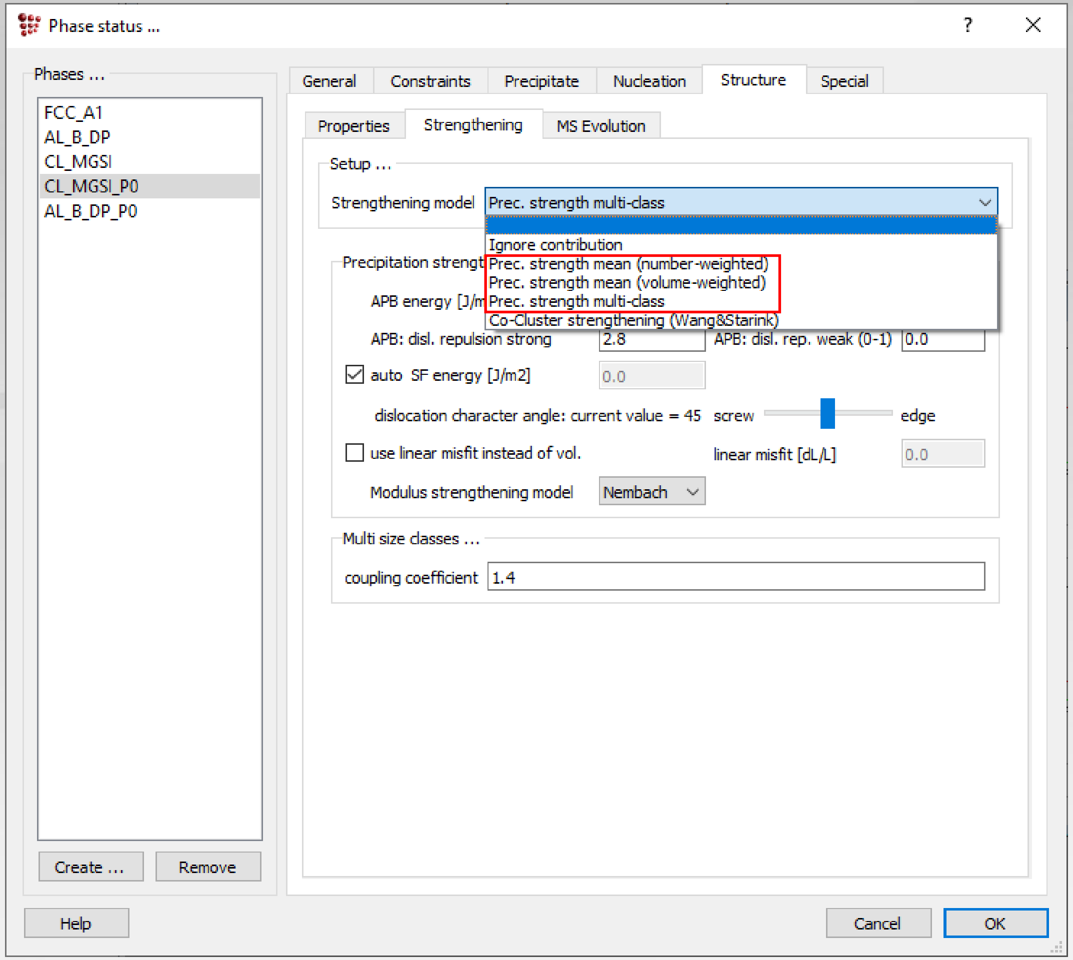
- 2 alternative models available
  - Size distribution dependent strengthening
  - Co-cluster strengthening



Size distribution dependent strengthening

- Precipitate size dependence
- Some general parameters/settings
- 2 scenarios for dislocation behavior:
  - Non-shearable particles (Orowan mechanism) → bypassing precipitate
  - Shearable particles (weak or strong) → cutting precipitate
- Critical stresses for both scenarios are evaluated

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Size distribution dependent strengthening

- Precipitate size dependence
  - Contributions dependent on precipitate size
  - Various choices for precipitate size parameter selection possible
    - Number weighted mean radius
    - Volume weighted mean radius
    - Size class radius

Size distribution dependent strengthening

- Various choices possible
  - Number-weighted mean radius, $r_{m,n}$

$$r_{m,n} = \frac{\sum_i N_i r_i}{\sum_i N_i}$$

  - Volume-weighted mean radius, $r_{m,v}$

$$r_{m,v} = \frac{\sum_i N_i r_i^4}{\sum_i N_i r_i^3}$$

  - Size class radius, r_i

Precipitate size distribution

Size class index i	Size class radius r_i	Size class number density N_i
0	r_0	N_0
1	r_1	N_1
2	r_2	N_2
3	r_3	N_3
…	…	…

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Size distribution dependent strengthening

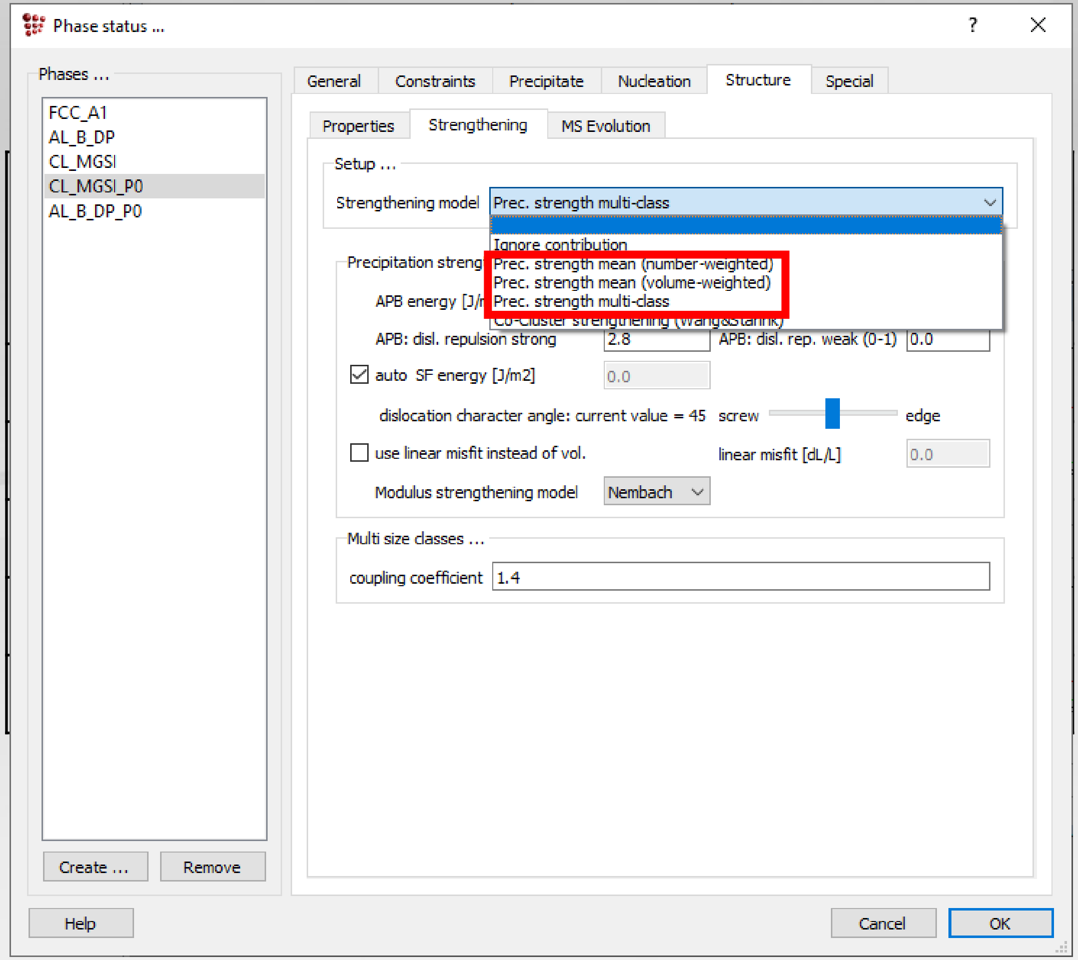
- Various choices possible
  - Number-weighted mean radius, $r_{m,n}$

$$r_{m,n} = \frac{\sum_i N_i r_i}{\sum_i N_i}$$

  - Volume-weighted mean radius, $r_{m,v}$

$$r_{m,v} = \frac{\sum_i N_i r_i^4}{\sum_i N_i r_i^3}$$

  - Size class radius, r_i (multi-class model)



Size distribution dependent strengthening

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Size distribution dependent strengthening

- Some general parameters/settings
  - Angle between dislocation line and Burger's vector, θ

    (edge/screw ratio; θ = 0 for pure screw; θ = π/2 for pure edge)
  - Equivalent radius, r_{eq} (describes precipitate-dislocation interference area)
  - Mean distance between the precipitate surfaces, L_S

Size distribution dependent strengthening

- Some general parameters/settings
  - Angle between dislocation line and Burger's vector θ

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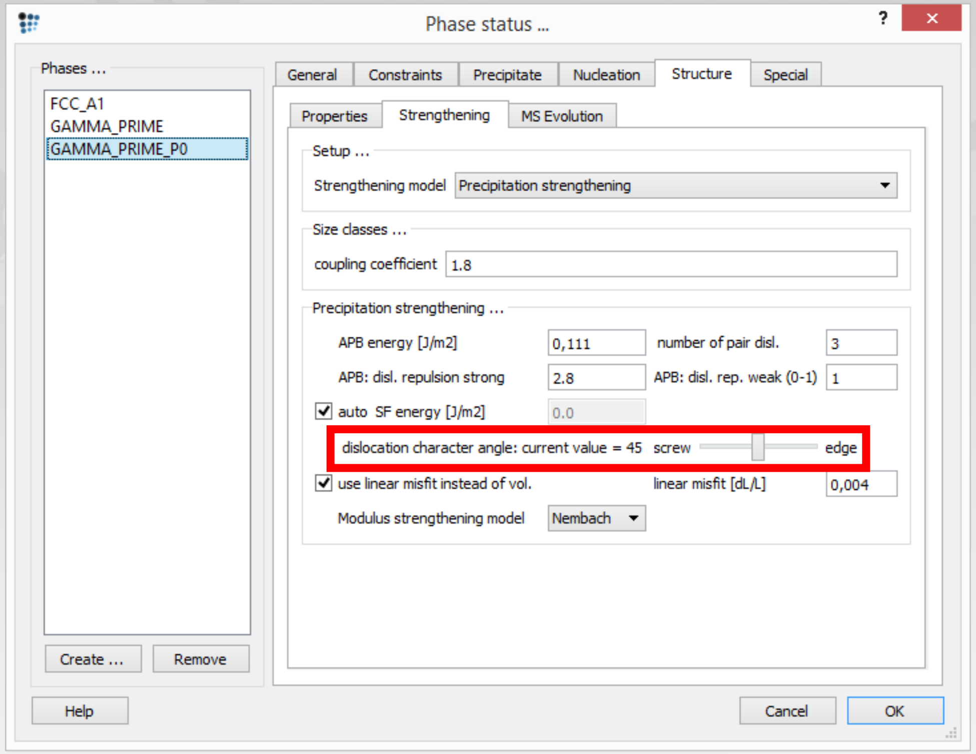

Size distribution dependent strengthening

- Some general parameters/settings
  - Equivalent radius, r_{eq} (describes precipitate-dislocation interference area)

$$r_{eq} = \frac{\pi}{4} r_m$$

r_m - Precipitate mean radius

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Size distribution dependent strengthening

- Some general parameters/settings
  - Mean distance between the precipitate surfaces, L_S

$$L_S = \sqrt{\frac{\ln 3}{2\pi \sum_{class} N_{V,class} r_{m,class}} + 4r_{ss}^2} - 2r_{ss}$$

$$r_{ss} = \sqrt{\frac{2}{3}\frac{\sum_{class} N_{V,class} r_{m,class}^2}{\sum_{class} N_{V,class} r_{m,class}}}$$

$N_{V,class}$ - Precipitate number density within the class

$r_{m,class}$ - Precipitate mean radius within the class

variables	value
◢ kinetics: precipitates	
◢ L_MEAN_2D$*	
L_MEAN_2D$GAMMA_PRIME_P0	2.02552e-08

category: kinetics: precipitates
expression: L_MEAN_2D$GAMMA_PRIME_P0
legal unit qualifiers: *none*
-> mean distance between randomly distributed precipitates on a single plane (2-dimensional)

Size distribution dependent strengthening

- Precipitate size dependence
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- 2 scenarios for dislocation behavior:
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Non-shearable particles

$$\tau_{nsh} = \frac{JGb}{2\pi L_S} ln\left(\frac{\pi}{2}\frac{r_{eq}}{r_i} f(\theta,h)\right)$$

$$J = \frac{1-\upsilon\left[cos^2\left(\frac{\pi}{2}-\theta\right)\right]}{1-\upsilon}$$

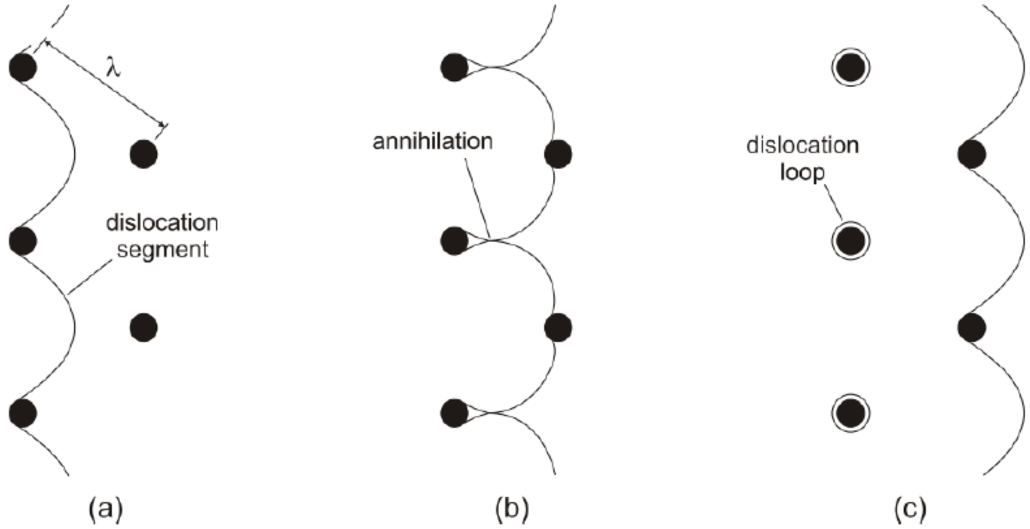

Figure 3.12. Bypassing of strong obstacles by a dislocation according to Orowan. λ denotes the mean planar spacing of precipitates[91].

$$f(\theta,h) = \frac{h^{2/3}}{3}\left[\left(\sqrt{\frac{3}{2+h^2}} + \sqrt{\frac{3}{h^2}+\frac{3}{2+h^2}}\right)sin^2\theta + \left(\sqrt{\frac{1}{h^2}} + \sqrt{\frac{9}{2+h^2}+\frac{1}{h^2}}\right)cos^2\theta\right]$$

Non-shearable particles

τ_{nsh} - Critical stress for a dislocation to by-pass the precipitate

$$\tau_{nsh} = \frac{JGb}{2\pi L_S} ln\left(\frac{\pi}{2}\frac{r_{eq}}{r_i} f(\theta, h)\right)$$

G - Shear modulus

b - Burgers vector

υ - Poisson‘s ratio

r_{eq} – Equivalent radius

θ - $\angle(b;$ dislocation line)

r_i – dislocation core radius

h - Shape factor

$$J = \frac{1 - \upsilon\left[cos^2\left(\frac{\pi}{2} - \theta\right)\right]}{1 - \upsilon}$$

$$f(\theta, h) = \frac{h^{2/3}}{3}\left[\left(\sqrt{\frac{3}{2 + h^2}} + \sqrt{\frac{3}{h^2} + \frac{3}{2 + h^2}}\right) sin^2\theta + \left(\sqrt{\frac{1}{h^2}} + \sqrt{\frac{9}{2 + h^2} + \frac{1}{h^2}}\right) cos^2\theta\right]$$

Non-shearable particles

τ_{nsh} - Critical stress for a dislocation to by-pass the precipitate

G - Shear modulus

b - Burgers vector

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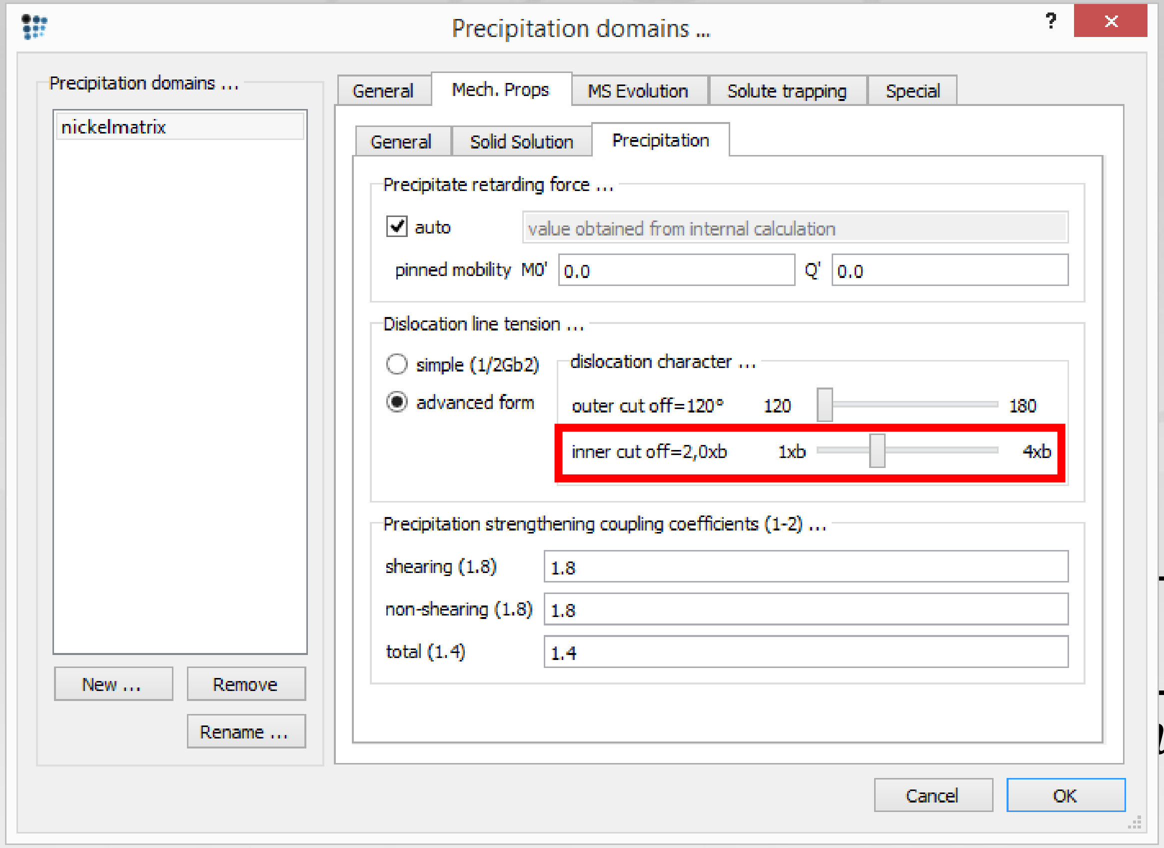

$$\ldots\Big)\sin^2\theta + \left(\sqrt{\frac{1}{h^2}} + \sqrt{\frac{9}{2+h^2} + \frac{1}{h^2}}\right)\cos^2\theta\Big]$$

Non-shearable particles

τ_{nsh} - Critical stress for a dislocation to by-pass the precipitate

G - Shear modulus

b - Burgers vector

υ - Poisson's ratio

r_{eq} – Equivalent radius

θ - $\angle(b;$ dislocation line)

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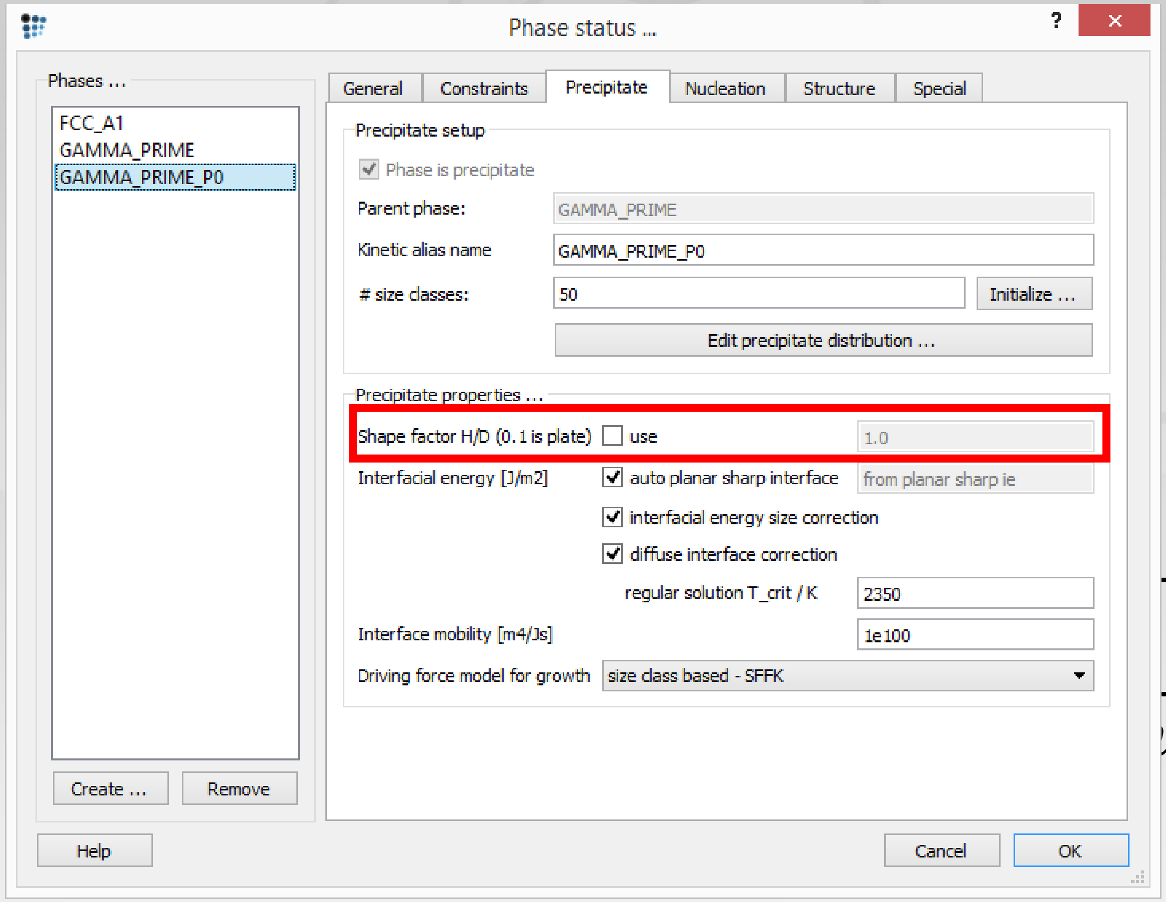


$$\ldots{}^{2}\Big)\, sin^2\theta + \left(\sqrt{\frac{1}{h^2}} + \sqrt{\frac{9}{2+h^2} + \frac{1}{h^2}}\right) cos^2\theta \Big]$$

Non-shearable particles

$$\tau_{nsh} = \frac{JGb}{2\pi L_S} ln\left(\frac{\pi}{2}\frac{r_{eq}}{r_i} f(\theta, h)\right)$$

$$J = \frac{1 - \upsilon \left[cos^2\left(\frac{\pi}{2} - \theta\right)\right]}{1 - \upsilon}$$

$$f(\theta, h) = \frac{h^{2/3}}{3}\left[\left(\sqrt{\frac{3}{2+h^2}} + \sqrt{\frac{3}{h^2} + \frac{3}{2+h^2}}\right) sin^2\theta + \left(\sqrt{\frac{1}{h^2}} + \sqrt{\frac{9}{2+h^2} + \frac{1}{h^2}}\right) cos^2\theta\right]$$

variables	value
kinetics: prec. strength	
TAO_OROWAN$*	
TAO_OROWAN$GAMMA_PRIME_P0	7.74823e+08

category: kinetics: prec. strength
expression: TAO_OROWAN$GAMMA_PRIME_P0
legal unit qualifiers: *none*
-> Ashby-Orowan shear stress for impenetrable precipitates of individual phase

Size distribution dependent strengthening

- Precipitate size dependence
- Some general parameters/settings
- 2 scenarios for dislocation behavior:
  - Non-shearable particles (Orowan mechanism) → bypassing precipitate
  - Shearable particles (weak or strong) → cutting precipitate
- Critical stresses for both scenarios are evaluated

Shearable particles

- Models for “weak” and “strong” particles
- Various effects (contributions) considered
  - Coherency effect
  - Modulus effect
  - Anti-phase boundary effect
  - Stacking fault effect
  - Interfacial effect

Shearable particles

- Models for “weak” and “strong” particles
- Various effects (contributions) considered
  - Coherency effect
  - Modulus effect
  - Anti-phase boundary effect
  - Stacking fault effect
  - Interfacial effect

„Weak“ vs. „strong“ particles

- Criterion: Dislocation bending angle ψ threshold
  - Strong resistance of particles → High curvature of dislocation line → small ψ

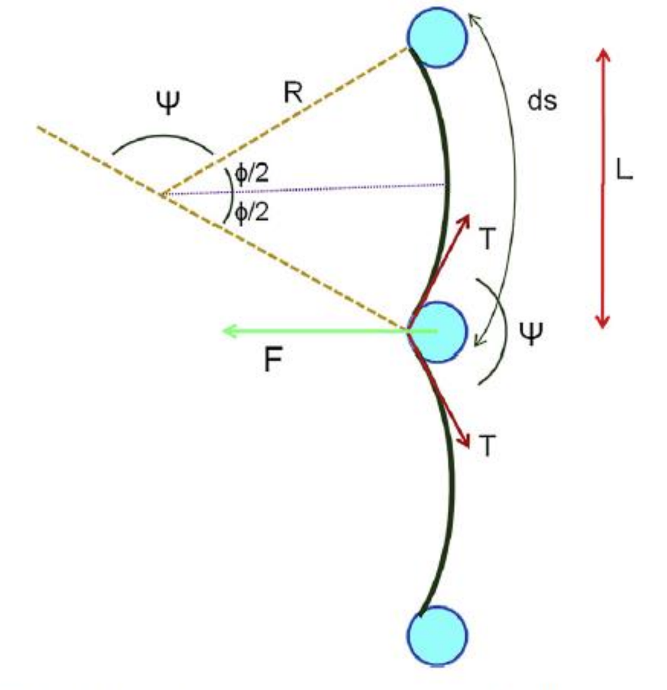


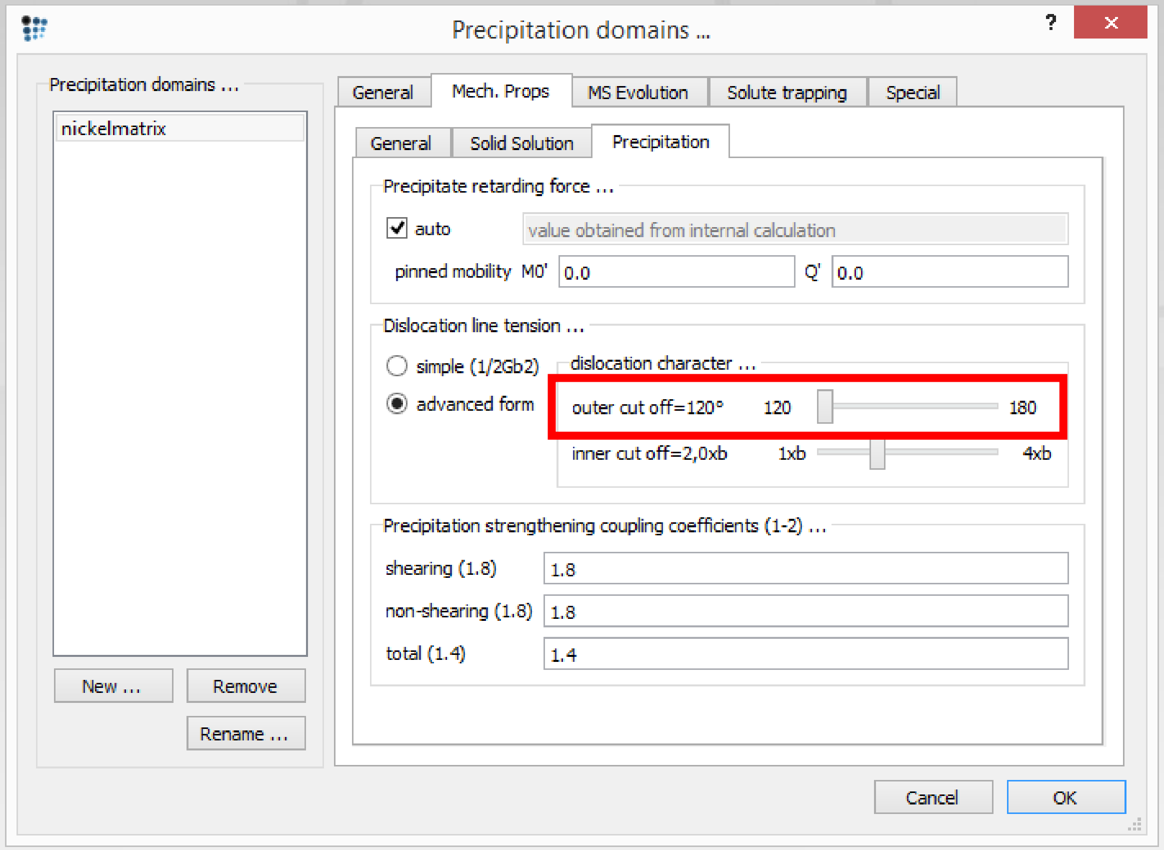
Fig. 1. Balance force between a precipitate and a dislocation.

0° - ψ → “strong” particles

ψ - 180° → “weak” particles

„Weak“ vs. „strong“ particles

- Criterion: Dislocation bending angle ψ threshold
  - Strong resistance of particles → High curvature of dislocation line → small ψ



0° - ψ → "strong" particles

ψ - 180° → "weak" particles

„Weak“ vs. „strong“ particles

- Criterion: Dislocation bending angle ψ threshold
  - Strong resistance of particles → High curvature of dislocation line → small ψ

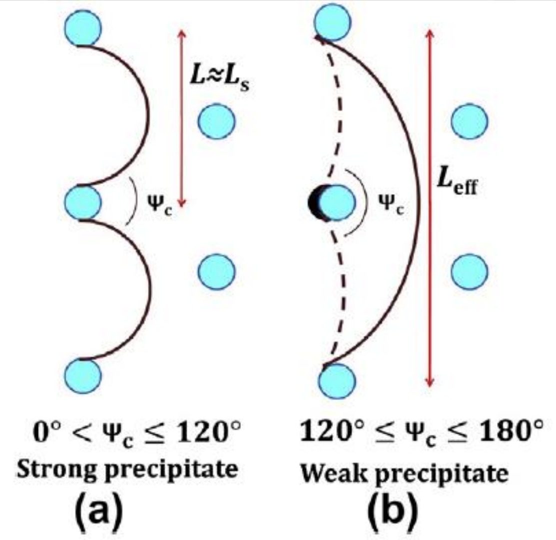


Fig. 2. Free distance between two precipitates along dislocation line in a random array. (A) The precipitates are shearable and strong and (B) the precipitates are shearable and weak.

Strong particles

$$L_S = \sqrt{\frac{\ln 3}{2\pi \sum_{class} N_{V,class} r_{m,class}} + 4r_{ss}^2} - 2r_{ss}$$

$$r_{ss} = \sqrt{\frac{2}{3}} \frac{\sum_{class} N_{V,class} r_{m,class}^2}{\sum_{class} N_{V,class} r_{m,class}}$$

„Weak“ vs. „strong“ particles

- Criterion: Dislocation bending angle ψ threshold
  - Strong resistance of particles → High curvature of dislocation line → small ψ

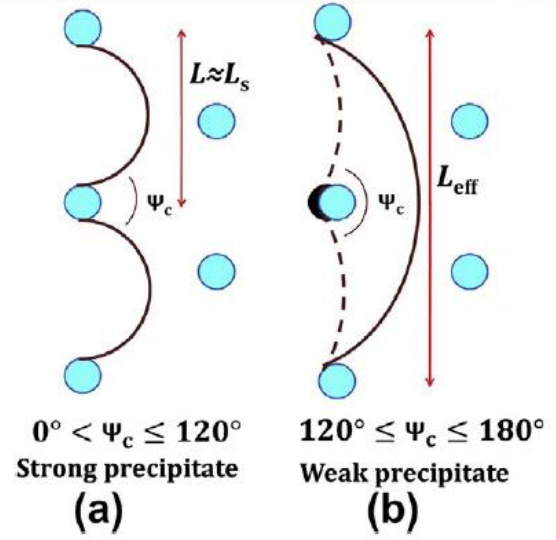


Fig. 2. Free distance between two precipitates along dislocation line in a random array. (A) The precipitates are shearable and strong and (B) the precipitates are shearable and weak.

Strong particles

$$L_S = \sqrt{\frac{\ln 3}{2\pi \sum_{class} N_{V,class} r_{m,class}} + 4r_{ss}^2} - 2r_{ss}$$

Weak particles

$$L_{eff} = L_S \left[\cos\left(\frac{\psi}{2} \right) \right]^{-1/2}$$

„Weak“ vs. „strong“ particles

- Dislocation line tension, T
  - Simple model

$$T = \frac{Gb^2}{2}$$

G - Shear modulus

b - Burgers vector

υ - Poisson‘s ratio

r_i – dislocation core radius

  - Advanced model (different values for „weak“ and „strong“ particles)

$$T_{strong} = \frac{Gb^2}{4\pi}\left(\frac{1+\upsilon-3\upsilon\sin^2\theta}{1-\upsilon}\right)\ln\left(\frac{L_S}{r_i}\right)$$

$$T_{weak} = \frac{Gb^2}{4\pi}\left(\frac{1+\upsilon-3\upsilon\sin^2\theta}{1-\upsilon}\right)\ln\left(\frac{L_{eff}}{r_i}\right)$$

„Weak“ vs. „strong“ particles

- Dislocation line tension, T
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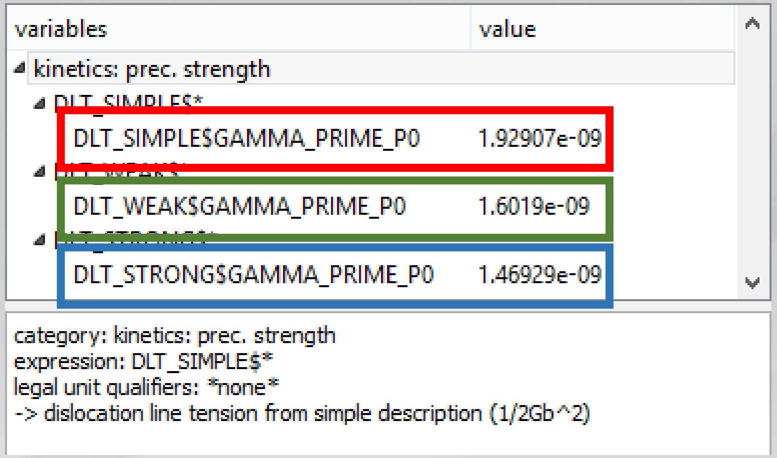


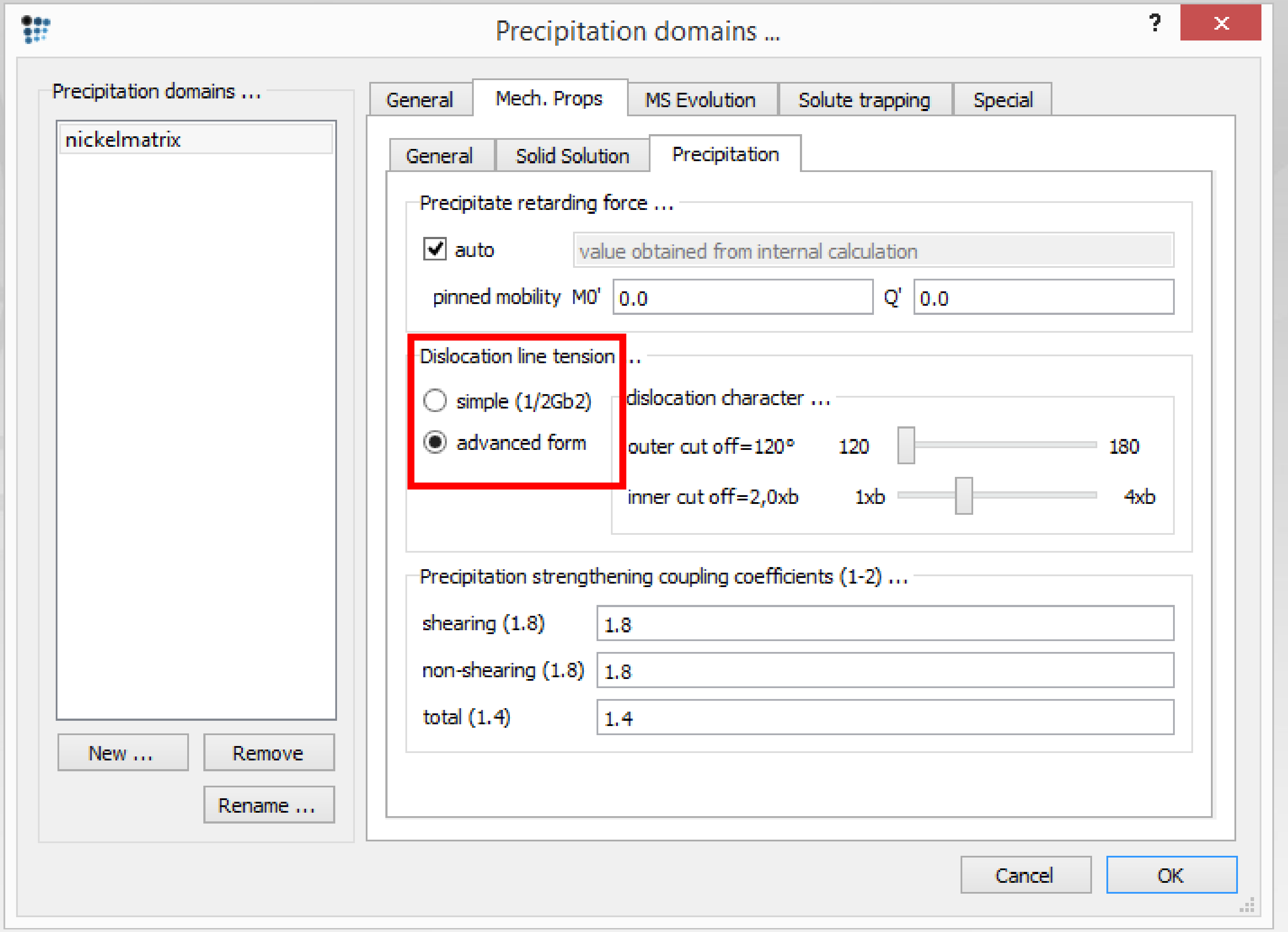
  - Advanced model (different values for „weak“ and „strong“ particles)

$$T_{strong} = \frac{Gb^2}{4\pi}\left(\frac{1+\upsilon-3\upsilon\sin^2\theta}{1-\upsilon}\right)\ln\left(\frac{L_S}{r_i}\right)$$

$$T_{weak} = \frac{Gb^2}{4\pi}\left(\frac{1+\upsilon-3\upsilon\sin^2\theta}{1-\upsilon}\right)\ln\left(\frac{L_{eff}}{r_i}\right)$$

„Weak“ vs. „strong“ particles

- Dislocation line tension, T
  - Simple
  - Advanced



Shearable particles

- Models for “weak” and “strong” particles
- Various effects (contributions) considered
  - Coherency effect
  - Modulus effect
  - Anti-phase boundary effect
  - Stacking fault effect
  - Interfacial effect

Coherency effect

- Strain field due to precipitation/matrix misfit
  - Strong particles

$$\tau_{coh,strong} = \frac{\left(2\cos^2\theta + 2.1352\sin^2\theta\right)}{L_S}\left(\frac{T_{strong}^3 G\varepsilon r_m}{b^3}\right)^{1/4}$$

$$\varepsilon = \frac{2}{3}\Delta_{lin} = \frac{2}{9}\Delta_{vol}$$

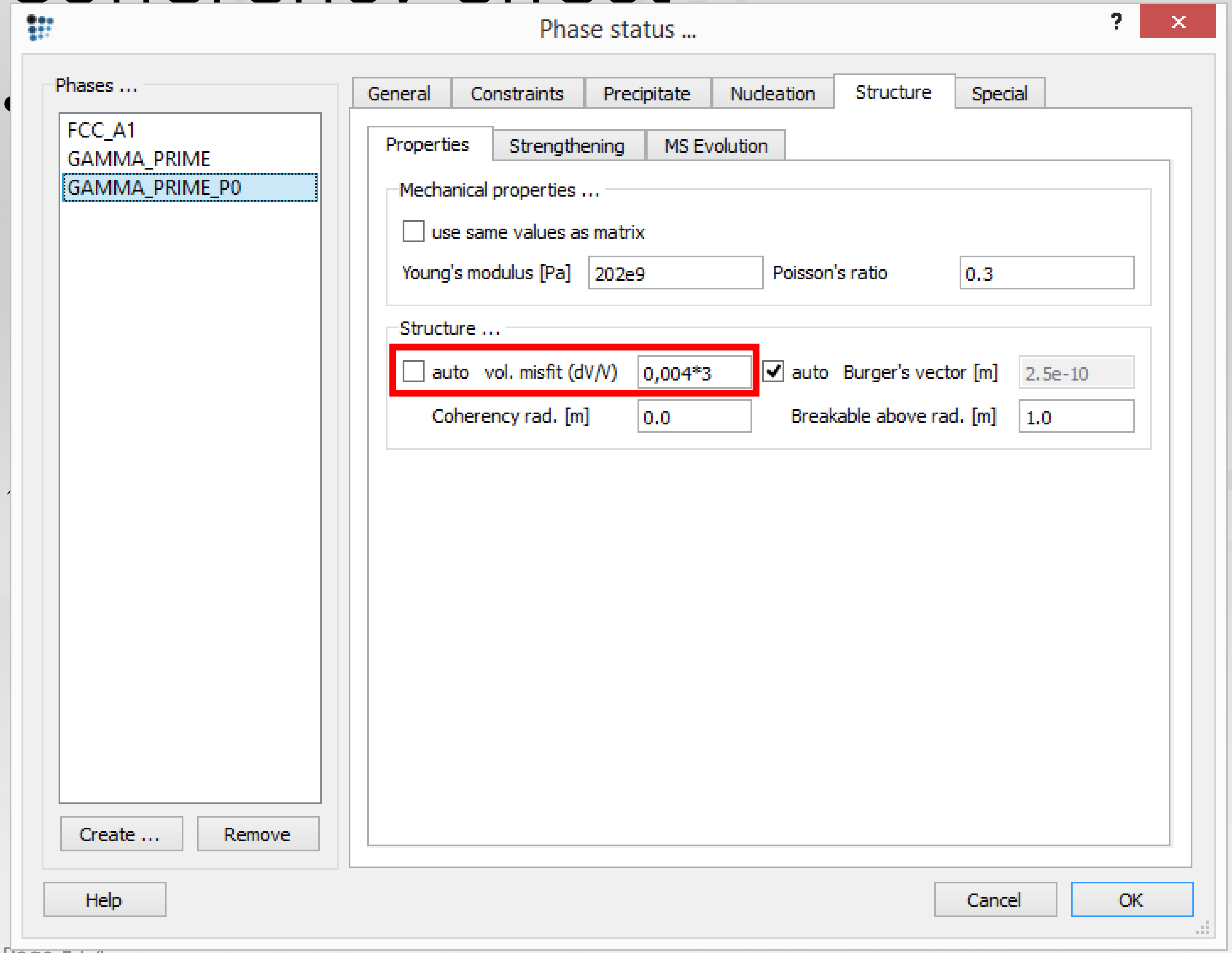
  - Weak particles

$$\tau_{coh,weak} = \frac{\left(1.3416\cos^2\theta + 4.1127\sin^2\theta\right)}{L_S}\left(\frac{G^3\varepsilon^3 r_{eq}^3 b}{T_{weak}}\right)^{1/2}$$

Δ_{lin} - Linear misfit

Δ_{vol} - Volumetric misfit

Coherency effect



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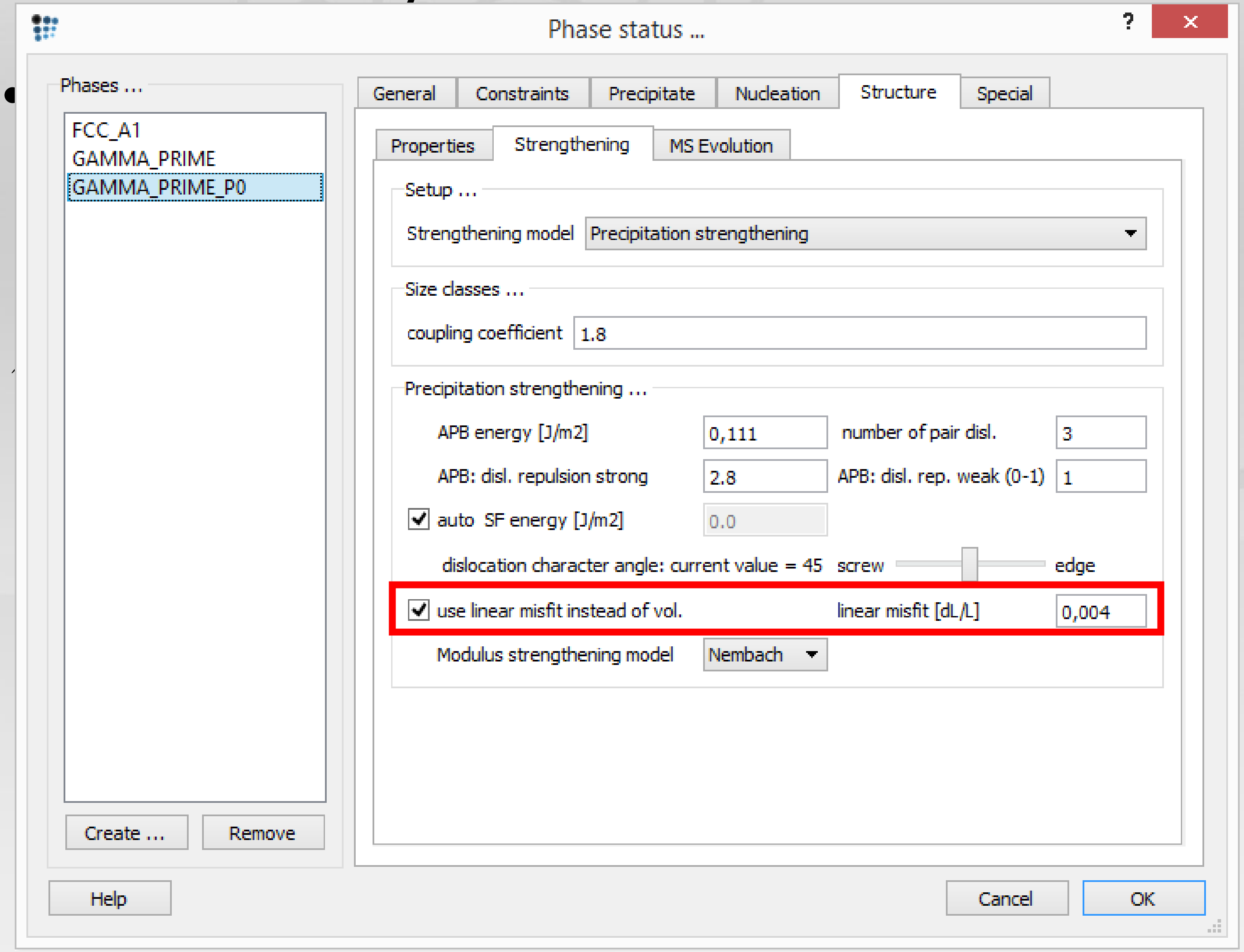

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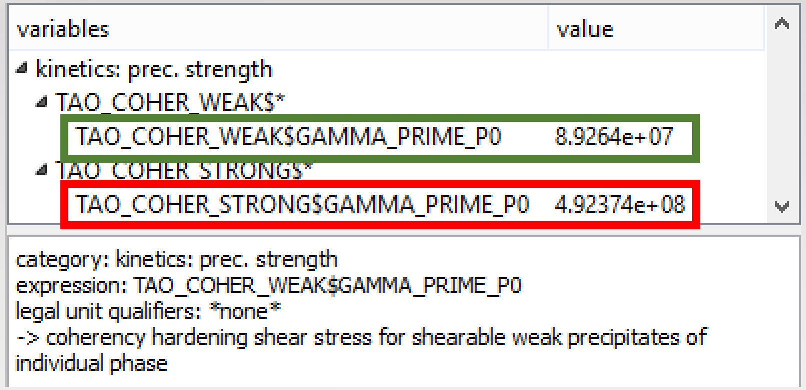

MatCalc Engineering

Shearable particles

- Models for “weak” and “strong” particles
- Various effects (contributions) considered
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  - Anti-phase boundary effect
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  - Interfacial effect

MatCalc Engineering

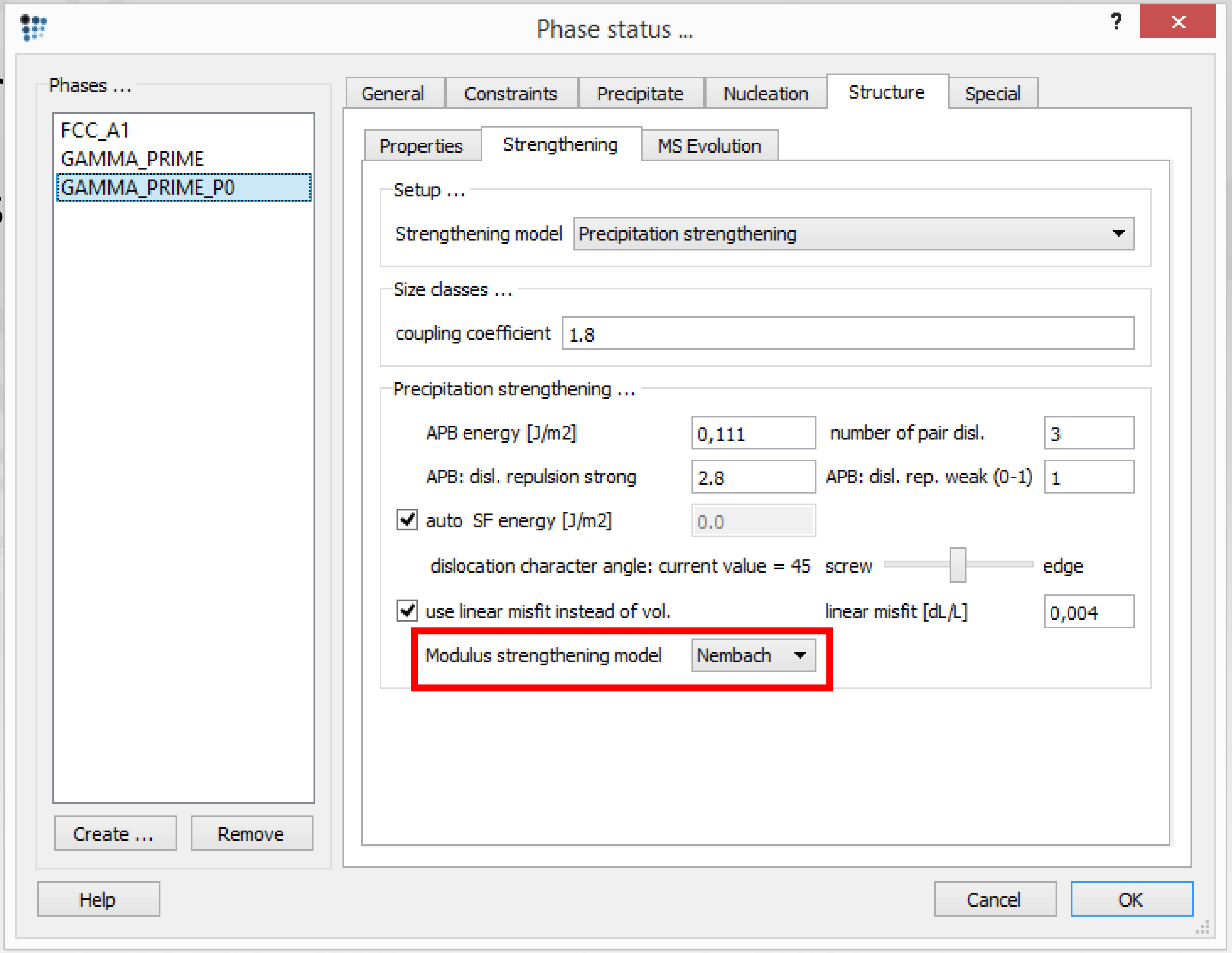
Modulus effect

- Elastic properties of precipitate and matrix differ → dislocation energy inside and outside the precipitate differ
- 2 models
  - Nembach
  - Siems

MatCalc
Engineering

Modulus effect

- Elastic properties of pr
  energy inside and outs
- 2 models
  - Nembach
  - Siems



Modulus effect

- Nembach model
  - Strong particles

$$\tau_{\mathrm{mod},strong} = \frac{F_{\mathrm{mod}}}{bL_S}$$

  - Weak particles

$$\tau_{\mathrm{mod},weak} = \frac{2T_{weak}}{bL_S}\left(\frac{F_{\mathrm{mod}}}{2T_{weak}}\right)^{3/2}$$

$$F_{\mathrm{mod}} = 0.05\left|G - G_P\right| b^2 \left(\frac{r_{eq}}{b}\right)^{0.85}$$

G_p - Particle shear modulus

Modulus effect

- Siems model

υ_p - Particle Poisson ratio

Strong

$$\tau_{\mathrm{mod},strong} = 0.8\frac{2T_{strong}}{bL_S}\left[1-\left(\frac{E_p}{E}\right)^2\right]^{1/2}$$

$$\frac{E_p}{E} = \frac{G_P(1-\upsilon)\log\frac{r_{eq}}{r_i} + G(1-\upsilon_p)\log\frac{L_S}{r_{eq}}}{G(1-\upsilon_p)\log\frac{L_S}{r_i}}$$

Weak

$$\tau_{\mathrm{mod},weak} = \frac{2T_{weak}}{bL_S}\left[1-\left(\frac{E_p}{E}\right)^2\right]^{3/4}$$

$$\frac{E_p}{E} = \frac{G_P(1-\upsilon)\log\frac{r_{eq}}{r_i} + G(1-\upsilon_p)\log\frac{L_{eff}}{r_{eq}}}{G(1-\upsilon_p)\log\frac{L_{eff}}{r_i}}$$

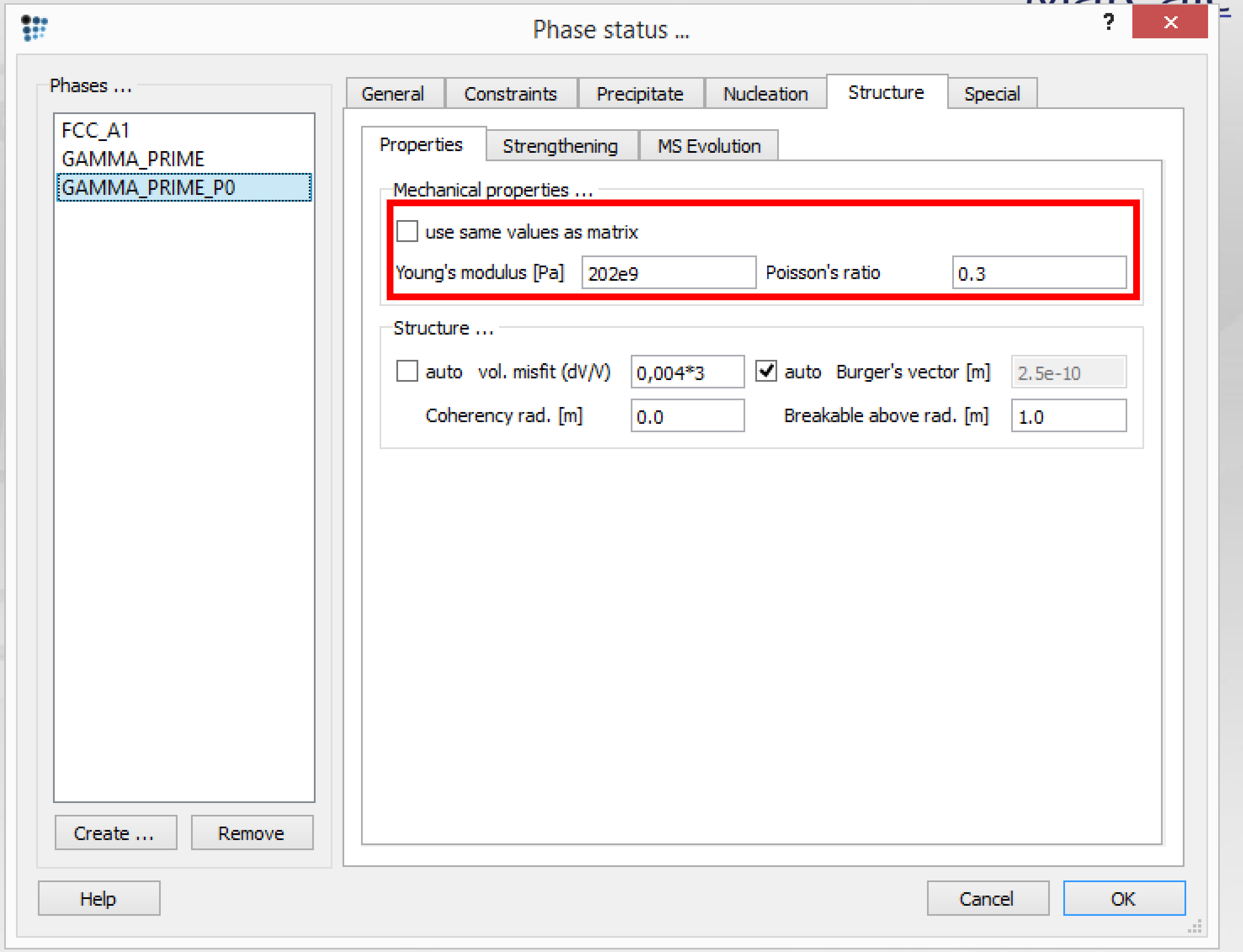
Modulus effect

- Nembach model
  - Strong particles

$$\tau_{\mathrm{mod},strong} = \frac{F_{\mathrm{mod}}}{bL_S}$$

  - Weak particles

$$\tau_{\mathrm{mod},weak} = \frac{2T_{weak}}{bL_S}\left(\frac{F_{\mathrm{mod}}}{2T_{weak}}\right)^{3/2}$$



υ_p - Particle Poisson ratio G_p - Particle shear modulus

Modulus effect

- Elastic properties of precipitate and matrix differ → dislocation energy inside and outside the precipitate differ
- 2 models
  - Nembach
  - Siems

$$\tau_{\mathrm{mod},weak}$$

$$\tau_{\mathrm{mod},strong}$$

variables	value
kinetics: prec. strength	
TAO_MOD_WEAK$*	
TAO_MOD_WEAK$GAMMA_PRIME_P0	1.80848e+06
TAO_MOD_STRONG$*	
TAO_MOD_STRONG$GAMMA_PRIME_P0	1.32552e+07

category: kinetics: prec. strength
expression: TAO_MOD_WEAK$GAMMA_PRIME_P0
legal unit qualifiers: *none*
-> modulus mismatch hardening shear stress for weak shearable precipitates of individual phase

MatCalc Engineering

Shearable particles

- Models for "weak" and "strong" particles
- Various effects (contributions) considered
  - Coherency effect
  - Modulus effect
  - Anti-phase boundary effect
  - Stacking fault effect
  - Interfacial effect

Anti-phase boundary (APB) effect

- Dislocation passing through ordered precipitate increases the energy by creating the APB
  - Strong particles

$$\tau_{APB,strong} = \frac{0.69}{bL_S}\left(\frac{8wT_{strong} r_{eq} \gamma_{APB}}{3}\right)^{1/2}$$

  - Weak particles

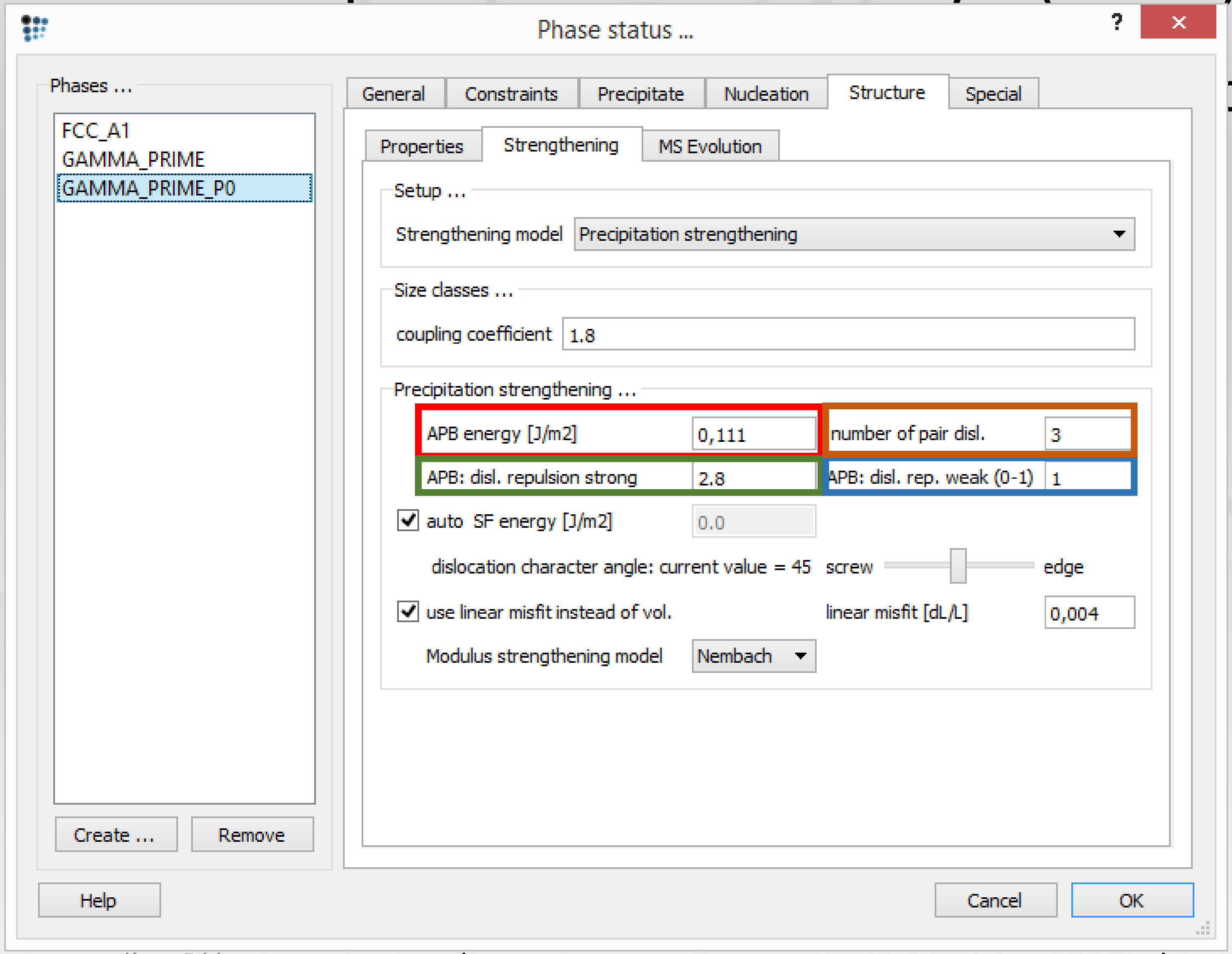
$$\tau_{APB,weak} = \frac{2}{sbL_S}\left[2T_{weak}\left(\frac{r_{eq}\gamma_{APB}}{T_{weak}}\right)^{3/2} - \frac{16\beta\gamma_{APB} r_{eq}^2}{3\pi L_S}\right]$$

γ_{APB} - APB energy

w, β - Interaction parameter between the leading and trailing dislocation

s - Number of pair dislocations

Anti-phase boundary (APB) effect



cipitate increases the energy

γ_{APB} - APB energy

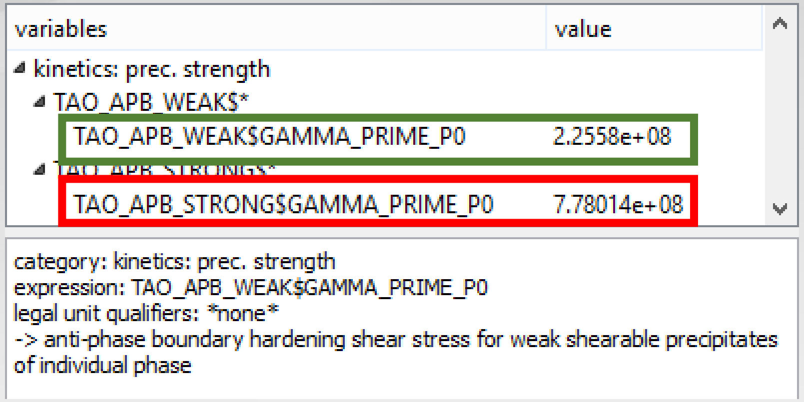
w, β - Interaction parameter between the leading and trailing dislocation

s - Number of pair dislocations

Anti-phase boundary (APB) effect

- Dislocation passing through ordered precipitate increases the energy by creating the APB
  - Strong particles

$$\tau_{APB,strong} = \frac{0.69}{bL_S}\left(\frac{8wT_{strong}r_{eq}\gamma_{APB}}{3}\right)^{1/2}$$



  - Weak particles

$$\tau_{APB,weak} = \frac{2}{sbL_S}\left[2T_{weak}\left(\frac{r_{eq}\gamma_{APB}}{T_{weak}}\right)^{3/2} - \frac{16\beta\gamma_{APB}r_{eq}^2}{3\pi L_S}\right]$$

Shearable particles

- Models for “weak” and “strong” particles
- Various effects (contributions) considered
  - Coherency effect
  - Modulus effect
  - Anti-phase boundary effect
  - Stacking fault effect
  - Interfacial effect

Stacking fault (SF) effect

- Passing dislocation creates a stacking fault – energy difference between the SF in the precipitate and matrix

$$K_{SF} = \frac{G b_p^2 \left(2 - \upsilon - 2\upsilon \cos(2\theta)\right)}{8\pi(1-\upsilon)}$$

$$W_{eff} = \frac{2K_{SF}}{\gamma_{SFM} + \gamma_{SFP}}$$

$$F_{SF} = 2(\gamma_{SFM} - \gamma_{SFP})\sqrt{W_{eff} r_{eq} - W_{eff}^2 / 4}$$

b_p - Burger's vector of particle

γ_{SFP} - Stacking fault energy of particle

γ_{SFM} - Stacking fault energy of matrix

Stacking fault (SF) effect

- Passing dislocation creates a stacking fault – energy difference between the SF in the precipitate and matrix
  - Strong particles

$$\tau_{SF,strong} = \frac{F_{SF}}{bL_S}$$

  - Weak particles

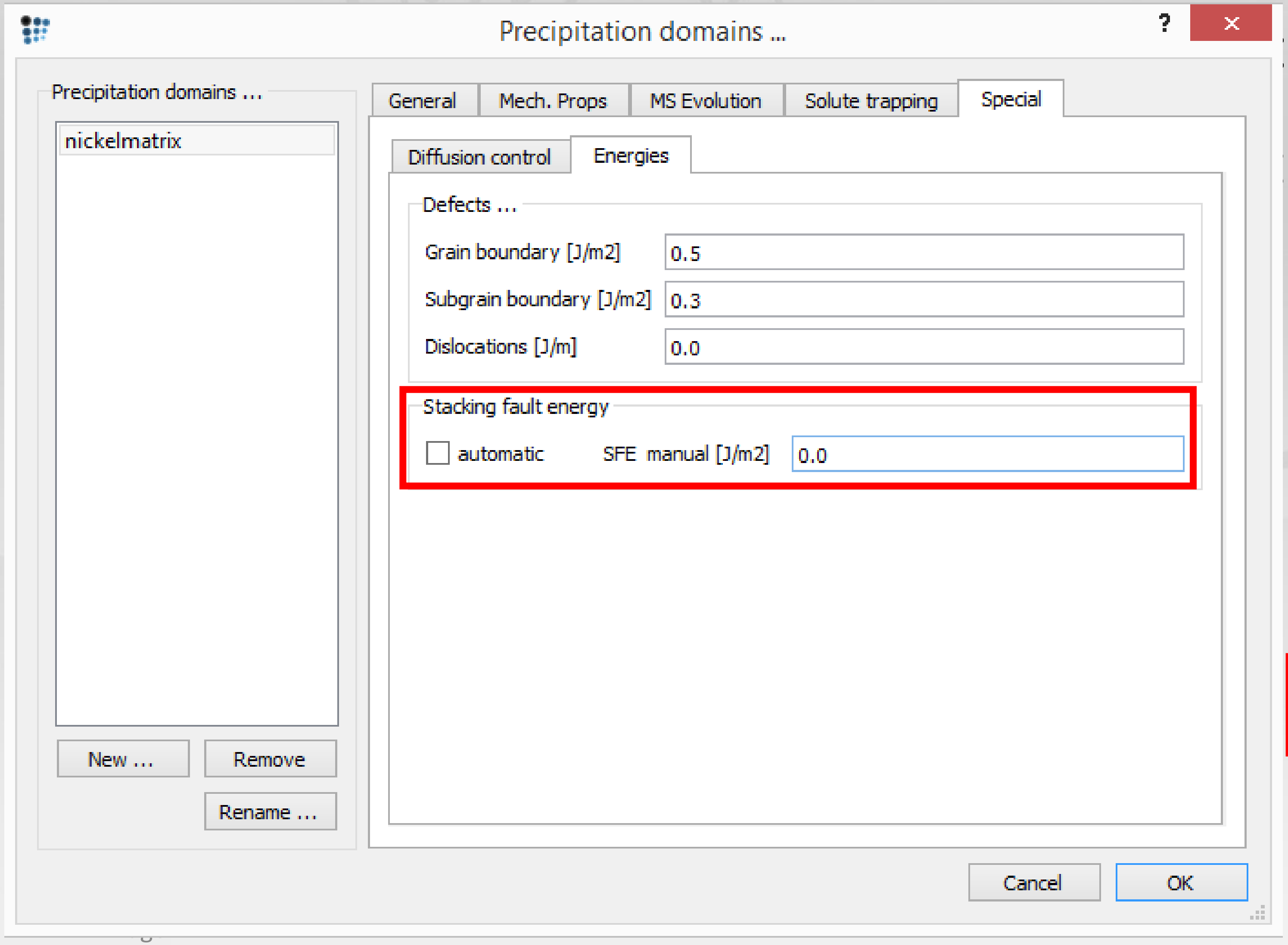
$$\tau_{SF,weak} = \frac{2T_{weak}}{bL_S}\left(\frac{F_{SF}}{2T_{weak}}\right)^{3/2}$$

$$K_{SF} = \frac{Gb_p^2\left(2-\upsilon-2\upsilon\cos(2\theta)\right)}{8\pi(1-\upsilon)}$$

$$W_{eff} = \frac{2K_{SF}}{\gamma_{SFM}+\gamma_{SFP}}$$

$$F_{SF} = 2(\gamma_{SFM}-\gamma_{SFP})\sqrt{W_{eff}r_{eq}-W_{eff}^2/4}$$

Stacking fault (SF) effect



– energy difference

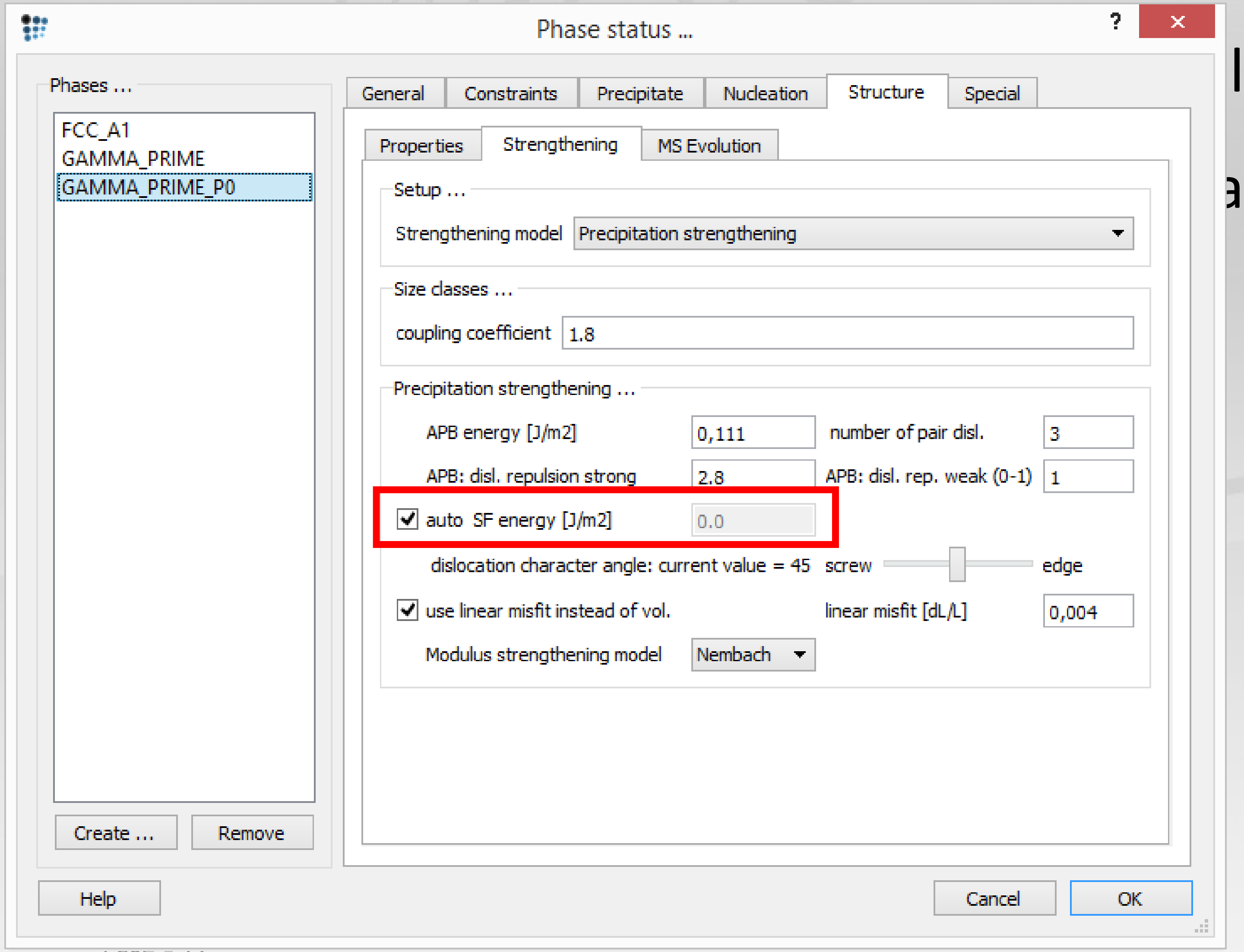
rix

b_p - Burger's vector of particle

γ_{SFP} - Stacking fault energy of particle

γ_{SFM} - Stacking fault energy of matrix

Stacking fault (SF) effect



lt – energy difference

atrix

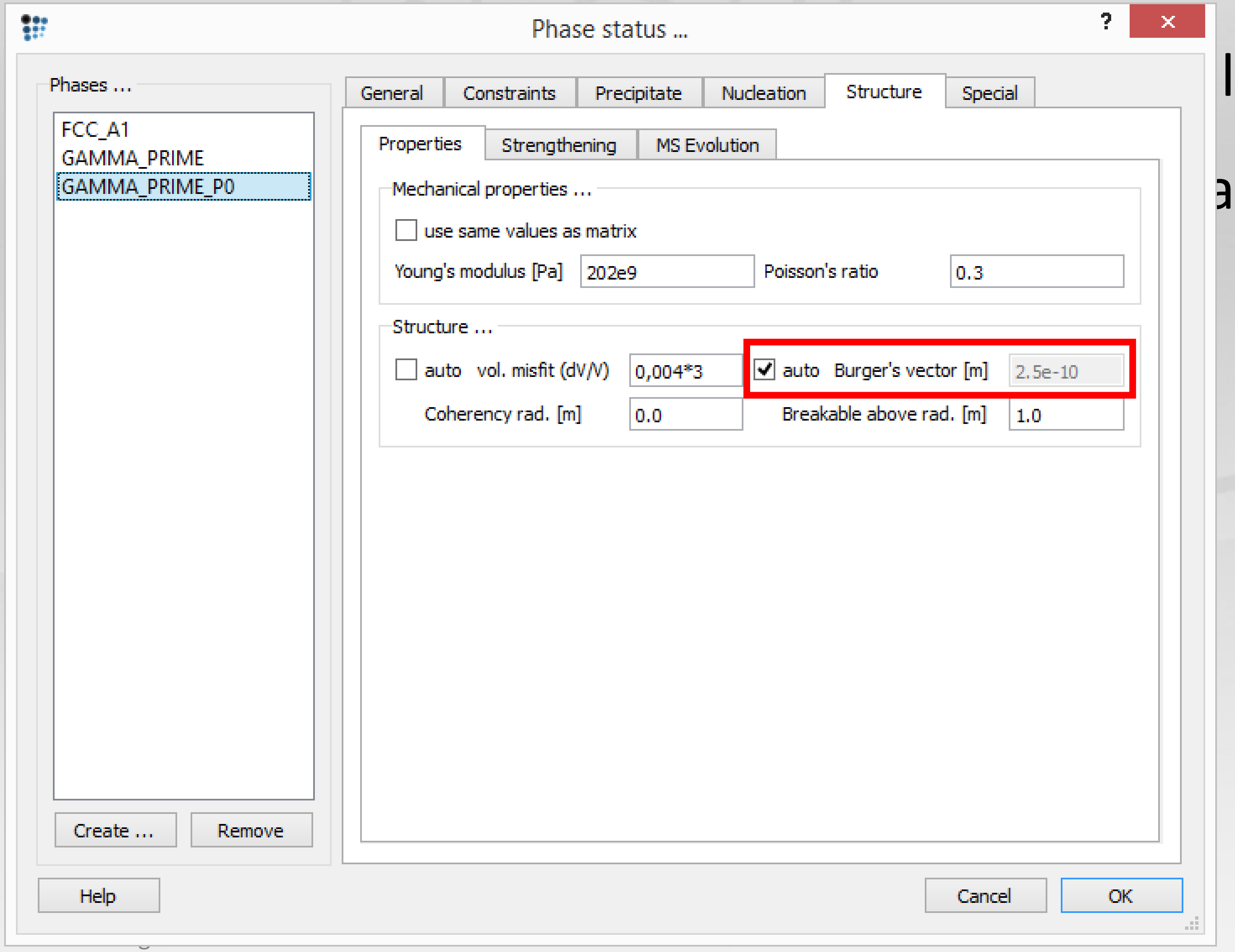
b_p - Burger's vector of particle

γ_{SFP} - Stacking fault energy of particle

γ_{SFM} - Stacking fault energy of matrix

Stacking fault (SF) effect

MatCalc Engineering



lt – energy difference

atrix

b_p - Burger’s vector of particle

γ_{SFP} - Stacking fault energy of particle

γ_{SFM} - Stacking fault energy of matrix

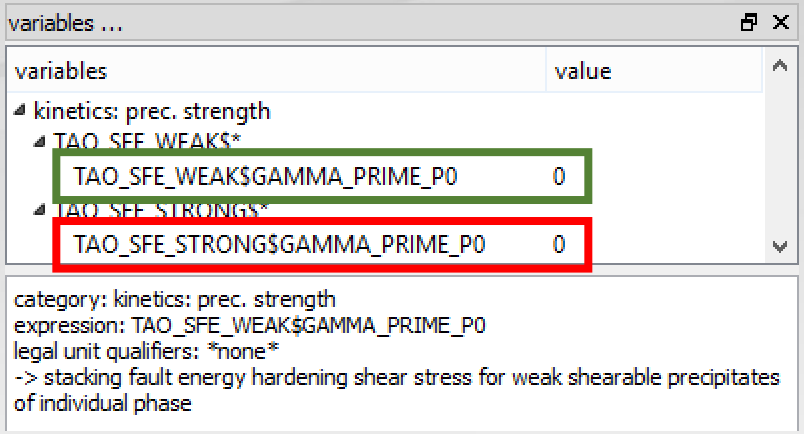
Stacking fault (SF) effect

- Passing dislocation creates a stacking fault – energy difference between the SF in the precipitate and matrix
  - Strong particles

$$\tau_{SF,strong} = \frac{F_{SF}}{bL_S}$$

  - Weak particles

$$\tau_{SF,weak} = \frac{2T_{weak}}{bL_S}\left(\frac{F_{SF}}{2T_{weak}}\right)^{3/2}$$



MatCalc Engineering

Shearable particles

- Models for “weak” and “strong” particles
- Various effects (contributions) considered
  - Coherency effect
  - Modulus effect
  - Anti-phase boundary effect
  - Stacking fault effect
  - Interfacial effect

Interfacial effect

- Passing dislocation increases the area of precipitate/matrix interface
  - Strong particles

$$\tau_{\mathrm{int},strong} = \frac{F_{\mathrm{int}}}{bL_S}$$

$$F_{\mathrm{int}} = 2\gamma_{PM} b$$

  - Weak particles

$$\tau_{\mathrm{int},weak} = \frac{2T_{weak}}{bL_S}\left(\frac{F_{\mathrm{int}}}{2T_{weak}}\right)^{3/2}$$

γ_{PM} - Precipitate/matrix interface energy

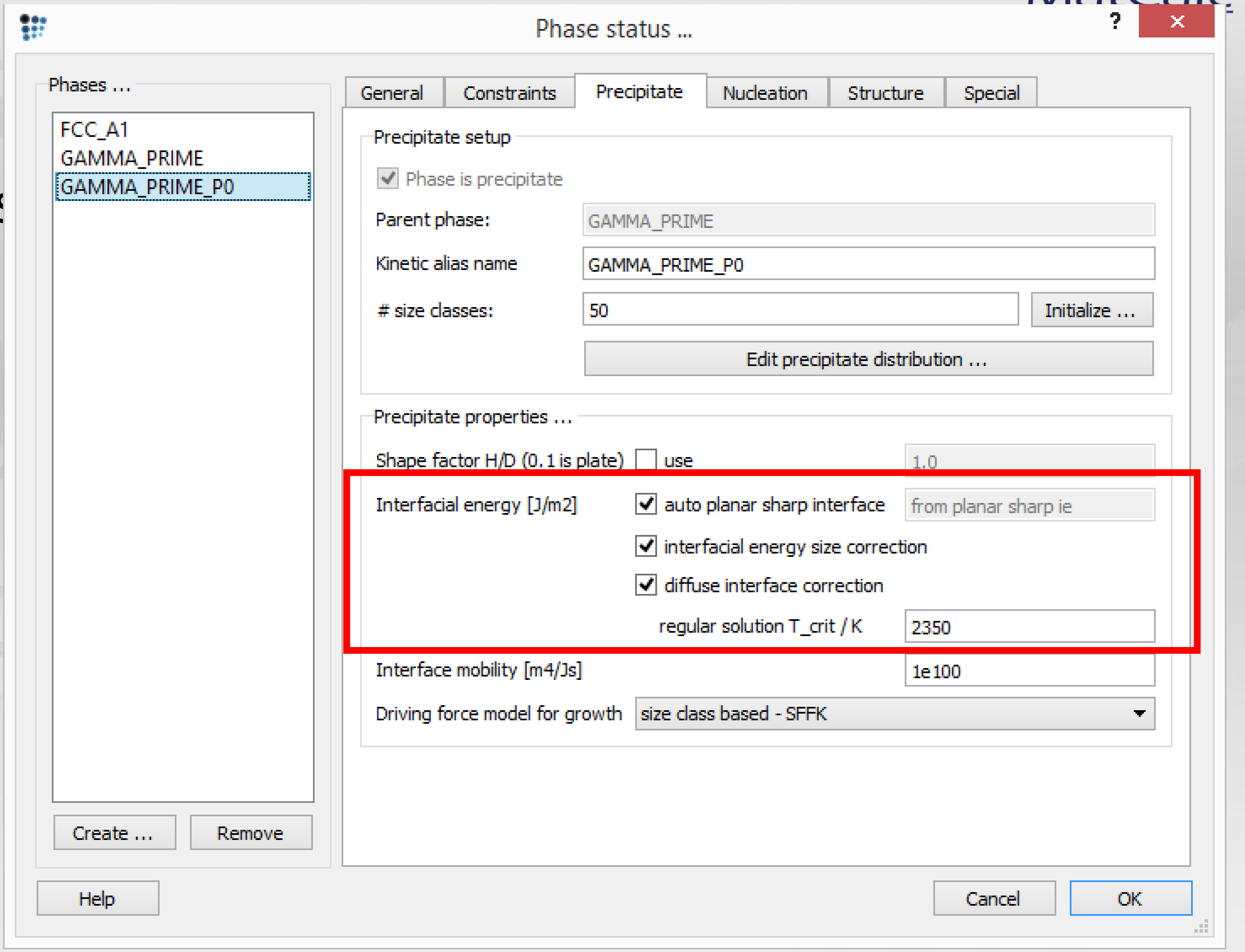
Interfacial effect

- Passing dislocation increases
  - Strong particles

$$\tau_{\text{int},strong} = \frac{F_{\text{int}}}{bL_S}$$

  - Weak particles

$$\tau_{\text{int},weak} = \frac{2T_{weak}}{bL_S}\left(\frac{F_{\text{int}}}{2T_{weak}}\right)^{3/2}$$



γ_{PM} - Precipitate/matrix interface energy

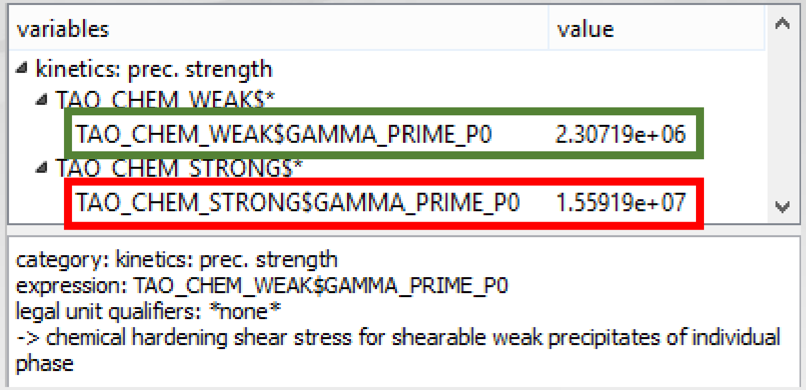
Interfacial effect

- Passing dislocation increases the area of precipitate/matrix interface
  - Strong particles

$$\tau_{\mathrm{int},strong} = \frac{F_{\mathrm{int}}}{bL_S}$$

  - Weak particles

$$\tau_{\mathrm{int},weak} = \frac{2T_{weak}}{bL_S}\left(\frac{F_{\mathrm{int}}}{2T_{weak}}\right)^{3/2}$$



Size distribution dependent strengthening

MatCalc Engineering

- Precipitate size dependence
- Some general parameters/settings
- 2 scenarios for dislocation behavior:
  - Non-shearable particles (Orowan mechanism) → bypassing precipitate
  - Shearable particles (weak or strong) → cutting precipitate
- Critical stresses for both scenarios are evaluated

Identifying the strengthening regime

- Values of τ evaluated for each of three regimes (Non-shearable, shearable weak, shearable strong)
  - Shearable model taken as a superposition of individual contributions

$$\tau_{i,strong} = \left(\tau_{i,coher,strong}^{m_{sh}} + \tau_{i,\mathrm{mod},strong}^{m_{sh}} + \tau_{i,APB,strong}^{m_{sh}} + \tau_{i,SF,strong}^{m_{sh}} + \tau_{i,\mathrm{int},strong}^{m_{sh}}\right)^{1/m_{sh}}$$

$$\tau_{i,weak} = \left(\tau_{i,coher,weak}^{m_{sh}} + \tau_{i,\mathrm{mod},weak}^{m_{sh}} + \tau_{i,APB,weak}^{m_{sh}} + \tau_{i,SF,weak}^{m_{sh}} + \tau_{i,\mathrm{int},weak}^{m_{sh}}\right)^{1/m_{sh}}$$

$$\tau_{i,nsh}$$

$i -$
- Precipitate phase (for „mean radius“ models)
- Size class (for „multi-class“ model)

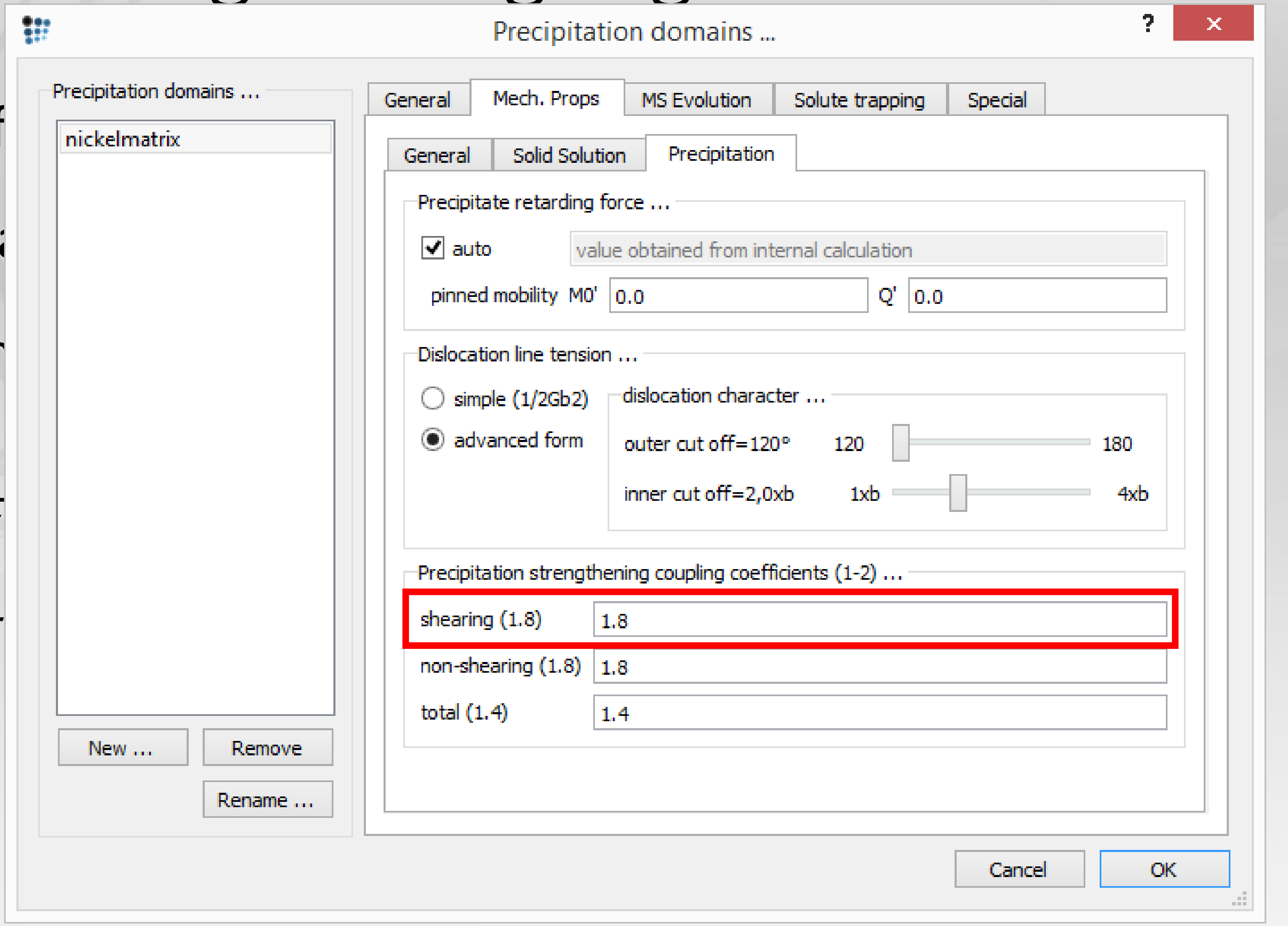
Identifying the strengthening regime

- Values of τ evaluated f
  shearable weak, sheara
  - Shearable model taken

$$\tau_{i,strong} = \left(\tau^{m_{sh}}_{i,coher,strong} + \tau\right.$$

$$\tau_{i,weak} = \left(\tau^{m_{sh}}_{i,coher,weak} + \tau\right.$$

$$\tau_{i,nsh}$$



Identifying the strengthening regime

- Lowest value regime taken as the operative one
  - Precipitate „releases“ passing dislocation according to „lowest resistance“scenario.

$$\tau_i = min.\left(\tau_{i,nsh}, \tau_{i,strong}, \tau_{i,weak}\right)$$

$$\tau_{i,strong} = \left(\tau_{i,coher,strong}^{m_{sh}} + \tau_{i,\mathrm{mod},strong}^{m_{sh}} + \tau_{i,APB,strong}^{m_{sh}} + \tau_{i,SF,strong}^{m_{sh}} + \tau_{i,\mathrm{int},strong}^{m_{sh}}\right)^{1/m_{sh}}$$

$$\tau_{i,weak} = \left(\tau_{i,coher,weak}^{m_{sh}} + \tau_{i,\mathrm{mod},weak}^{m_{sh}} + \tau_{i,APB,weak}^{m_{sh}} + \tau_{i,SF,weak}^{m_{sh}} + \tau_{i,\mathrm{int},weak}^{m_{sh}}\right)^{1/m_{sh}}$$

$$\tau_{i,nsh}$$

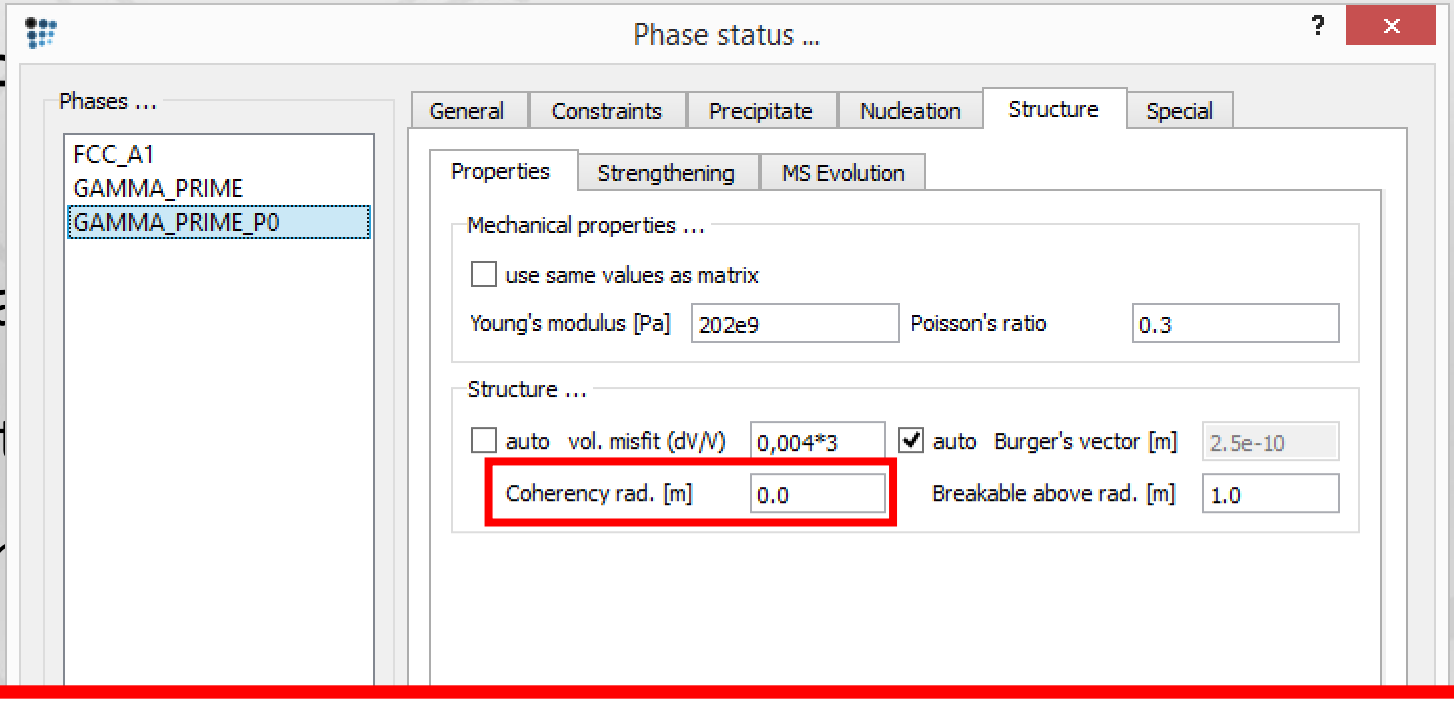
$i -$ { Precipitate phase (for „mean radius“ models) / Size class (for „multi-class“ model)

Identif

- Lowest va
  - Precipit

    resistar

τ_i



If coherency radius ≠ 0 and the respective radius (mean value or size class) is greater than the coherency radius ➔

the non-shearable regime is taken for further calculation ($\tau_i = \tau_{i,nsh}$)

Calculating strenghtening contribution of individual precipitate phase, τ_j

- “Multi-class” strengthening model selected
  - Superposition of individual size class contributions

$$\tau_j = \left[\left(\sum_{i,sh}(\tau_{i,sh})^{m_{sh}}\right)^{m_{sum}/m_{sh}} + \left(\sum_{i,nsh}(\tau_{i,nsh})^{m_{nsh}}\right)^{m_{sum}/m_{nsh}}\right]^{1/m_{sum}}$$

$$\tau_{i,strong}, \tau_{i,weak} \rightarrow \tau_i \rightarrow \tau_{i,sh}$$

$$\tau_{i,nsh} \rightarrow \tau_i \rightarrow \tau_{i,nsh}$$

- Other strengthening models

$$\tau_j = \tau_i$$

Calculating strenghtening contribution of individual precipitate phase, τ_j

- "Multi-class" strengthening m
  - Superposition of individual size

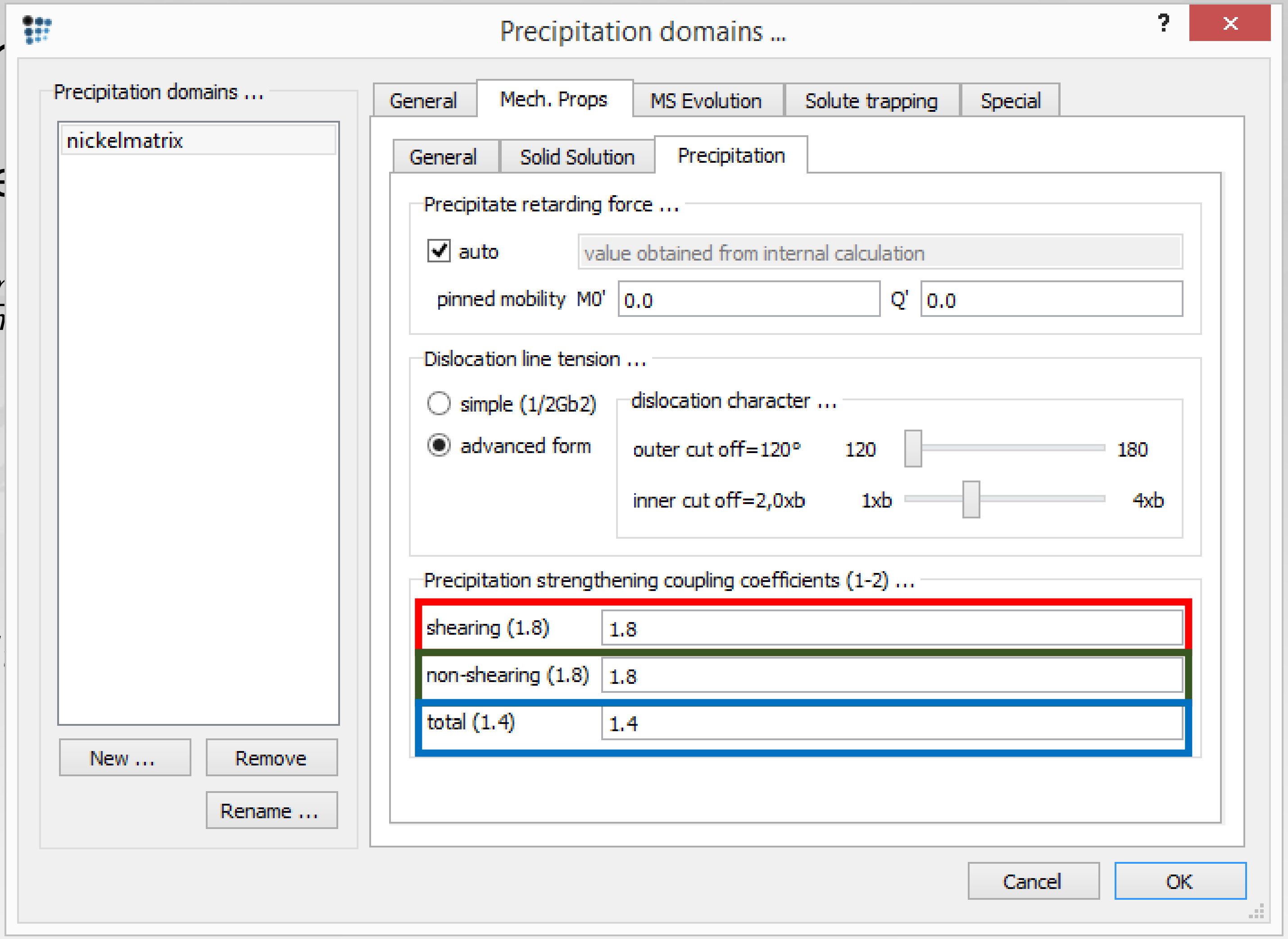
$$\tau_j = \left[\left(\sum_{i,sh}(\tau_{i,sh})^{m_{sh}}\right)^{\frac{m_{sum}}{m_{sh}}} + \left(\sum_{i,nsh}(\tau_{i,nsh})^{m_{nsh}}\right)^{\frac{m}{n}}\right.$$

$$\tau_{i,strong}, \tau_{i,weak} \rightarrow$$

$$\tau_{i,nsh} \rightarrow \tau_i \rightarrow \tau$$

- Other strengthening models

$$\tau_j = \tau_i$$



Total precpitation shear stress, τ_{prec}

- Superposition of individual precipitate phase contributions

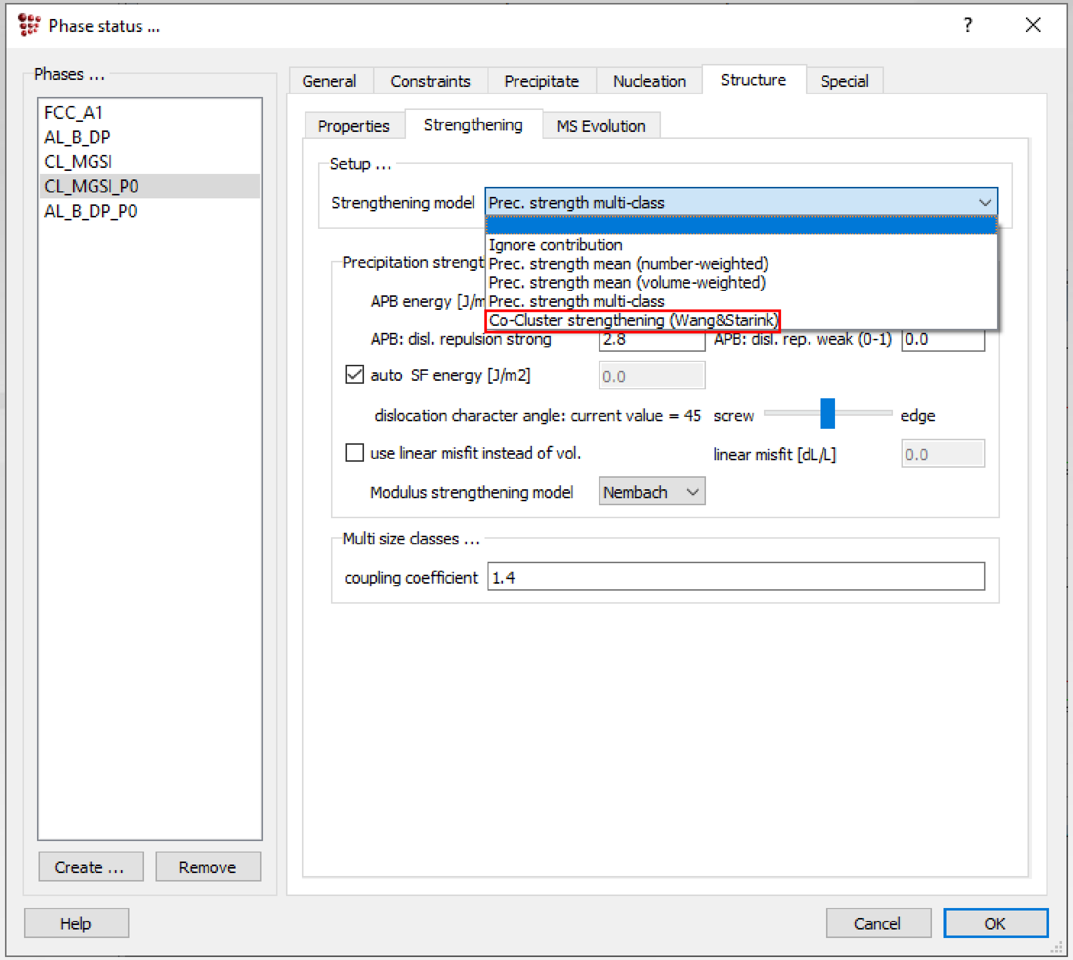
$$\tau_{prec} = \left[\sum_j \tau_j^{9/5}\right]^{5/9}$$

- Precipitate phases with “grain boundaries” (including “edges” and “corners”) as nucleation sites are ignored ($\tau_j = 0$)

Precipitation strengthening, σ_{prec}

MatCalc Engineering

- 2 alternative models available
  - Size distribution dependent strengthening
  - Co-cluster strengthening



Co-cluster strengthening

MatCalc Engineering

- Related to binding enthalpy of co-cluster elements

(applicable only for phases containing two elements)

$$\tau_{prec} = \frac{8}{3\sqrt{3}} \frac{\Delta H_{ccl}}{N_A b^3} \left[f_{ccl} y_A (1 - x_B) + f_{ccl} y_B (1 - x_A) - 3 x_A x_B \right]$$

ΔH_{ccl} - Binding enthalpy of heteroatomic bond in co-cluster

b - Burgers vector

N_A - Avogadro number

y_i - Content of element *i* in co-cluster

x_i - Content of element *i* in matrix

f_{ccl} - Co-cluster phase fraction

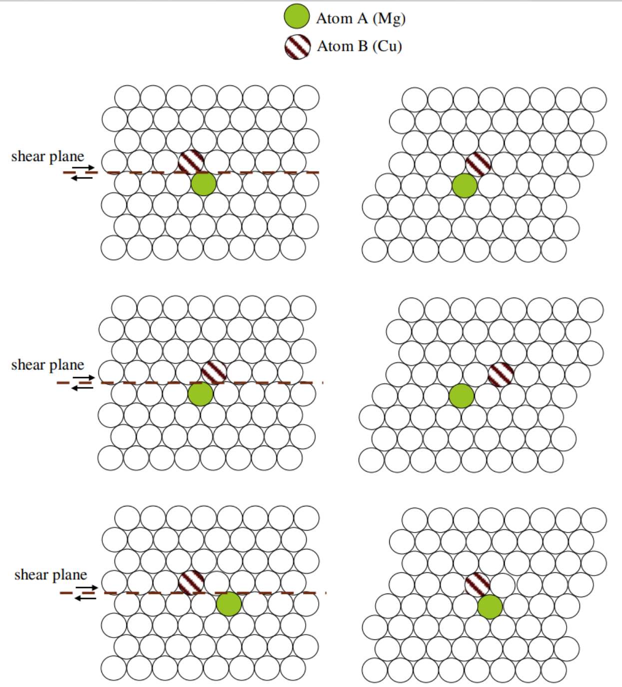


Fig. 2. A 111 plane in an FCC lattice with a 2-atom co-cluster being cut by a dislocation. Top shows before and after with the co-cluster remaining intact in a rotated form; middle shows before and after with the co-cluster being eliminated, which requires an energy input; and bottom shows before and after in the case where the passing of one dislocation creates a co-cluster, which releases energy.

M.J. Starink, S.C. Wang, Acta Mater. 57 (2009) 2376-2389

Co-cluster strengthening

MatCalc Engineering

- Related to binding enthalpy of co-

(applicable only for phases containing two ele

$$\tau_{prec} = \frac{8}{3\sqrt{3}} \frac{\Delta H_{ccl}}{N_A b^3} [f_{ccl} y_A (1 - x_B) + f_{ccl} y_B (1$$

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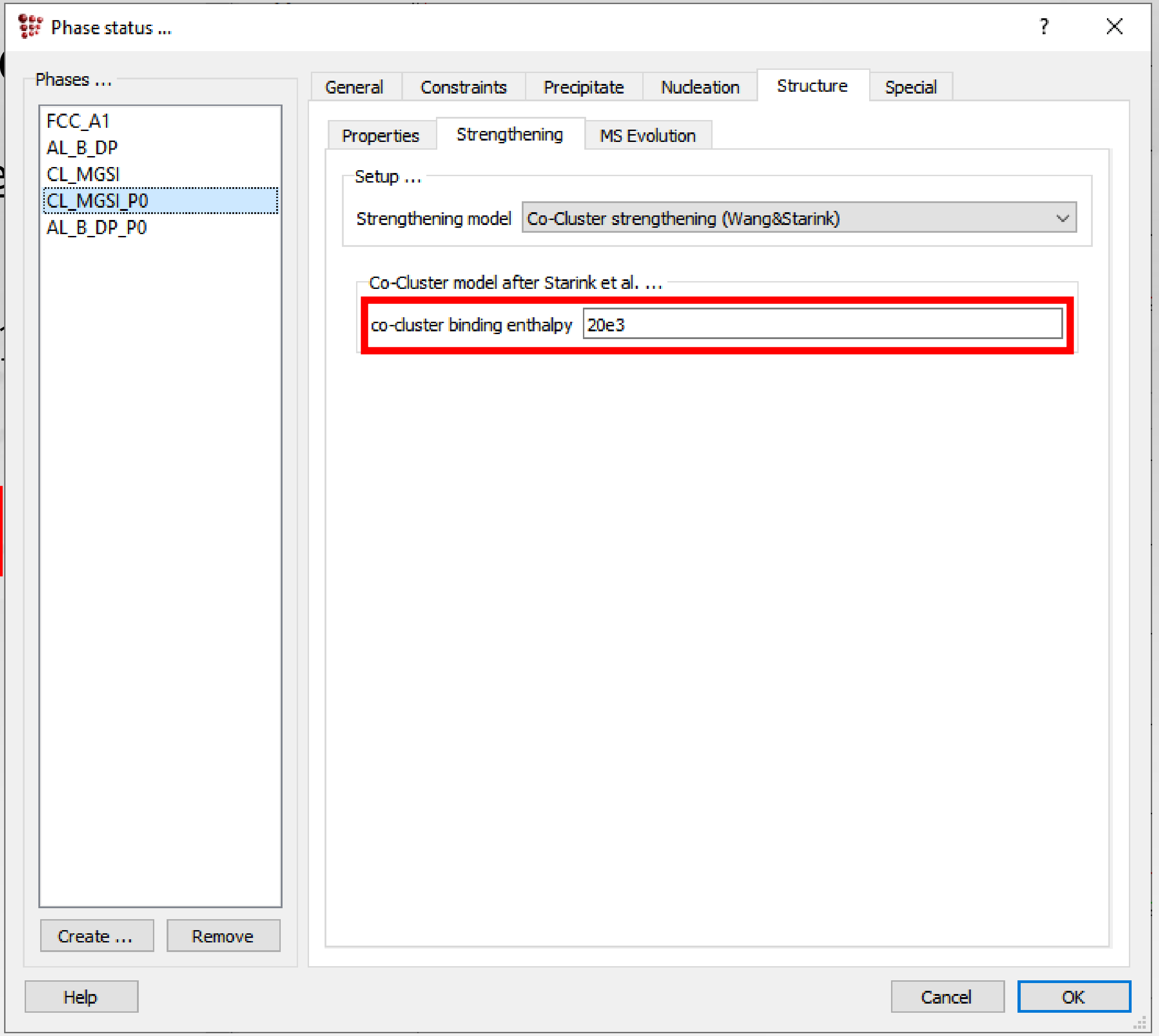

Co-cluster strengthening

MatCalc Engineering

- Related to binding enthalpy of co-cluster elements

  (<u>applicable only for phases containing two elements</u>)

$$\tau_{prec} = \frac{8}{3\sqrt{3}} \frac{\Delta H_{ccl}}{N_A b^3} \left[f_{ccl} y_A (1 - x_B) + f_{ccl} y_B (1 - x_A) - 3 x_A x_B \right]$$

ΔH_{ccl} - Binding enthalpy of heteroatomic bond in co-cluster

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N_A - Avogadro number

y_i - Content of element *i* in co-cluster

x_i - Content of element *i* in matrix

f_{ccl} - Co-cluster phase fraction

variable	value
precipitates strength	
TAU_CO_CLUST$*	
TAU_CO_CLUST$CL_MGSI_P0	1,99827e+07

Precipitation strengthening, σ_{prec}

- 2 alternative models available
  - Size distribution dependent strengthening
  - Co-cluster strengthening
- $\tau_{prec} \rightarrow \sigma_{prec}$

$$\sigma_{prec} = M_T \tau_{prec}$$

M_T - Taylor factor

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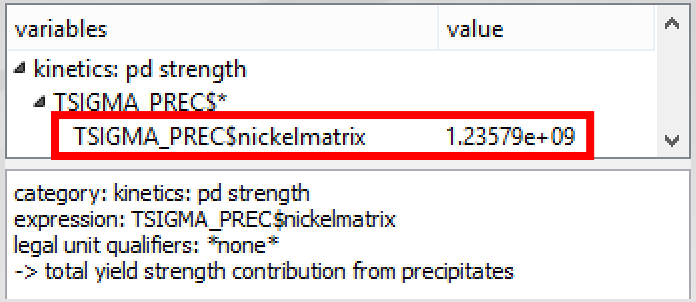


M_T - Taylor factor

Mechanical threshold, σ_0

- Yield stress at temperature 0 K
- Thermal & athermal contributions

$$\sigma_{ath} = \sigma_i + \sigma_{gb} + \sigma_{sgb} + \sigma_{ss} + \sigma_{prec}$$

$$\sigma_{th} = \sigma_{disl}$$

$$\sigma_0 = f\left(\sigma_i, \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \sigma_{ss}, \sigma_{prec}\right)$$

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

Thank you for your attention !

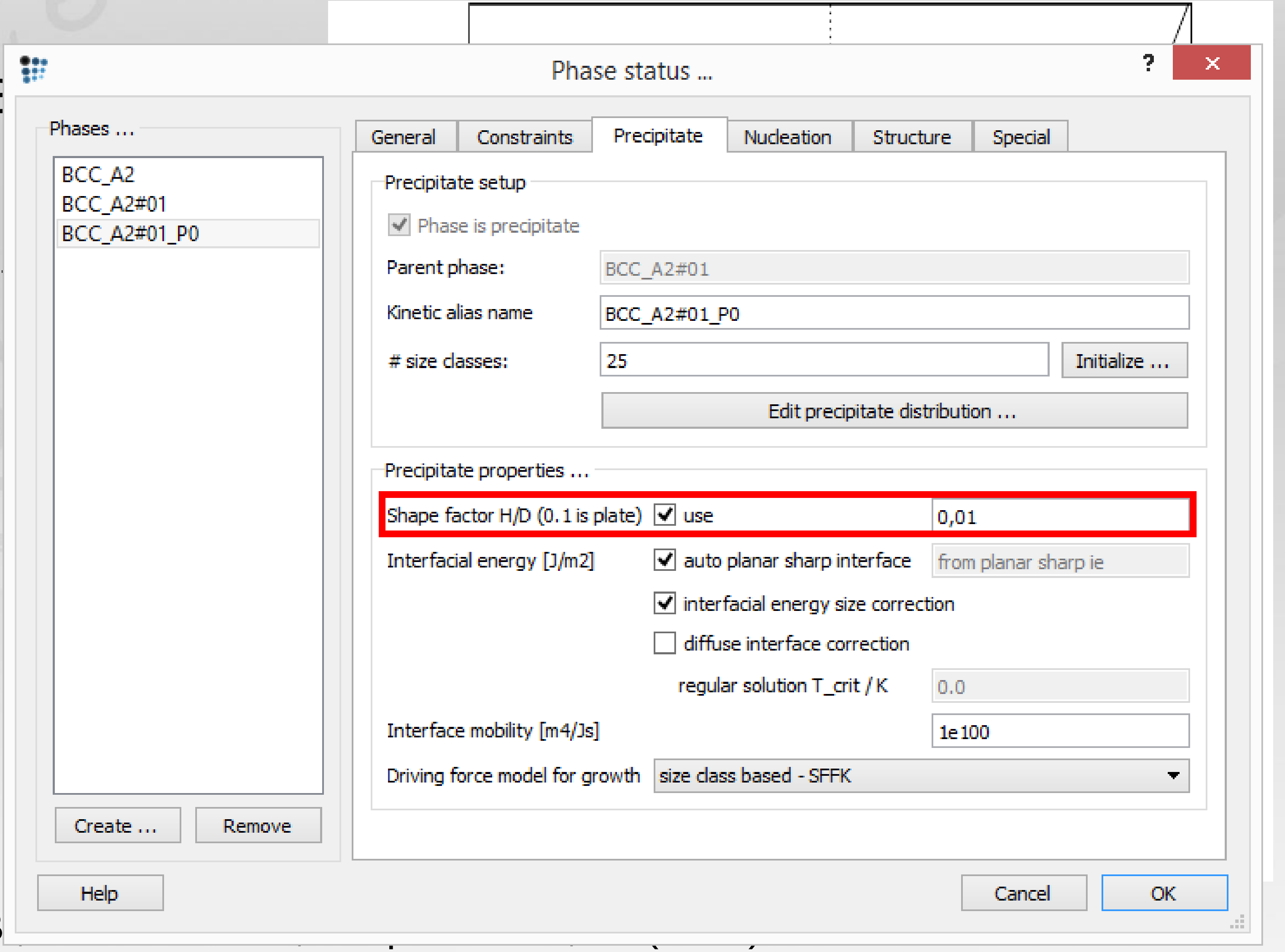
Precipitation hardening

Shape factor influence

$$L_S = K\left(\sqrt{\frac{\ln 3}{2\pi\sum_{class} N_{V,class} r_{m,class}} + 4r_{ss}^2}\right.$$

$$K = h^{1/6}\left(\frac{2+h^2}{3}\right)^{-1/4}$$

h - Shape factor



Sonderegger B

Precipitation hardening

Shape factor influence on L_S

$$L_S = K\left(\sqrt{\frac{\ln 3}{2\pi\sum_{class} N_{V,class} r_{m,class}} + 4r_{ss}^2} - 2r_{ss}\right)$$

$$K = h^{1/6}\left(\frac{2+h^2}{3}\right)^{-1/4}$$

h - Shape factor

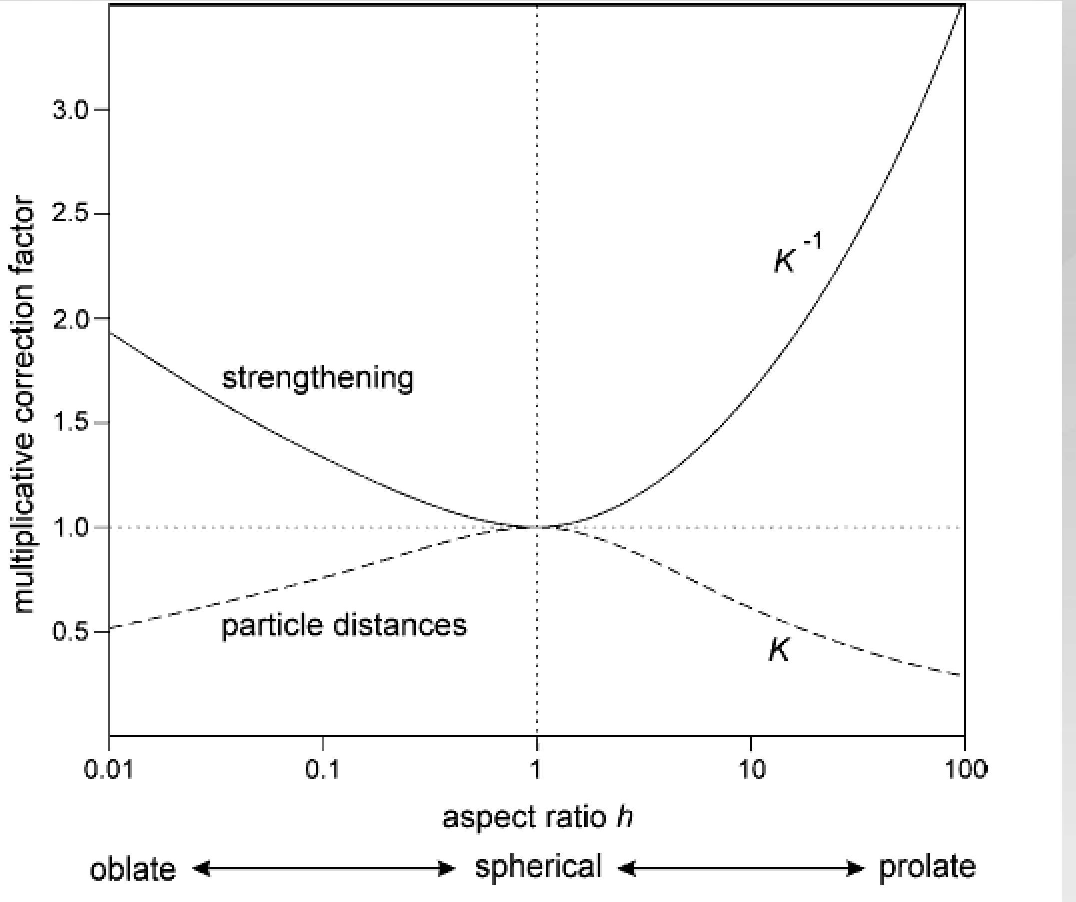


Figure 2. Variation in particle distances and strengthening for prolate and oblate precipitates relative to spherical particles.

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Precipitation hardening

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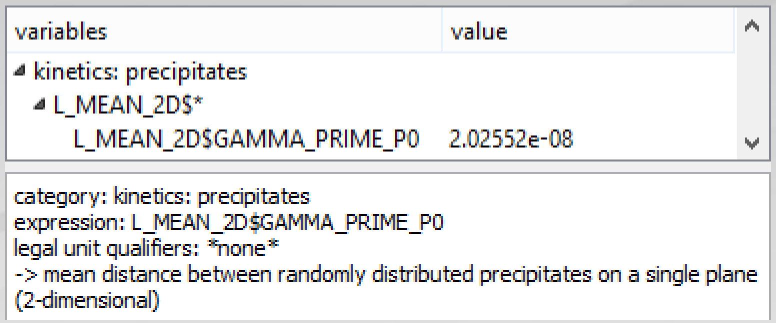

h - Shape factor

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Precipitation hardening

- Shearable particles – (e.g. coherency effect)

$$\tau_{coh,weak} = \frac{f(\theta)}{L_S}\left(\frac{G^3\varepsilon^3 r_{eq}^3 b}{27T_{weak}}\right)^{1/2} h$$

$$r_{eq} = \left(P_{edge} r_{eq,edge,sh} + P_{screw} r_{eq,screw,sh}\right)$$

$$r_{eq,edge,sh} = \left[\frac{h^{2/3}}{3}\left(\sqrt{\frac{3}{2+h^2}} + 2\sqrt{\frac{6}{1+5h^2}}\right)\right]\frac{\pi}{4} r_m$$

$$r_{eq,screw,sh} = \left[\frac{h^{2/3}}{3}\left(\frac{1}{h} + 2\sqrt{\frac{2}{1+h^2}}\right)\right]\frac{\pi}{4} r_m$$

$r_{eq,edge,sh}$ - Equivalent radius for edge disl.

$r_{eq,screw,sh}$ - Equivalent radius for screw disl.

Precipitation hardening

- Shearable particles – Coherency effect for non-spherical particles

  - Strong particles

$$\tau_{coh,strong} = \frac{\left(1.1101\cos^2\theta + 2.1488\sin^2\theta\right)}{L_S}\left(\frac{T_{strong}^3 G\varepsilon r_m}{b^3}\right)^{1/4} K \qquad K = h^{1/6}\left(\frac{2+h^2}{3}\right)^{-1/4}$$

  - Weak particles

$$\tau_{coh,weak} = \frac{\left(2.7310\cos^2\theta + 3.4736\sin^2\theta\right)}{L_S}\left(\frac{G^3\varepsilon^3 r_{eq}^3 b}{27T_{weak}}\right)^{1/2} h \quad \text{,if} \quad h \le \frac{\left(1.3416\cos^2\theta + 4.1127\sin^2\theta\right)}{\left(2.7310\cos^2\theta + 3.4736\sin^2\theta\right)}$$

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- Yao Shan

MatCalc
Engineering

Thank you for your attention!