MatCalc
Engineering

Alloy yield strength modeling with MatCalc
(rel. 5.61.0057)

P. Warczok

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}

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

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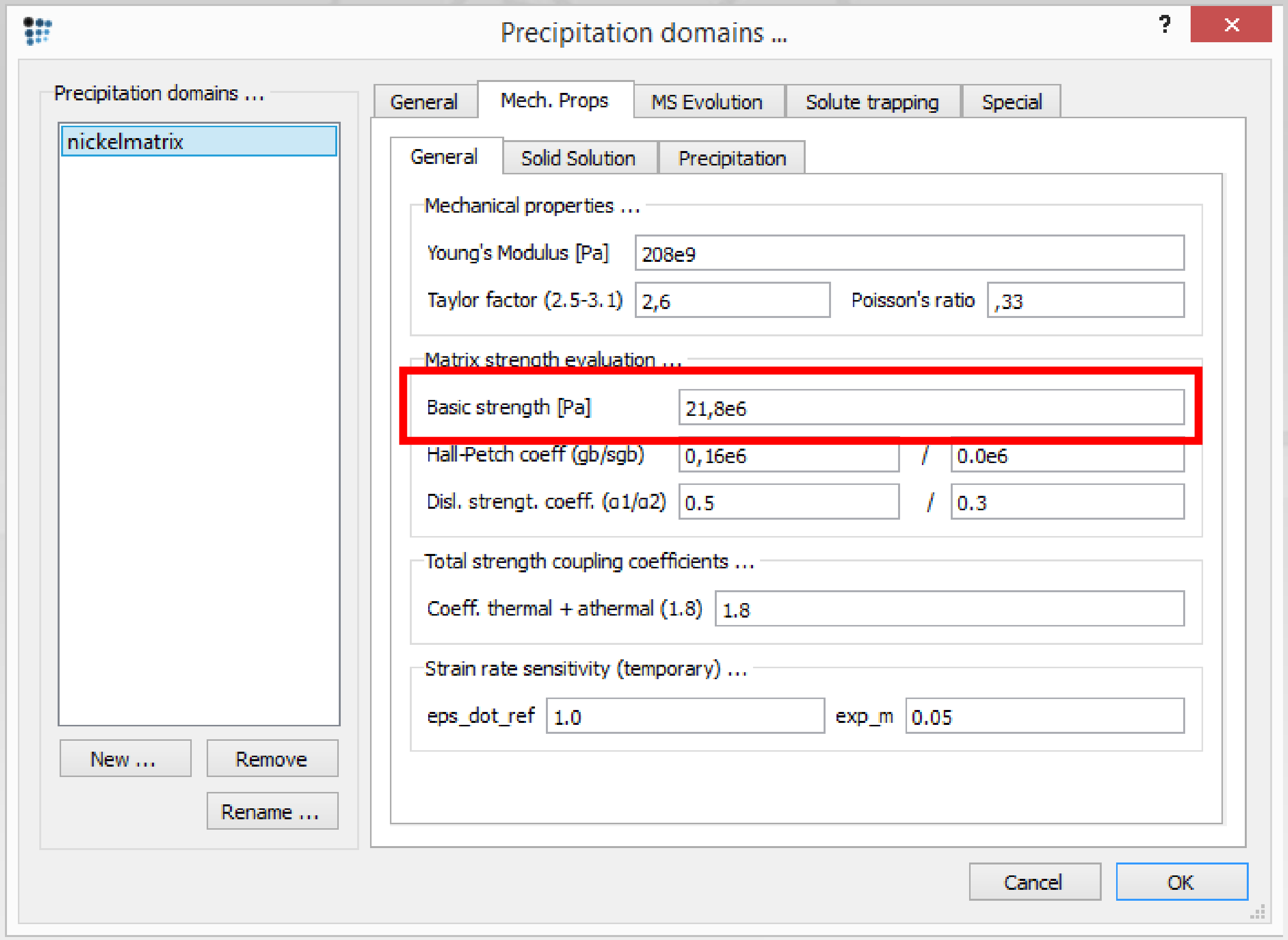
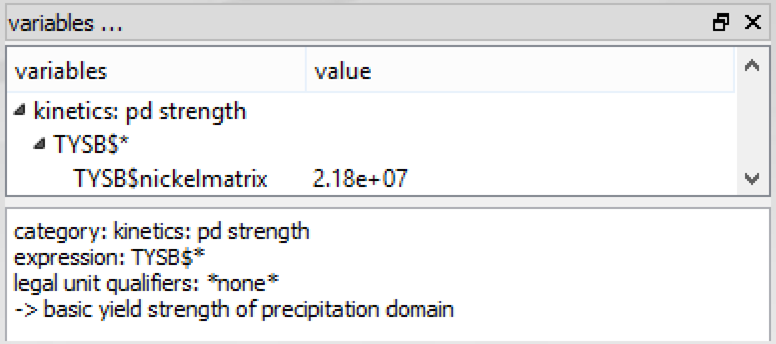
Intrinsic strength, σ_i





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

Work hardening, σ_{disl}

- Taylor equation

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

α - Taylor factor

G - Shear stress

b - Burger's vector

ρ - Dislocation density

Work hardening, σ_{disl}

- Taylor equation

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

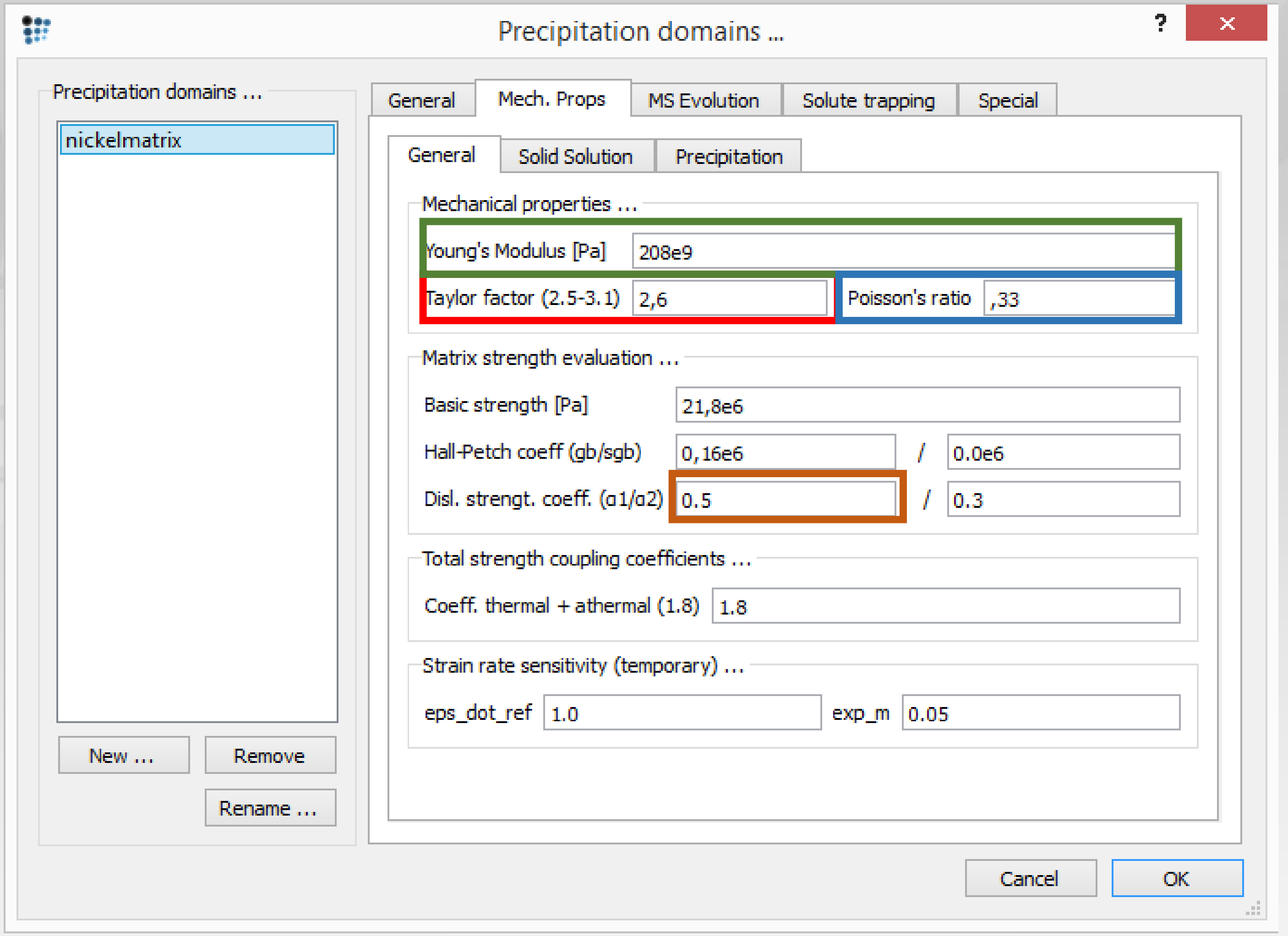
$\boxed{\alpha \text{ - Taylor factor}}$

G - Shear stress

b - Burger's vector

ρ - Dislocation density

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



Work hardening, σ_{disl}

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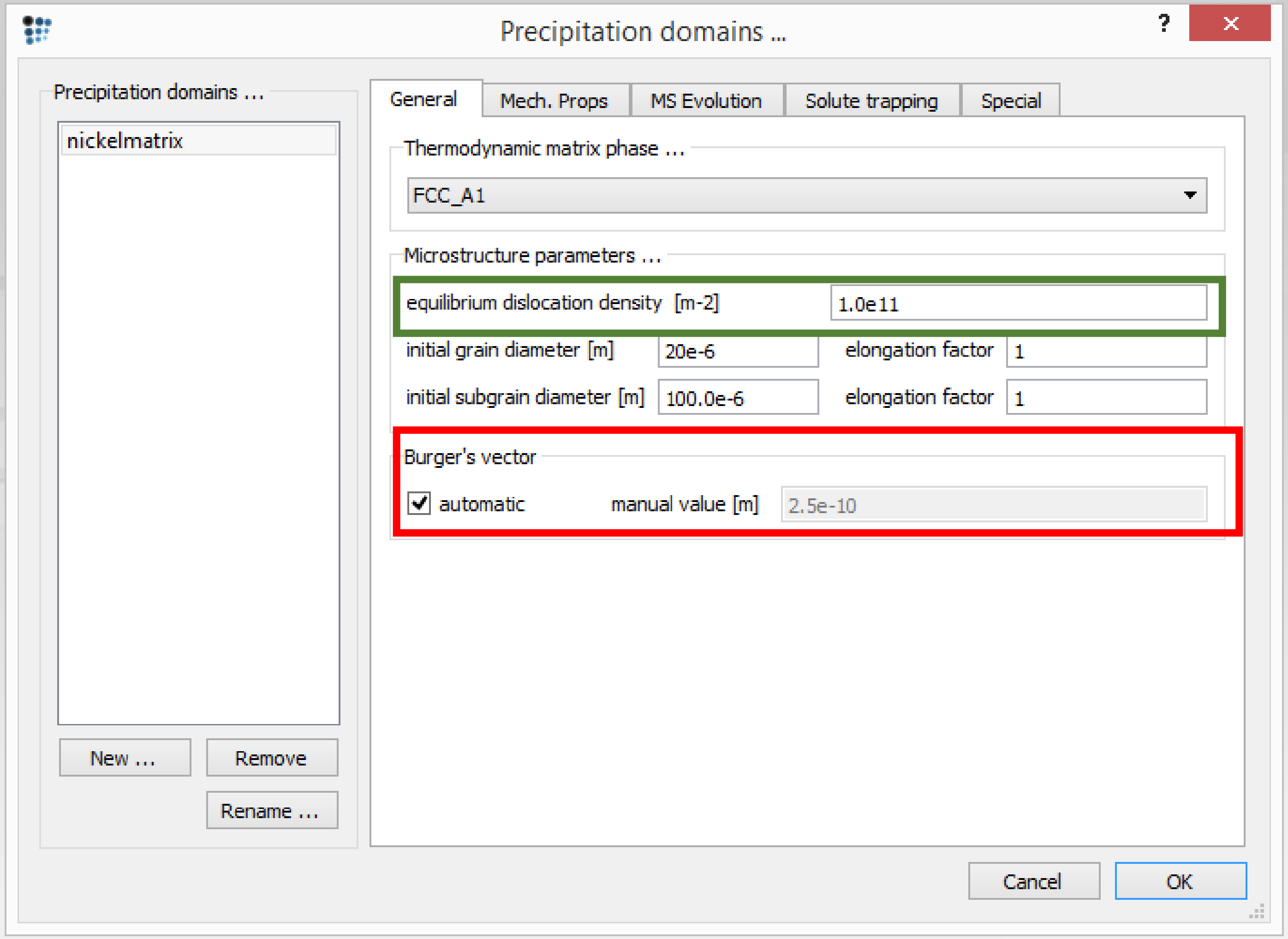

Work hardening, σ_{disl}

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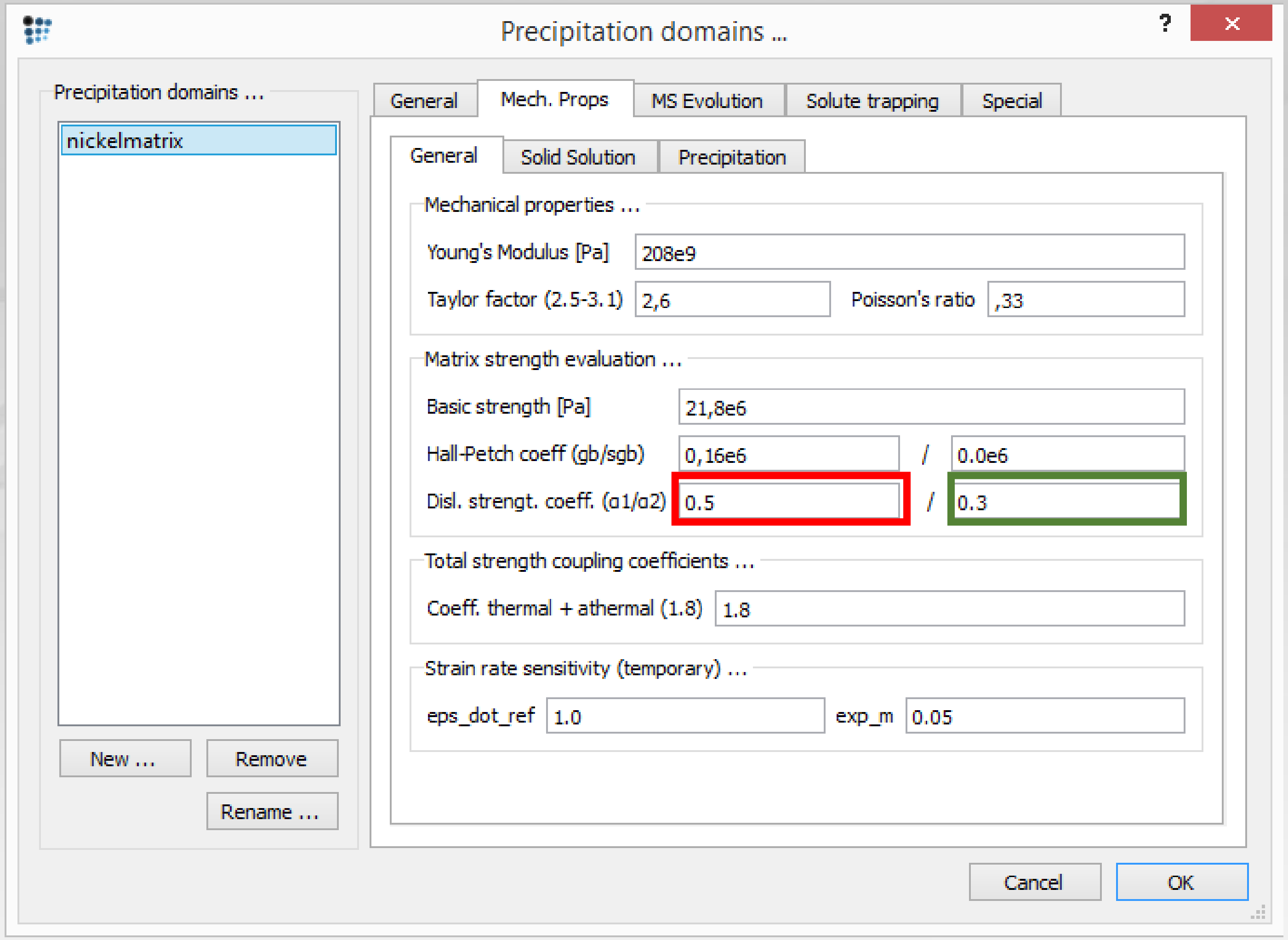
- Taylor equation
  - Two parameter model

$$\sigma_{disl} = \boxed{A_1}\alpha G b\sqrt{\rho_1} + \boxed{A_2}\alpha G b\sqrt{\rho_2}$$



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Work hardening, σ_{disl}

- Taylor equation
  - Two parameter model

$$\boxed{\sigma_{disl}} = A_1 \alpha G b \sqrt{\rho_1} + A_2 \alpha G b \sqrt{\rho_2}$$

variables	value
kinetics: pd strength	
TDS$*	
TDS$nickelmatrix	7.1404e+06

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

Model overview

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

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

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

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

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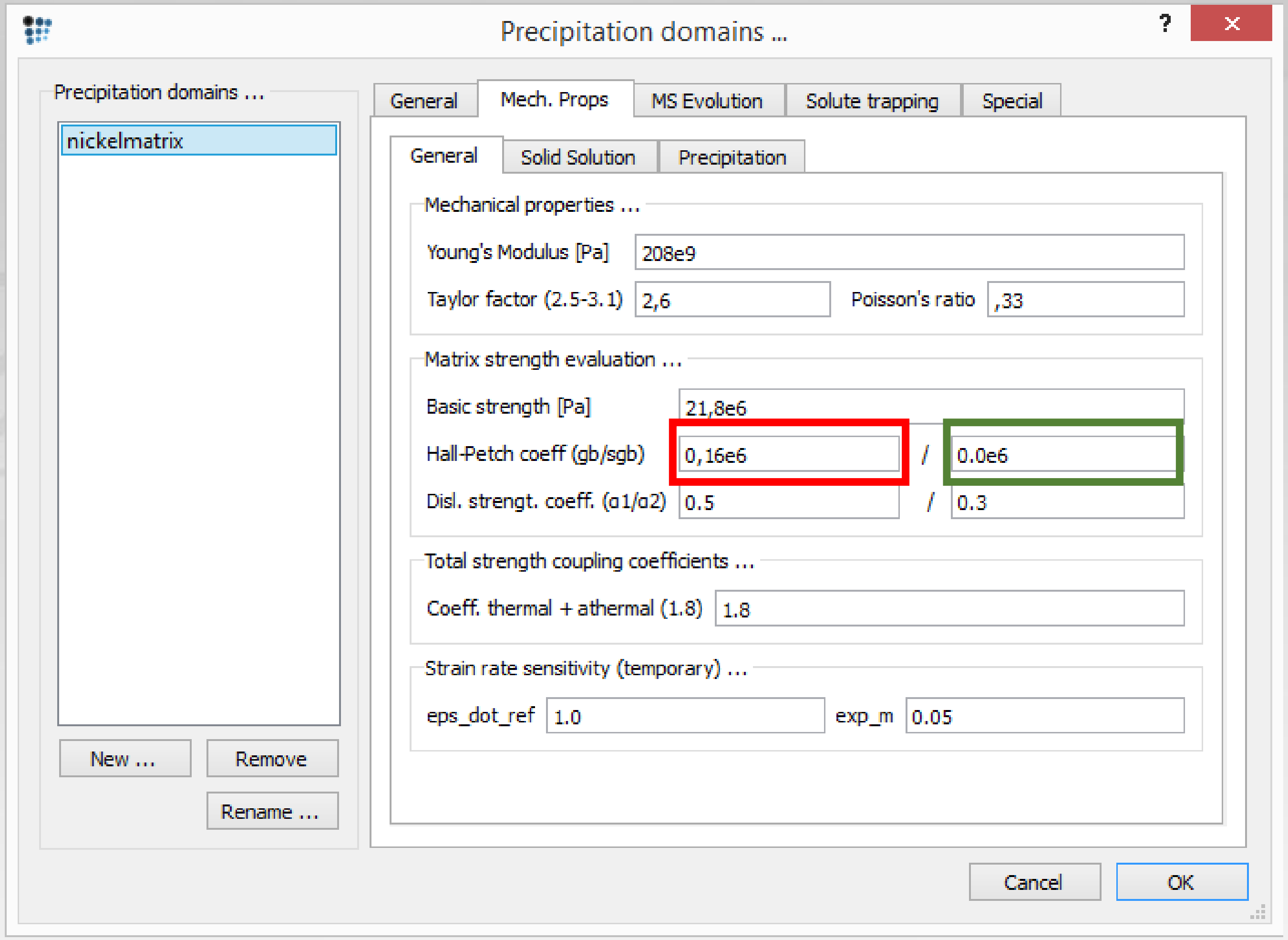

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Grain/subgrain boundary strengthening, σ_{gb} , σ_{sgb}

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

D - Grain diameter

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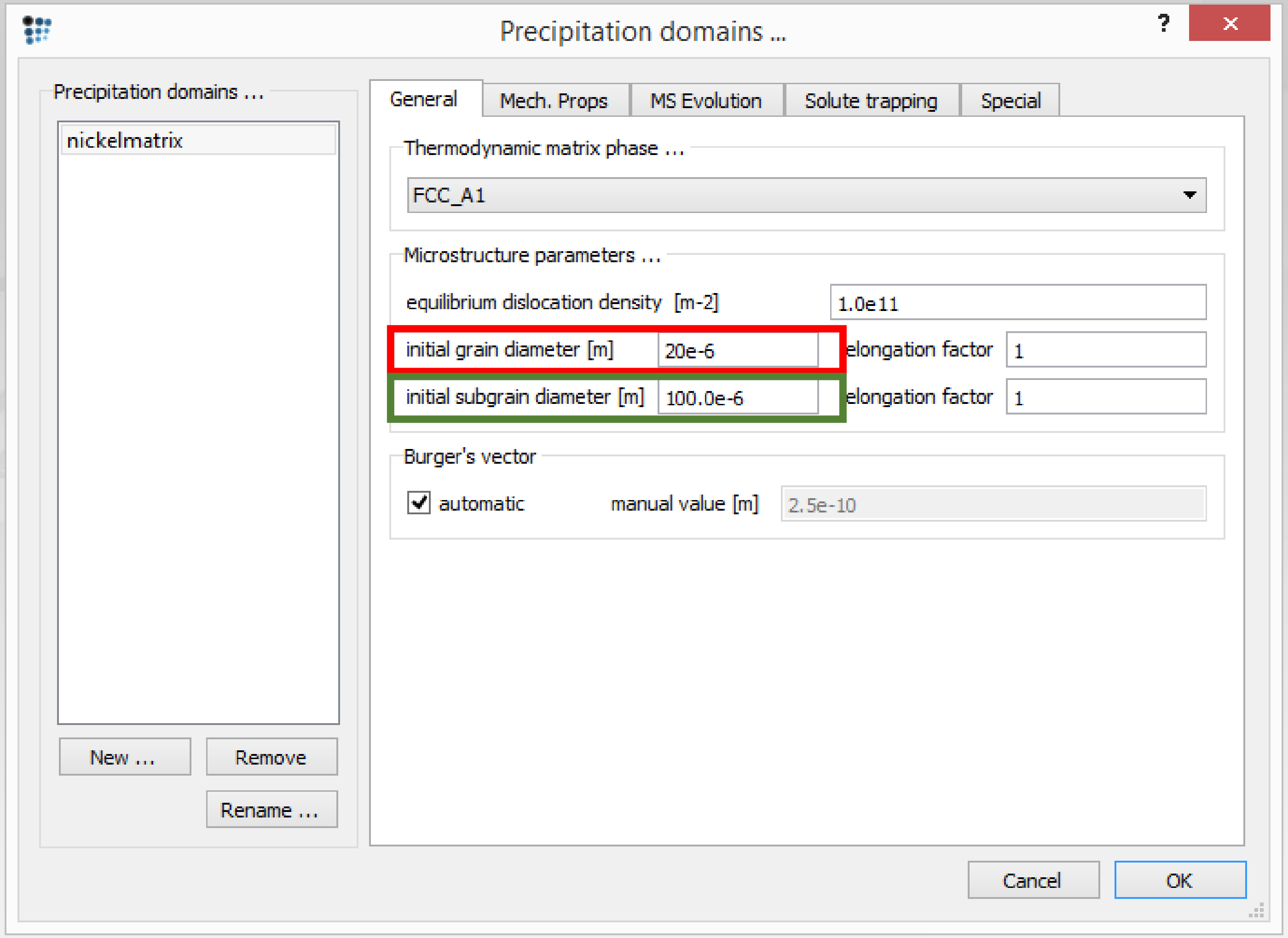

Grain/subgrain boundary strengthening, σ_{gb} , σ_{sgb}

- Hall-Petch equation

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

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

D - Grain diameter

δ - Subgrain diameter

k_n - Constant

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}

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

Solid solution strengthening, σ_{ss}

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

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

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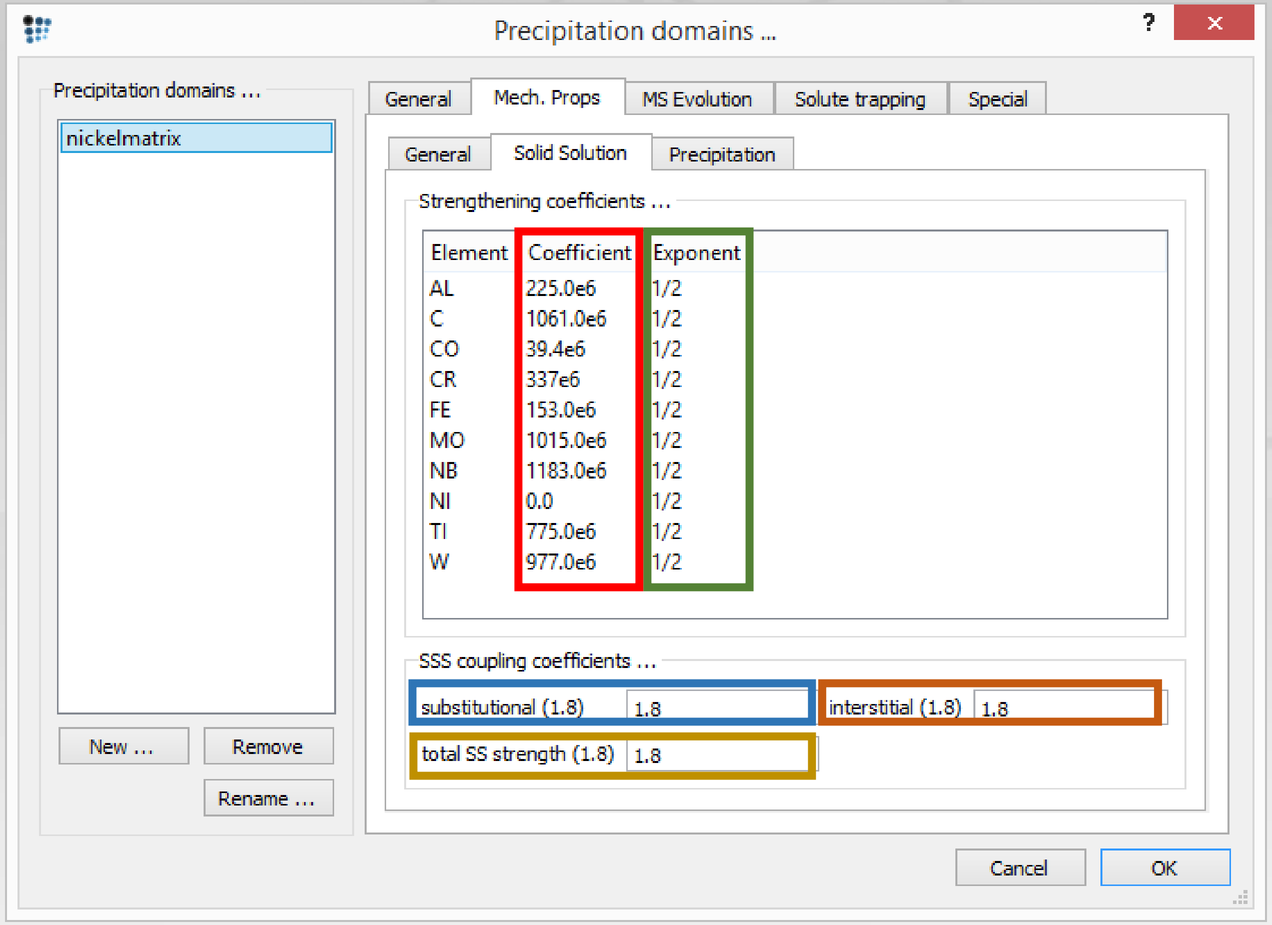
Solid solution strengthening, σ_{ss}



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

k_i - Coefficient for element *i*

c_i - Element i content in the prec. domain

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}

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

variables	value
kinetics: pd strength	
TSSS$*	
TSSS$nickelmatrix	2.82649e+08

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

Solid solution strengthening, σ_{ss}

- Solid solution strengthening, σ_{ss}

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

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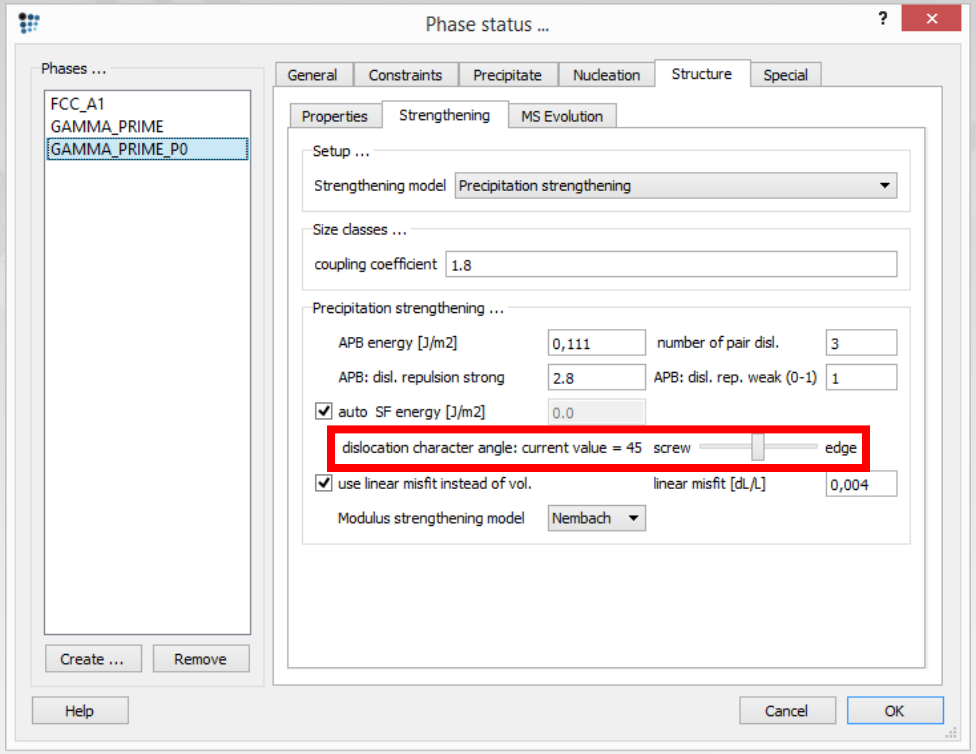
$$\sigma_{YS} = f\left(\sigma_i, \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \sigma_{ss}, \sigma_{prec}\right)$$

Precipitation strengthening, σ_{prec}

- Some general parameters/settings
  - Angle between dislocation line and Burger's vector θ (edge:screw ratio, θ = 0 for pure screw, θ = $\pi/2$ for pure edge)



Precipitation strengthening, σ_{prec}

- 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

Precipitation strengthening, σ_{prec}

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

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

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

$N_{V,class}$ - 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)

Precipitation strengthening, σ_{prec}

- Derived from τ_{prec}
  - Non-shearable particles (Orowan mechanism)
  - Shearable particles (weak or strong)
    - Coherency effect
    - Modulus effect
    - Anti-phase boundary effect
    - Stacking fault effect
    - Interfacial effect

Precipitation strengthening, σ_{prec}

- Derived from τ_{prec}
  - Non-shearable particles (Orowan mechanism)
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    - Interfacial effect

Non-shearable particles

$$\tau_{nsh} = \frac{JGb}{2\pi\sqrt{1-\upsilon}L_s}\ln\left(\frac{2r_{eq}}{r_i}\right)$$

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

$$r_i = 2b$$

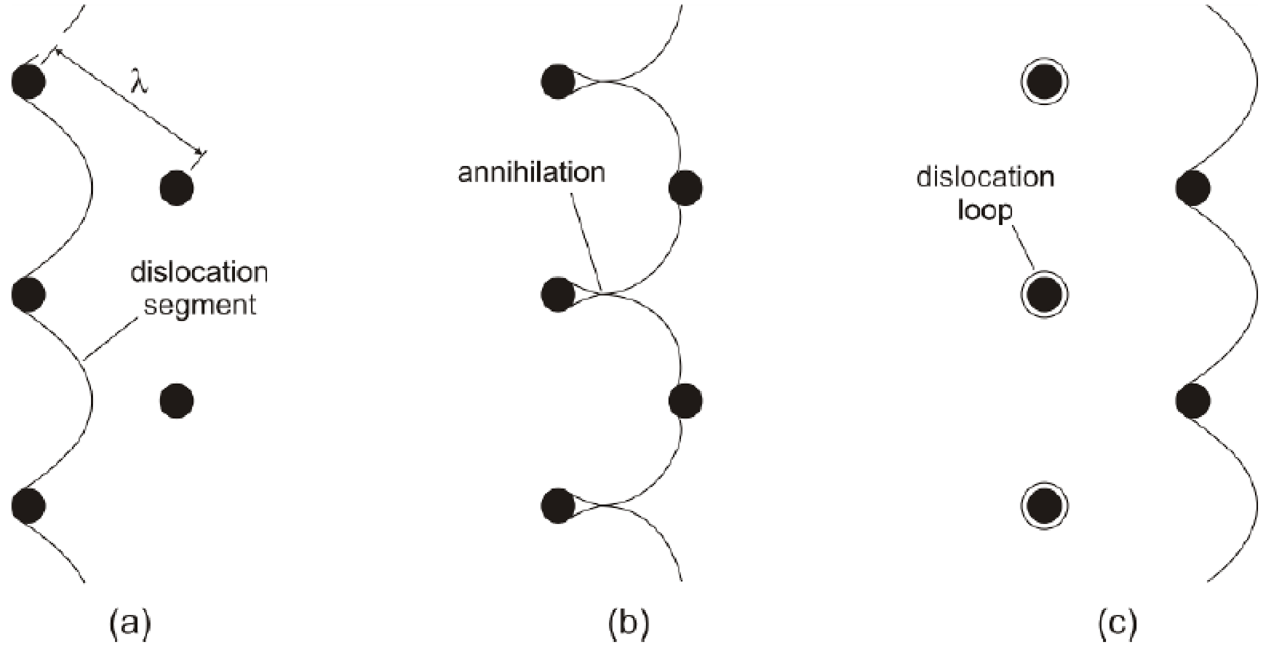


Figure 3.12. Bypassing of strong obstacles by a dislocation according to Orowan. λ denotes the mean planar spacing of precipitates[91].

Non-shearable particles

$$\tau_{nsh} = \frac{JGb}{2\pi\sqrt{1-\upsilon}L_s}\ln\left(\frac{2r_{eq}}{r_i}\right)$$

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

$$r_{eq} = \frac{\pi}{4}r_m \qquad r_i = 2b$$

If $r_{eq} < 2r_i$, then

$$\tau_{nsh} = \frac{JGb}{2\pi\sqrt{1-\upsilon}L_s}\ln(2)$$

Non-shearable particles

$$\boxed{\tau_{nsh}} = \frac{JGb}{2\pi\sqrt{1-\upsilon}L_s}\ln\left(\frac{2r_{eq}}{r_i}\right)$$

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

$$r_{eq} = \frac{\pi}{4}r_m \qquad r_i = 2b$$

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

Precipitation strengthening, σ_{prec}

- Derived from τ_{prec}
  - Non-shearable particles (Orowan mechanism)
  - Shearable particles (weak or strong)
    - Coherency effect
    - Modulus effect
    - Anti-phase boundary effect
    - Stacking fault effect
    - Interfacial effect

Shearable particles

- Some general parameters/settings
  - Dislocation bending angle, ψ - weak and strong particles

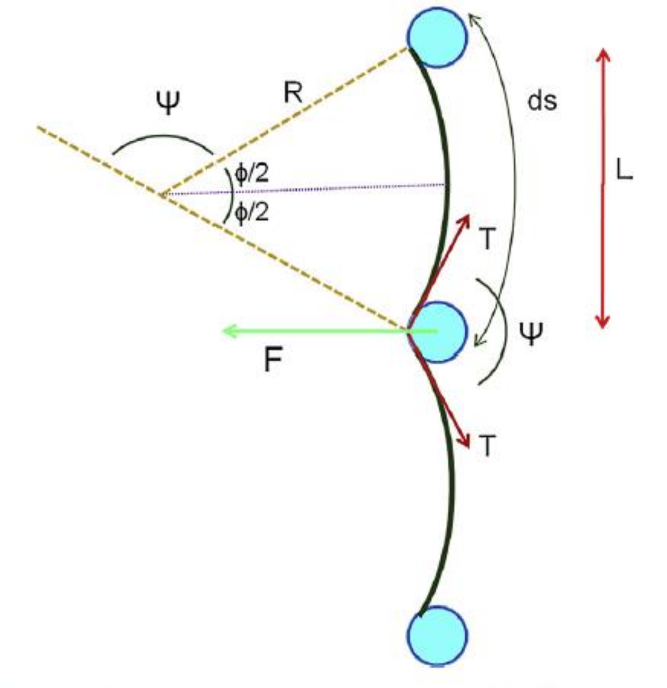


Fig. 1. Balance force between a precipitate and a dislocation.

$0° \leq \psi \leq 120°$ → "strong" particles

$120° \leq \psi \leq 180°$ → "weak" particles

Shearable particles

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

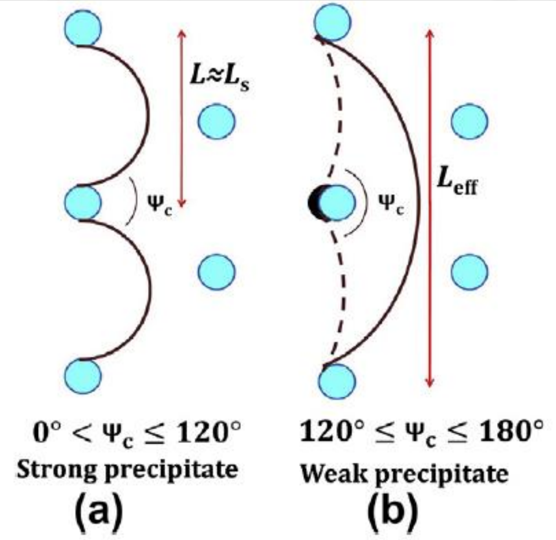


Fig. 2. Free distance between two precipitates along dislocation line in a random array. (A) The precipitates are shearable and strong and (B) the precipitates are shearable and weak.

Strong particles

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

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

Shearable particles

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

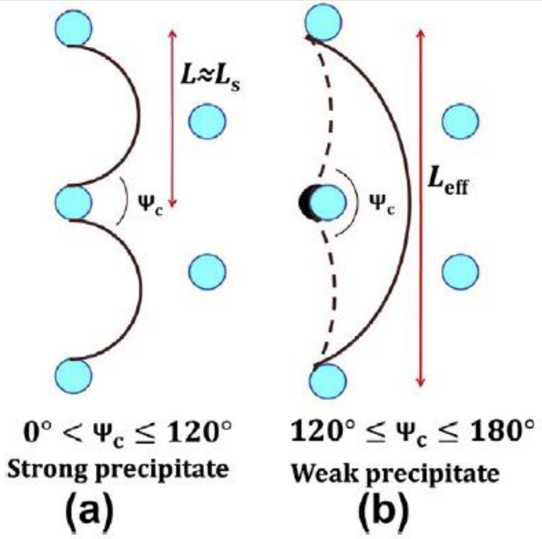


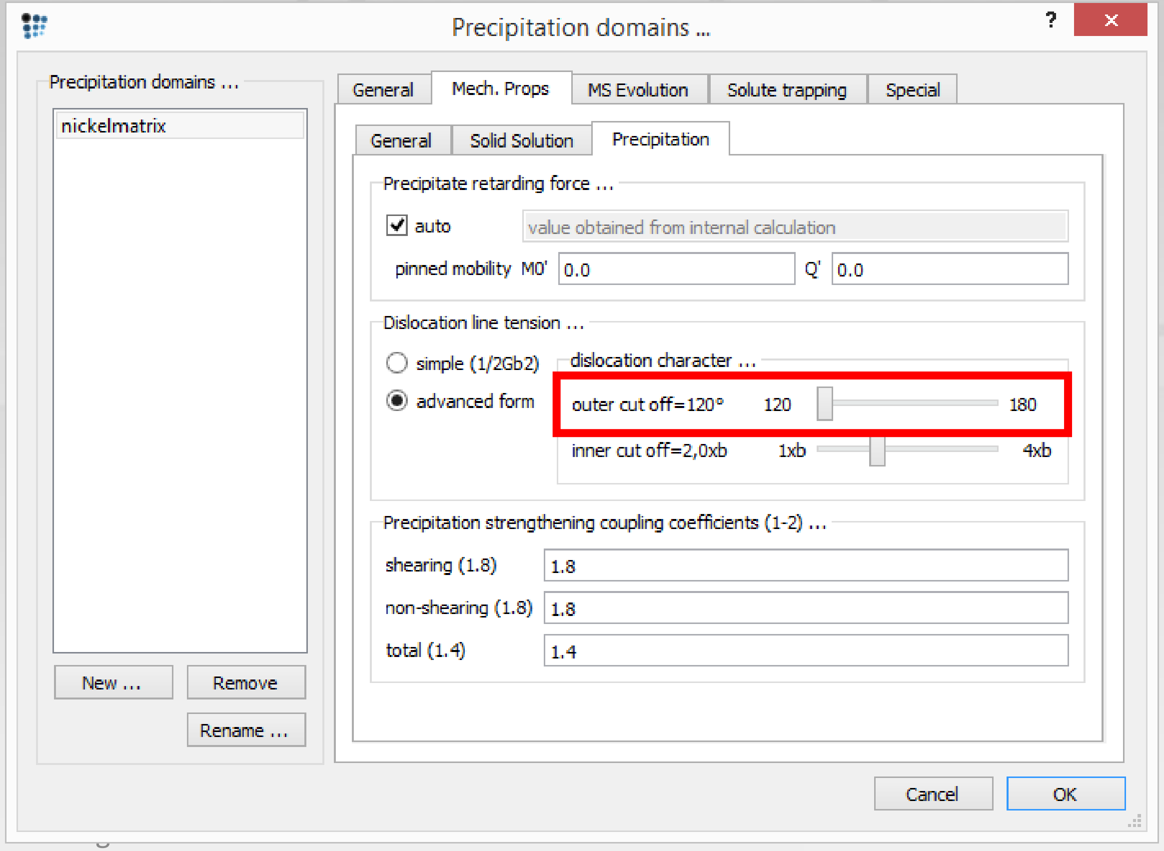
Fig. 2. Free distance between two precipitates along dislocation line in a random array. (A) The precipitates are shearable and strong and (B) the precipitates are shearable and weak.

Weak particles

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

Shearable particles

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



Weak particles

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

Shearable particles

- Some general parameters/settings
  - Dislocation line tension, T
    - Simple model

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

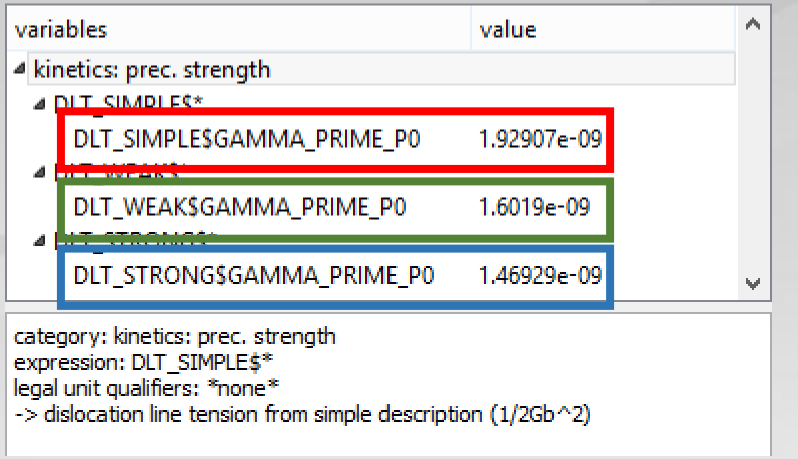
    - Advanced model

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

Shearable particles

- Some general parameters/settings
  - Dislocation line tension, T
    - Simple model

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



    - Advanced model

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

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

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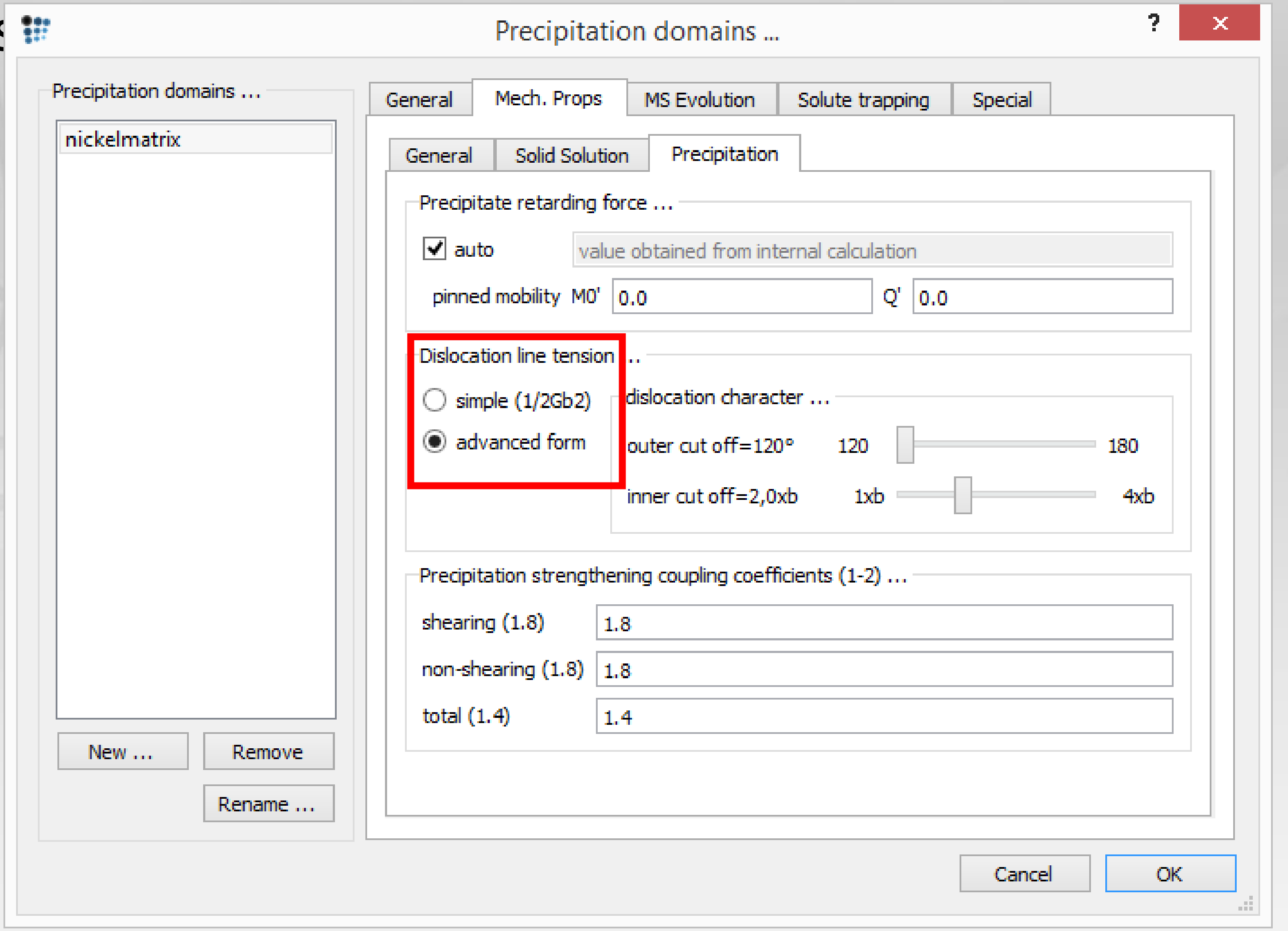
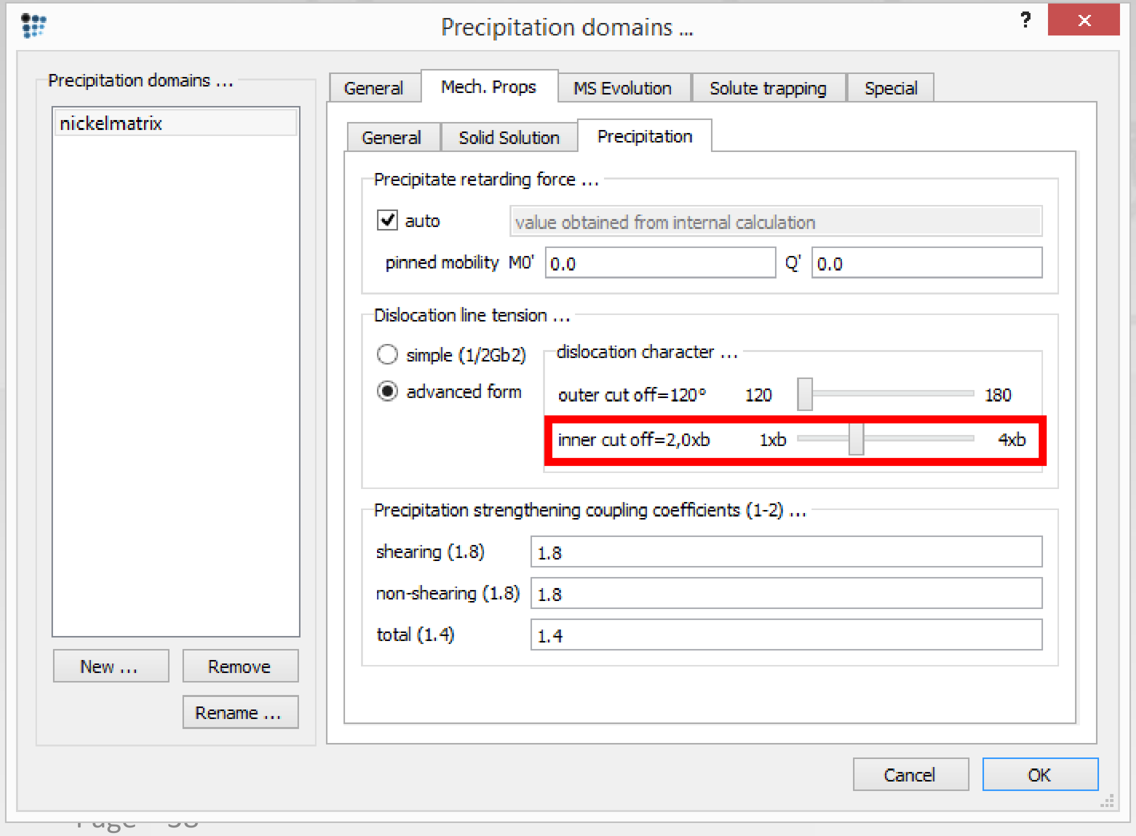
Shearable particles

- Some general parameters/s
  - Dislocation line tension, T
    - Simple
    - Advanced



Shearable particles

- Some general parameters/settings
  - Inner cut-off radius, r_i (multiplication of Burger's vector)



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

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

Precipitation strengthening, σ_{prec}

- Derived from τ_{prec}
  - Non-shearable particles (Orowan mechanism)
  - Shearable particles (weak or strong)
    - Coherency effect
    - Modulus effect
    - Anti-phase boundary effect
    - Stacking fault effect
    - Interfacial effect

Coherency effect

- Strain field due to precipitation/matrix misfit

  - Strong particles

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

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

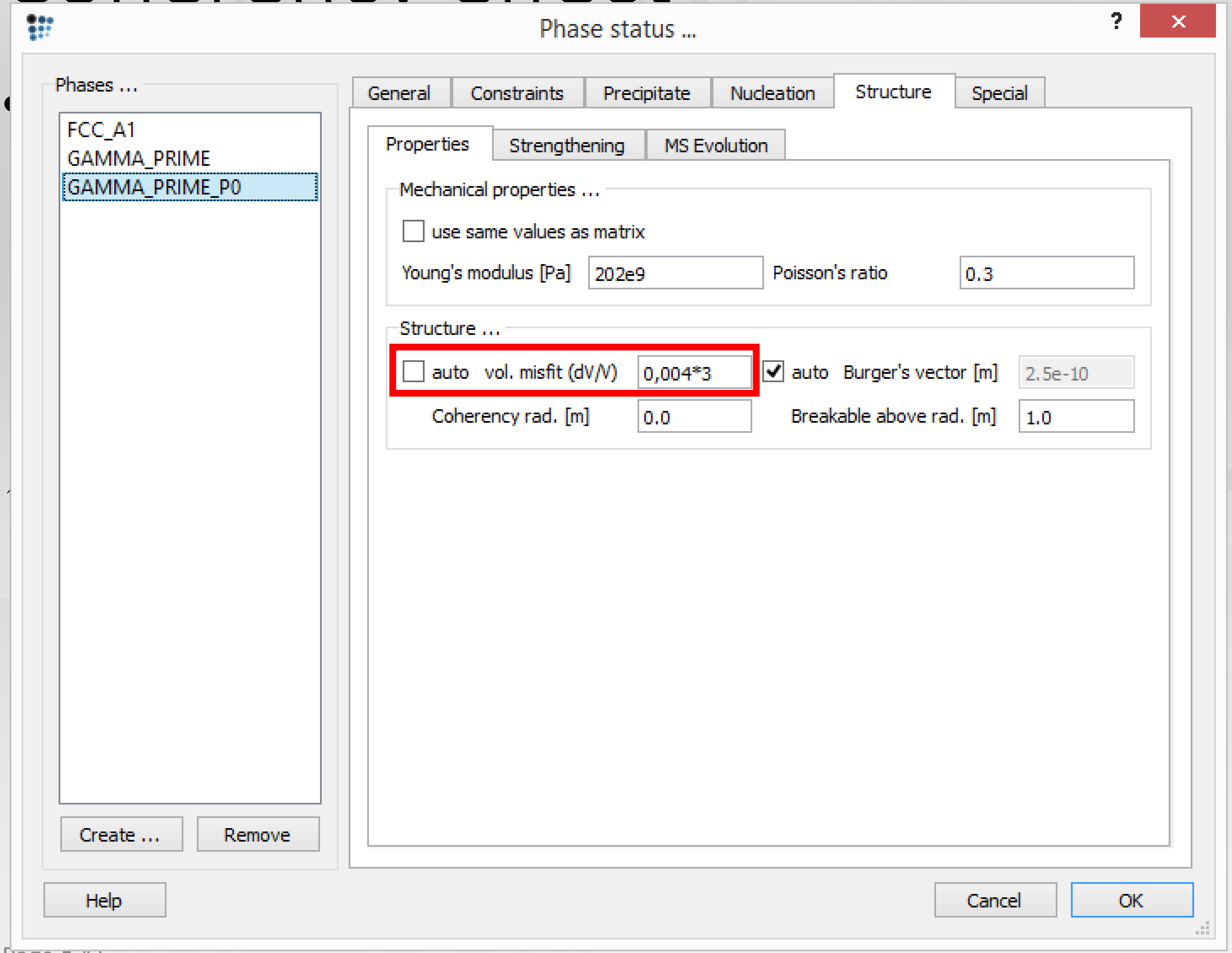
  - Weak particles

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

Δ_{lin} - Linear misfit

Δ_{vol} - Volumetric misfit

Coherency effect



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

Δ_{lin} - Linear misfit

Δ_{vol} - Volumetric misfit

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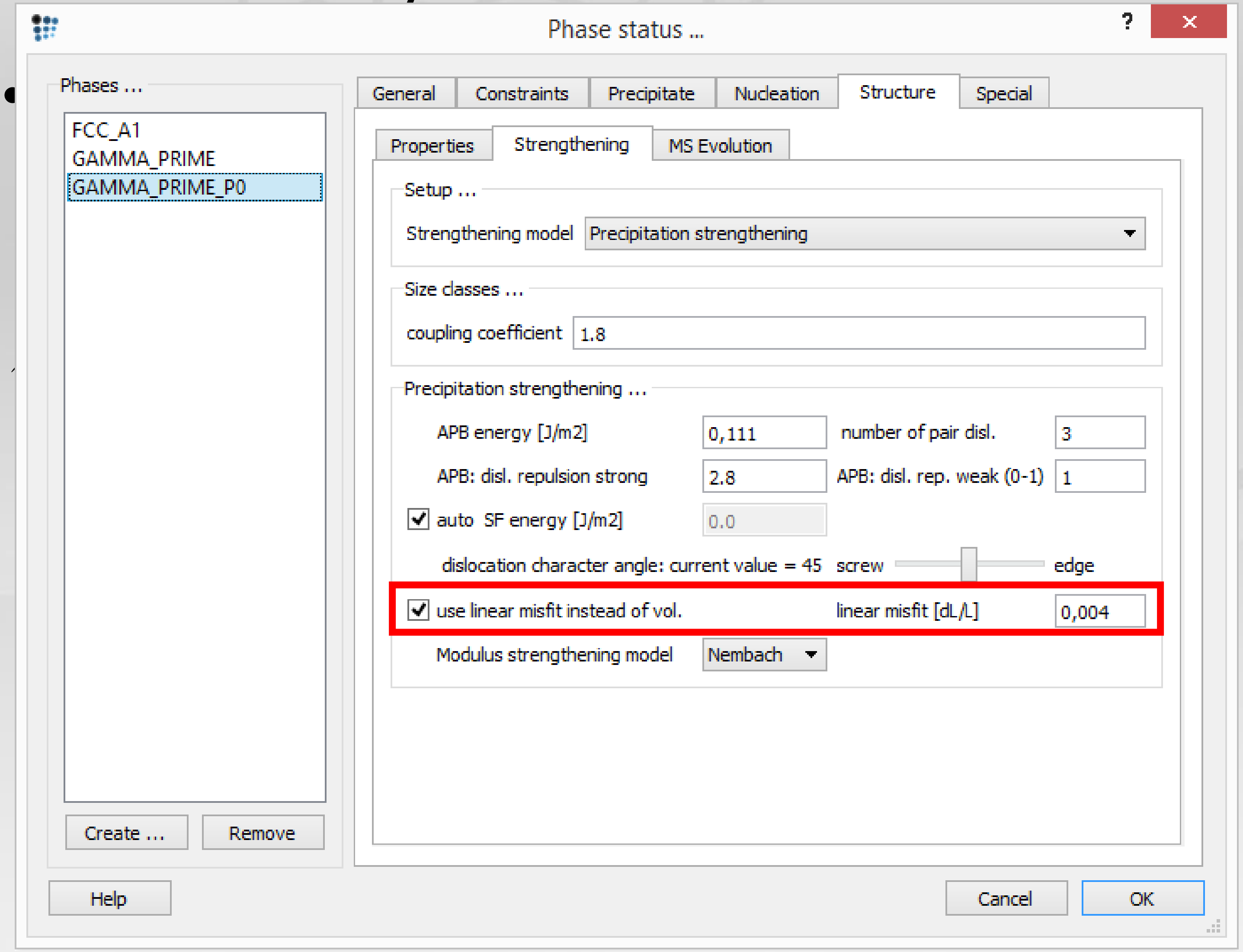
Coherency effect



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

$\boxed{\Delta_{lin} \text{ - Linear misfit}}$

Δ_{vol} - Volumetric misfit

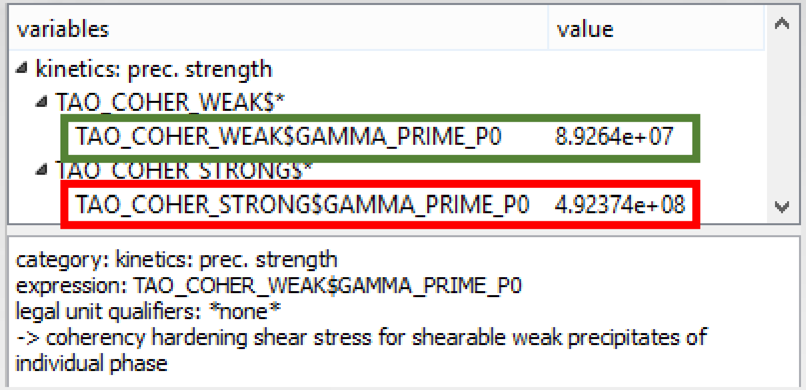
Coherency effect

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

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

  - Weak particles

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



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Precipitation strengthening, σ_{prec}

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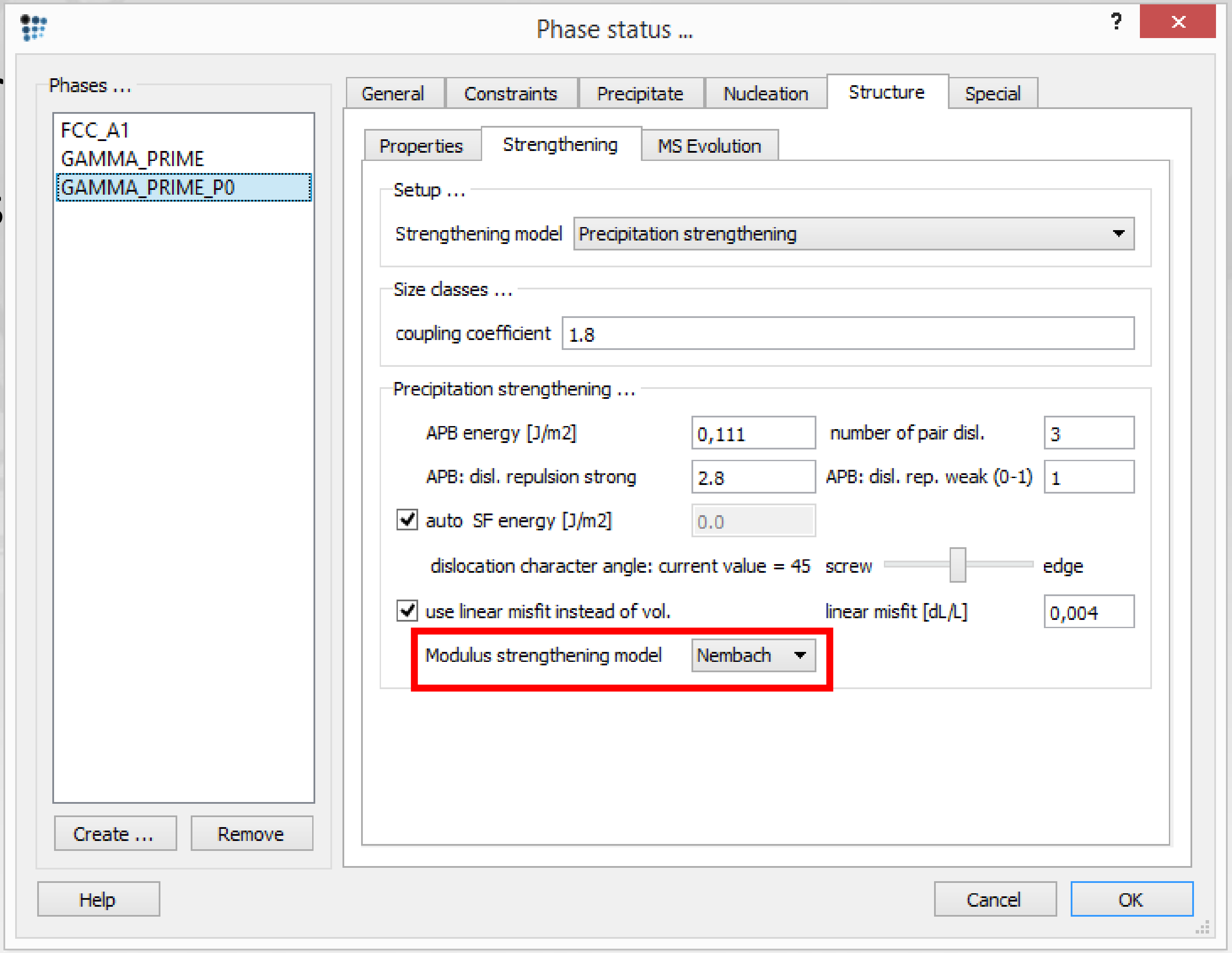
  - Non-shearable particles (Orowan mechanism)
  - Shearable particles (weak or strong)
    - Coherency effect
    - Modulus effect
    - Anti-phase boundary effect
    - Stacking fault effect
    - Interfacial effect

Modulus effect

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

Modulus effect

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



Modulus effect

- Nembach model
  - Strong particles

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

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

  - Weak particles

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

G_p - Particle shear modulus

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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

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

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

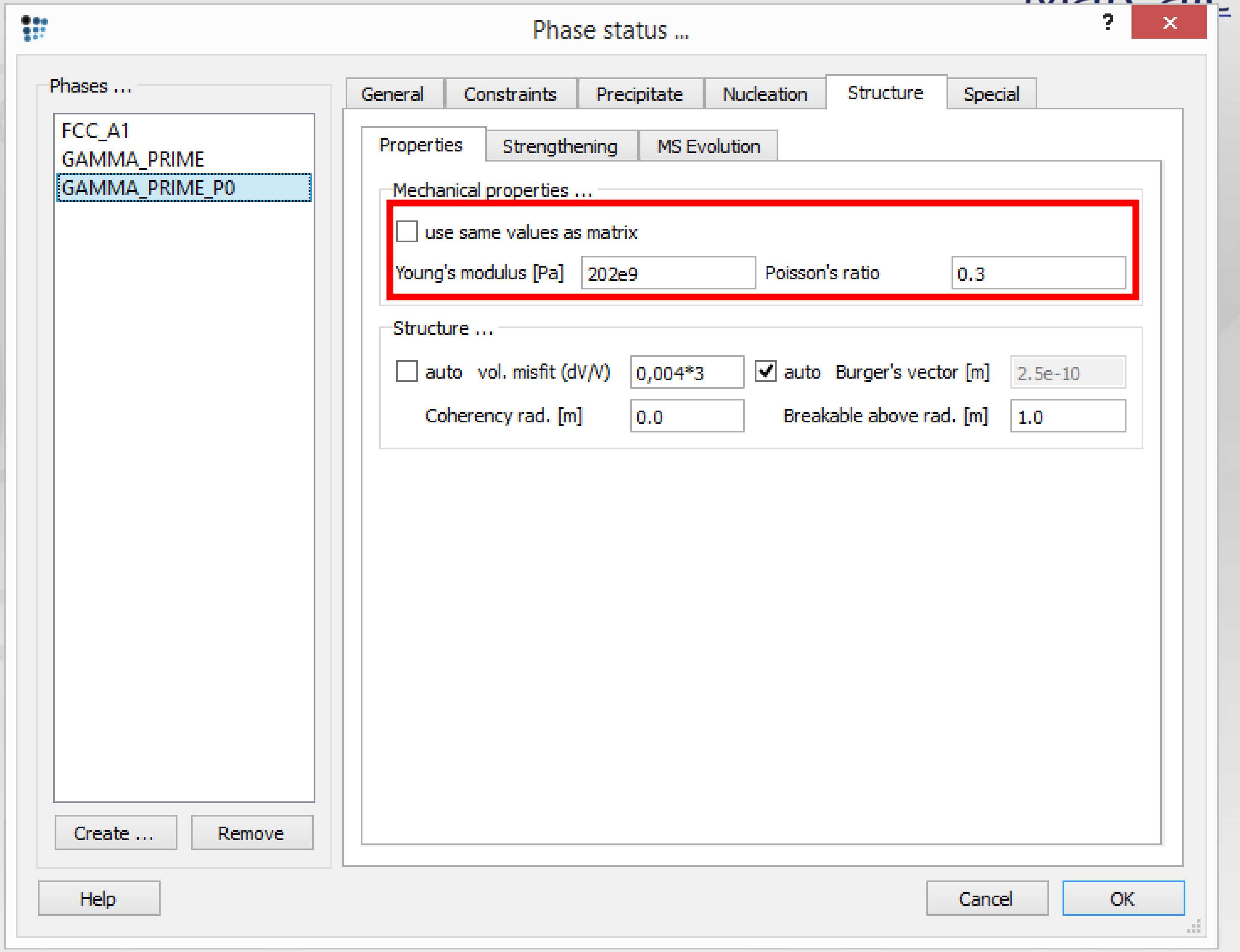
Modulus effect

- Nembach model
  - Strong particles

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

  - Weak particles

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



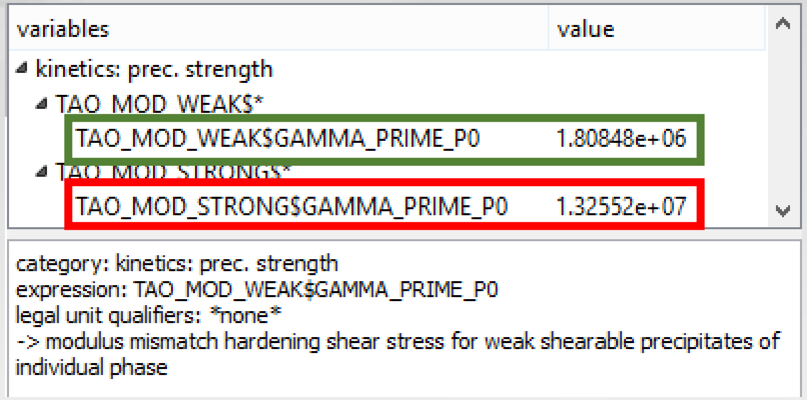
υ_p - Particle Poisson ratio G_p - Particle shear modulus

Modulus effect

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

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

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



Precipitation strengthening, σ_{prec}

- Derived from τ_{prec}
  - Non-shearable particles (Orowan mechanism)
  - Shearable particles (weak or strong)
    - 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

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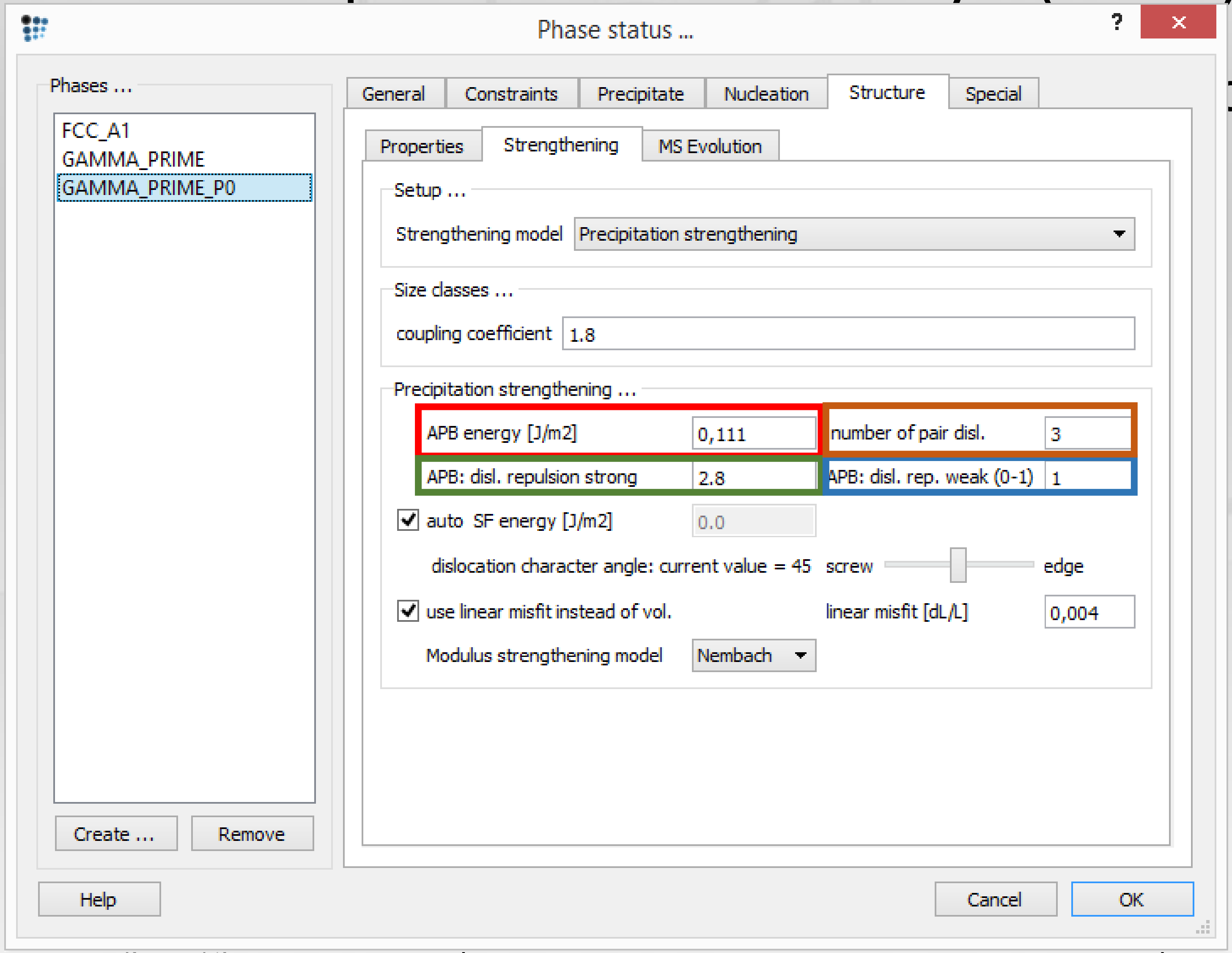

cipitate increases the energy

$\boxed{\gamma_{APB}}$ - APB energy

$\boxed{w}$, $\boxed{\beta}$ - Interaction parameter between the leading and trailing dislocation

$\boxed{s}$ - Number of pair dislocations

Anti-phase boundary (APB) effect

- Dislocation passing through ordered precipitate increases the energy by creating the APB
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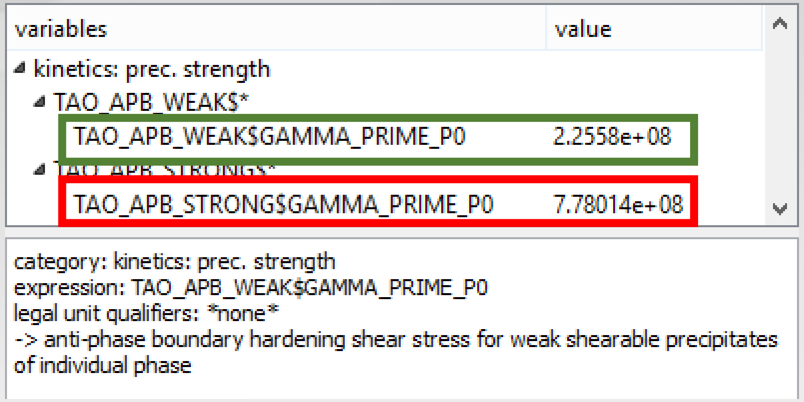
$$\boxed{\tau_{APB,strong}} = \frac{0.69}{bL_S}\left(\frac{8wT_{strong}r_{eq}\gamma_{APB}}{3}\right)^{1/2}$$

  - Weak particles

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



Precipitation strengthening, σ_{prec}

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    - 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

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

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

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

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

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

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

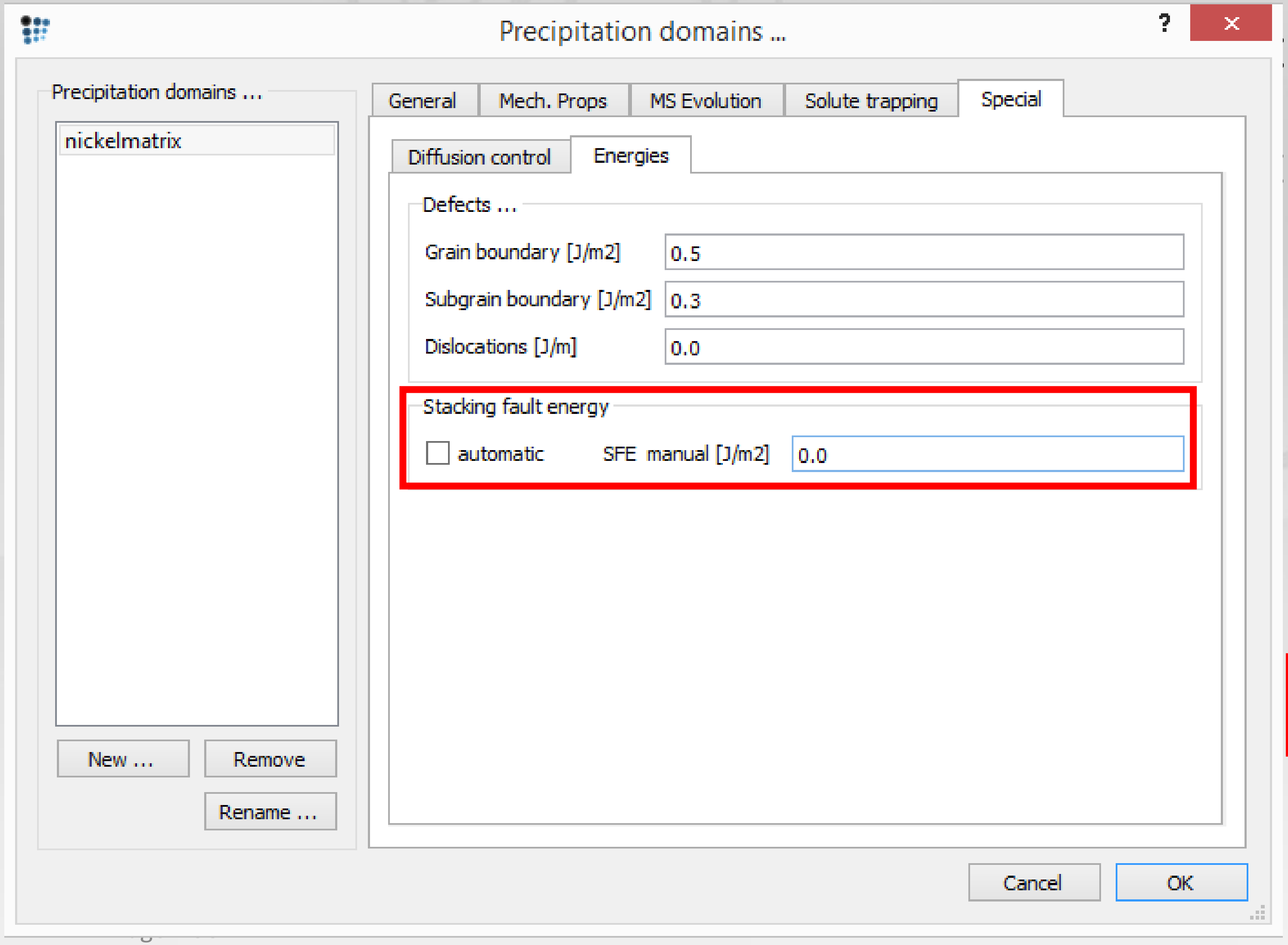
  - Weak particles

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

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

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

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

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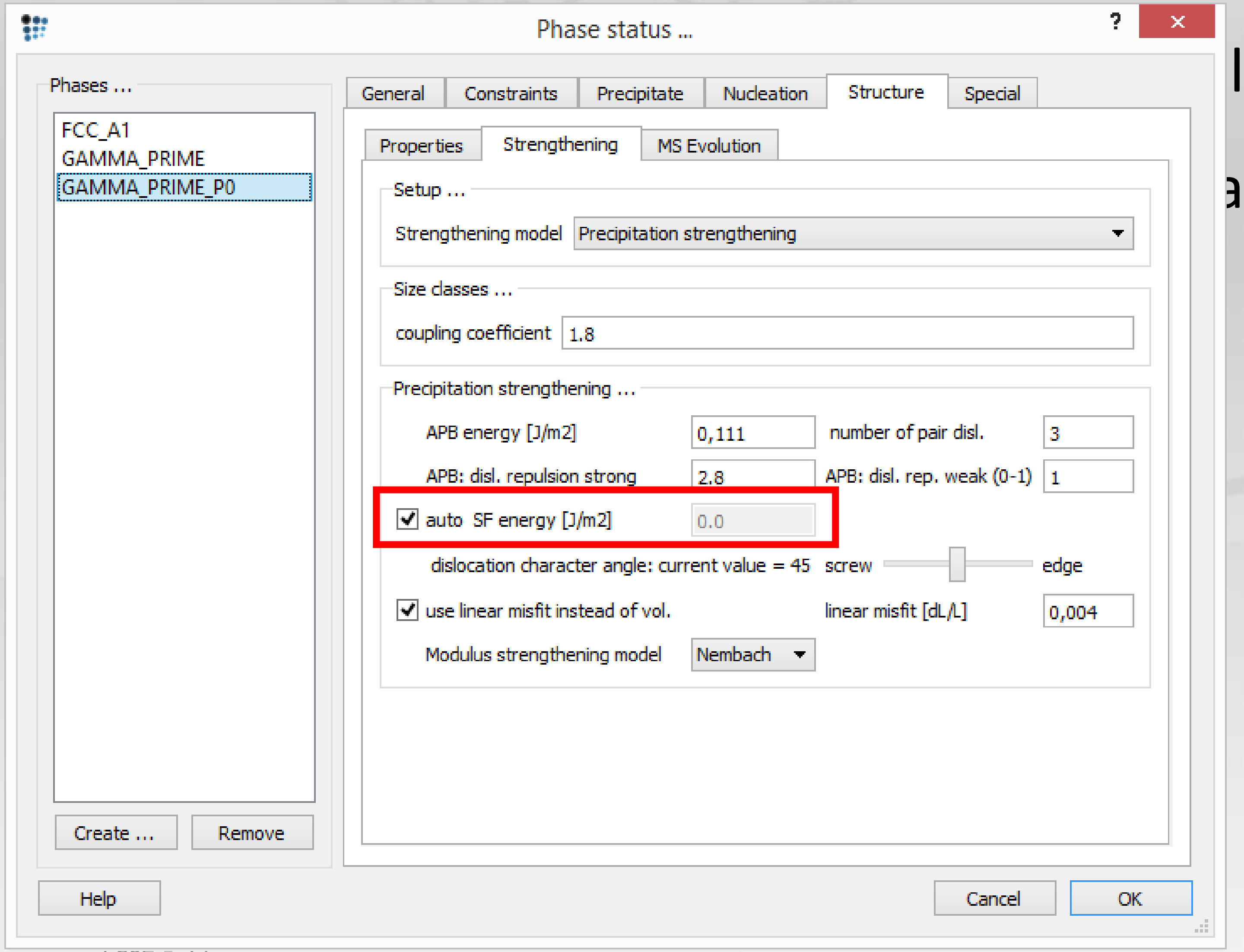
Stacking fault (SF) effect



lt – energy difference

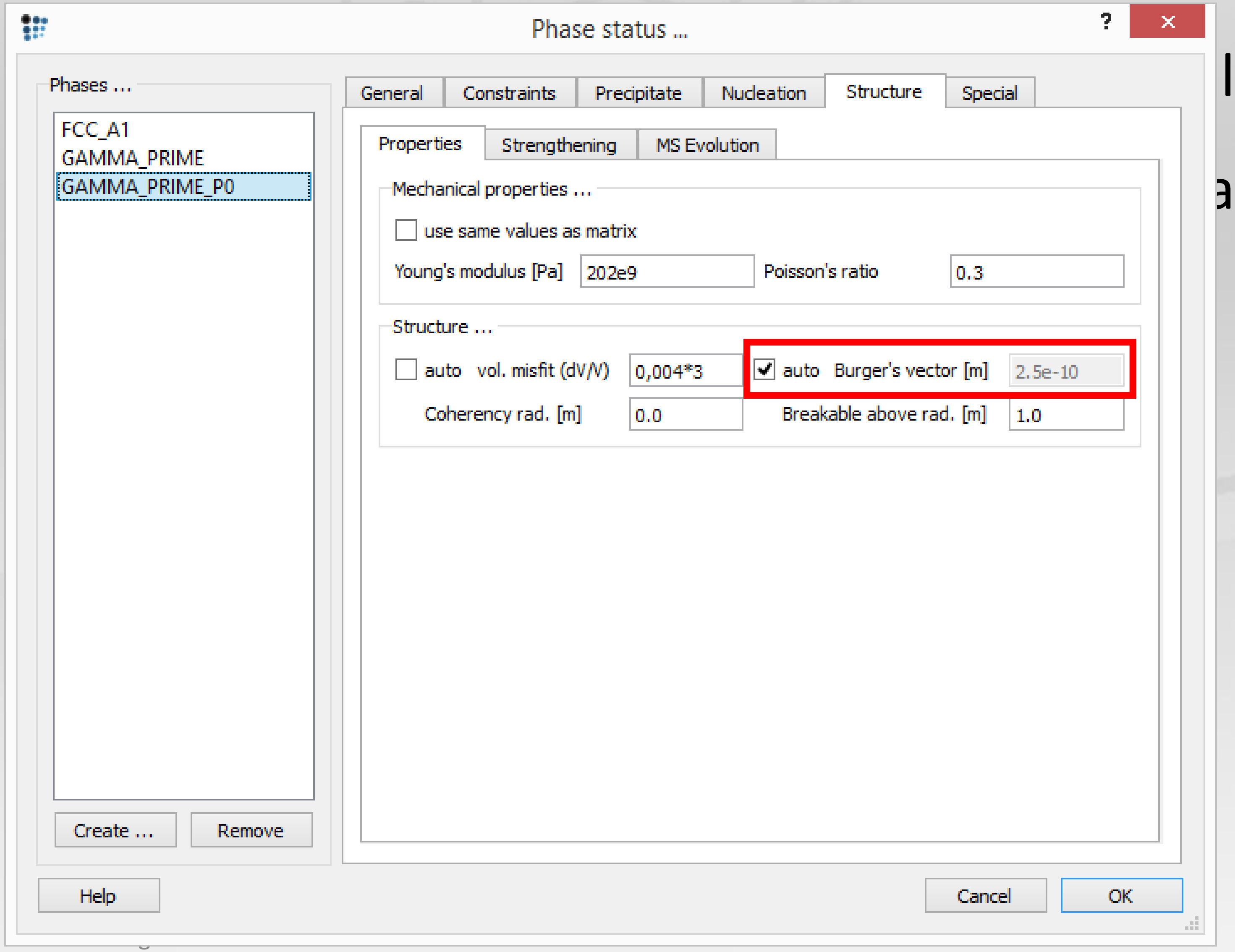
atrix

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



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

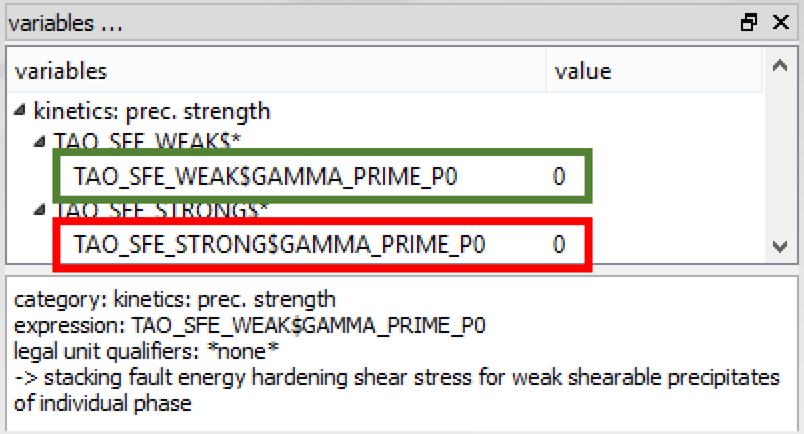
Stacking fault (SF) effect

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

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

  - Weak particles

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



Precipitation strengthening, σ_{prec}

- Derived from τ_{prec}
  - Non-shearable particles (Orowan mechanism)
  - Shearable particles (weak or strong)
    - 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

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

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

  - 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

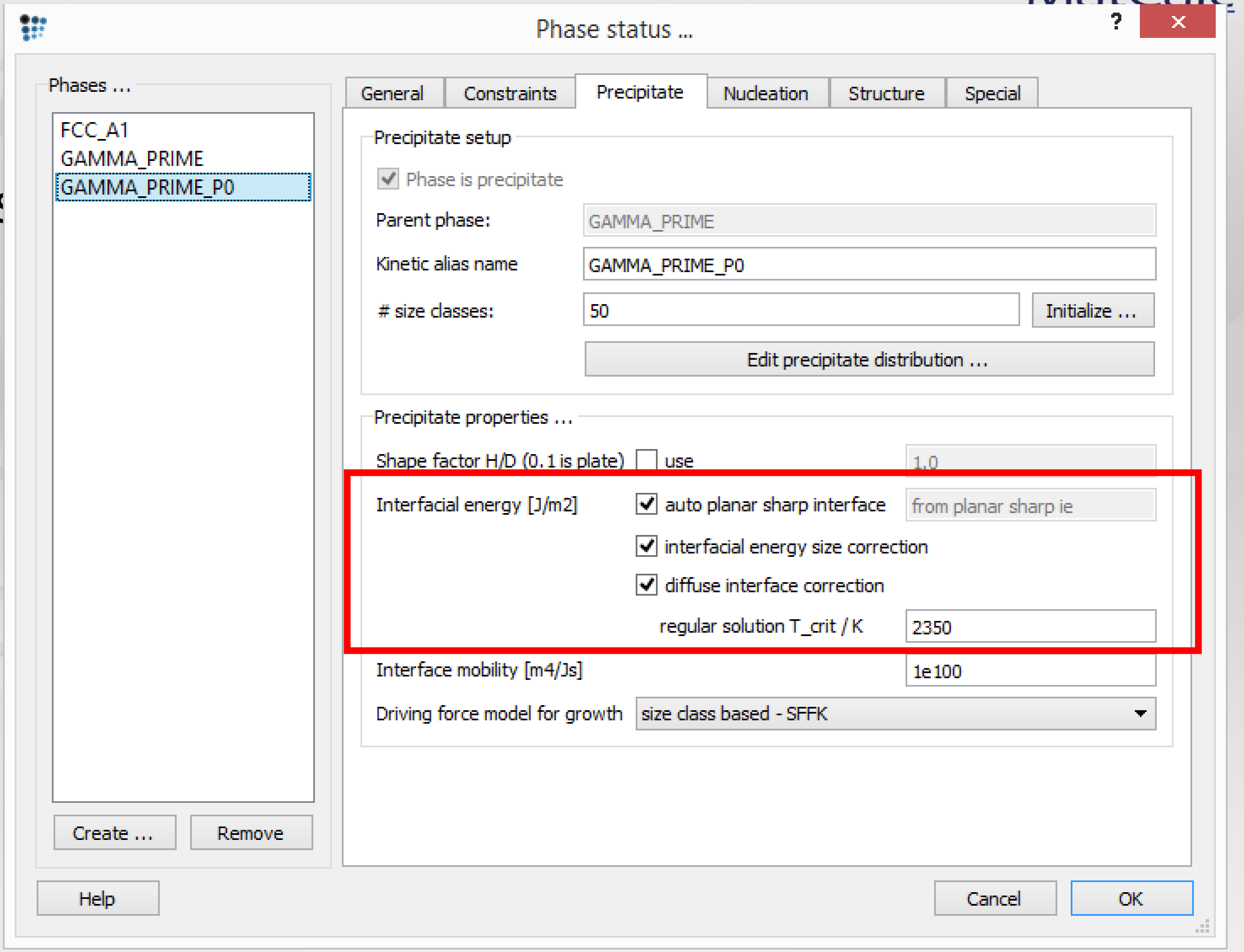
Interfacial effect

- Passing dislocation increases
  - Strong particles

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

  - Weak particles

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



γ_{PM} - Precipitate/matrix interface energy

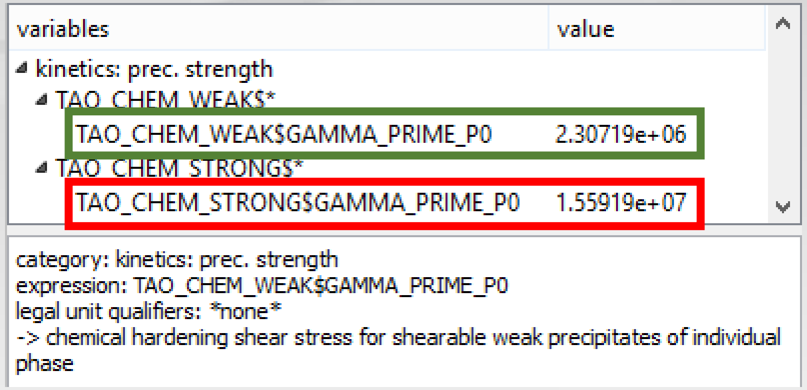
Interfacial effect

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

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

  - Weak particles

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



Precipitation strengthening, σ_{prec}

- Evaluation
  - Identifying the regime for each precipitate separately
  - Summation of the calculated τ_{regime} of each precipitate
  - Conversion of τ_{prec} to σ_{prec}

Precipitation strengthening, σ_{prec}

- Evaluation
  - Identifying the regime for each precipitate separately
  - Summation of the calculated $\tau_{i,regime}$ of each precipitate
  - Conversion of τ_{prec} to σ_{prec}

Regime of each precipitate

- For every precipitate phase *i*: Values of τ evaluated for each of three regimes (Non-shearable, shearable weak, shearable strong)

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

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

$$\tau_{i,nsh}$$

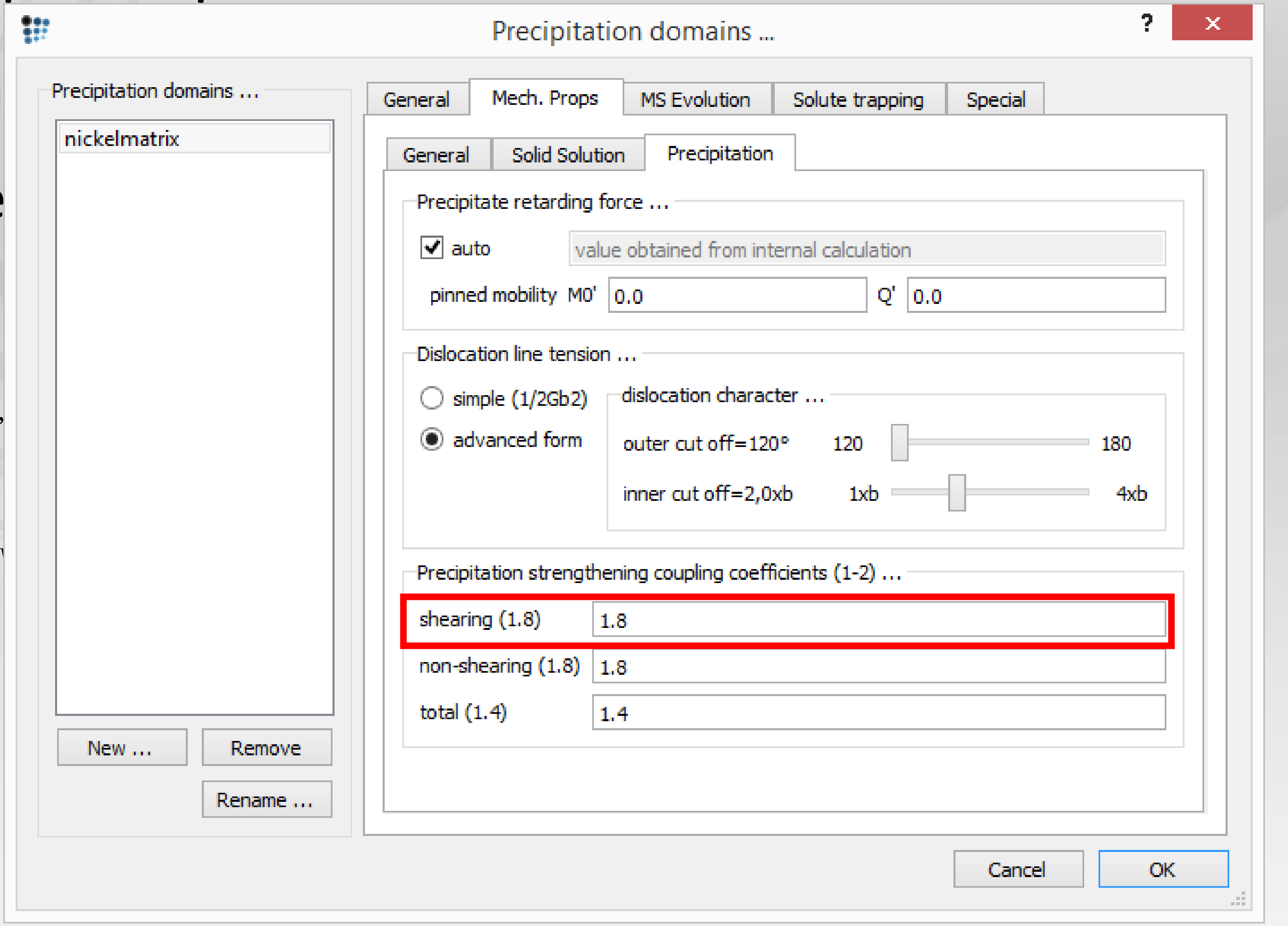
Regime of each precipitate

- For every precipitate ph

  regimes (Non-shearable

$$\tau_{i,strong} = \Big(\tau^{\boxed{m_{sh}}}_{i,coher,strong} + \tau^{m_{sh}}_{i,\mathrm{mod},}$$

$$\tau_{i,weak} = \Big(\tau^{m_{sh}}_{i,coher,weak} + \tau^{m_{sh}}_{i,\mathrm{mod},}$$



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Regime of each precipitate

- For every precipitate phase *i*: Values of τ evaluated for each of three regimes (Non-shearable, shearable weak, shearable strong)

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

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

$$\boxed{\tau_{i,nsh}}$$

variables	value
kinetics: prec. strength	
TAO_OROWAN$*	
TAO_OROWAN$GAMMA_PRIME_P0	7.74823e+08
TAO_SHEAR_WEAK$*	
TAO_SHEAR_WEAK$GAMMA_PRIME_P0	2.48342e+08
TAO_SHEAR_STRONG$*	
TAO_SHEAR_STRONG$GAMMA_PRIME_P0	9.52877e+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

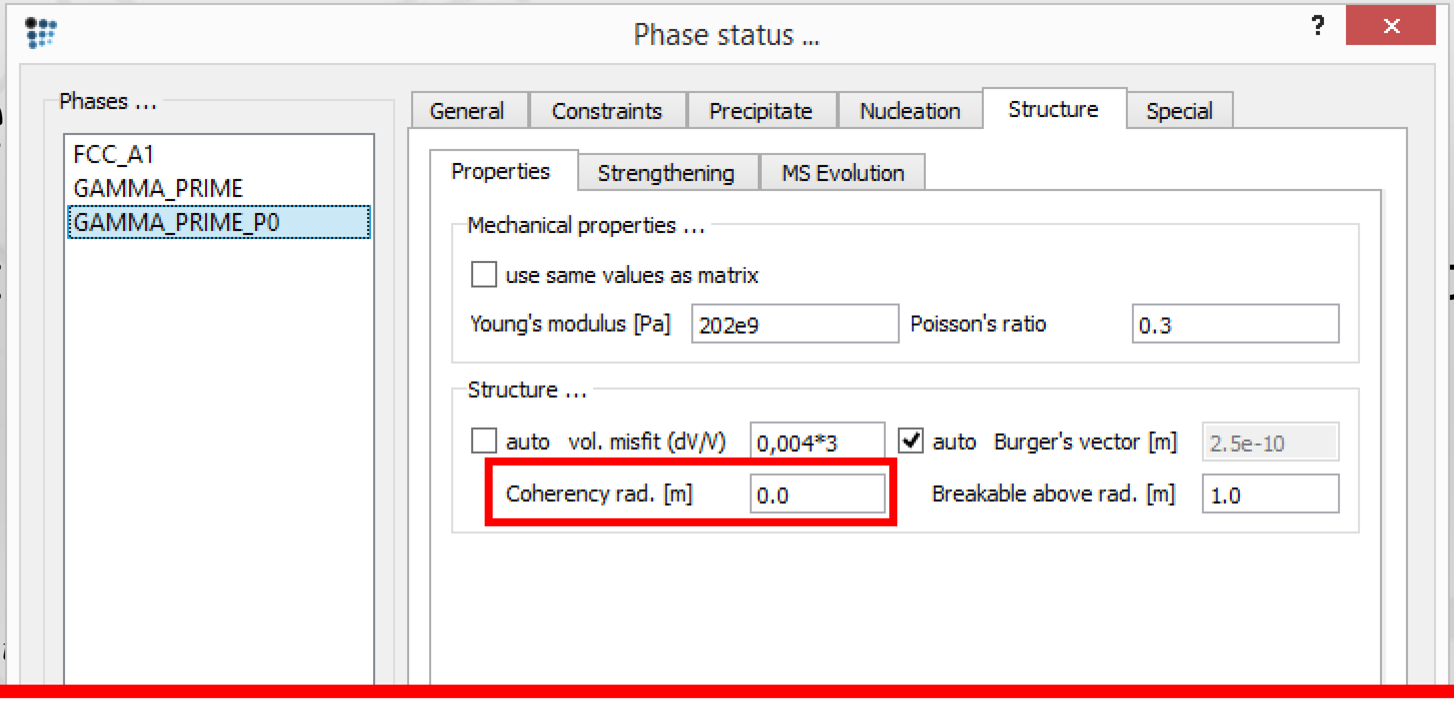
Regime

- $\tau_{i,regime}$ wit ... taken for the furthe

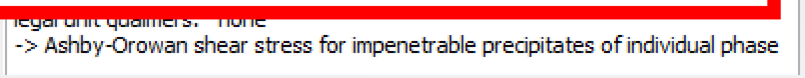
$\boxed{\tau_{i,strong}} = \left(\tau_{i,coher,s}^{m_{sh}} \right.$

$\boxed{\tau_{i,weak}} = ($

$\boxed{\tau_{i,nsh}}$



If coherency radius ≠ 0 and the mean radius of precipitate is greater than the coherency radius ➔ the non-shearable regime is taken for further calculation



Precipitation strengthening, σ_{prec}

- Evaluation
  - Identifying the regime for each precipitate separately
  - Summation of the calculated $\tau_{i,regime}$ of each precipitate
  - Conversion of τ_{prec} to σ_{prec}

Summation of $\tau_{i,regime}$

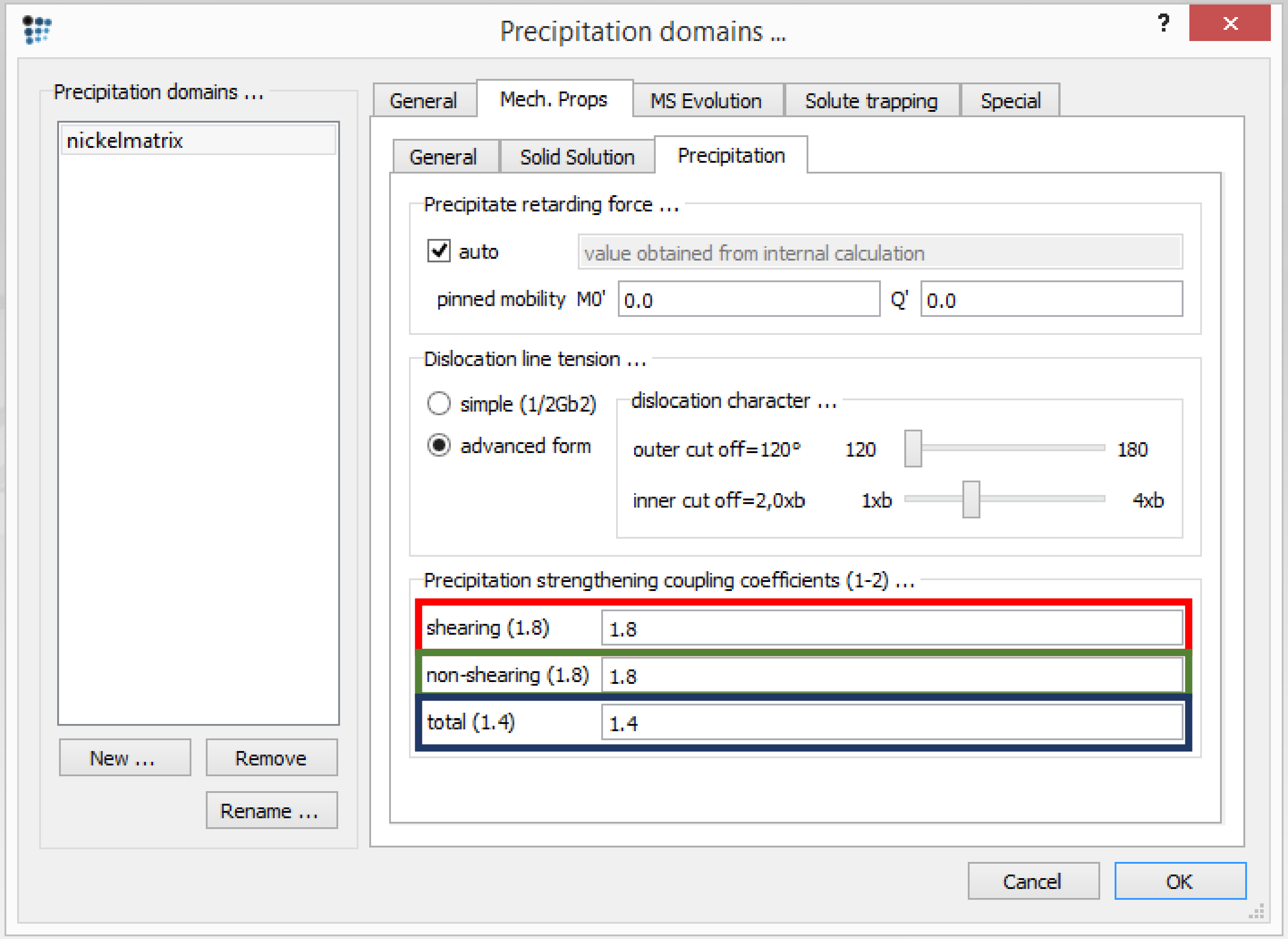
$$\tau_{prec} = \left[\left(\left(\sum_i \tau_{i,sh}^{m_{sh}} \right)^{\frac{1}{m_{sh}}} \right)^{m_{sum}} + \left(\left(\sum_i \tau_{i,nsh}^{m_{nsh}} \right)^{\frac{1}{m_{nsh}}} \right)^{m_{sum}} \right]^{\frac{1}{m_{sum}}}$$

$\tau_{i,sh}$ -Shearable particles contribution (weak and strong regime)

$\tau_{i,nsh}$ -Non-shearable particles contribution

Summation of $\tau_{i,regime}$

$$\tau_{prec} = \left[\left(\sum_i \tau_{i,sh}^{m_{sh}} \right)^{\frac{m_{sum}}{\boxed{m_{sh}}}} + \left(\sum_i \tau_{i,nsh}^{m_{nsh}} \right)^{\frac{m_{sum}}{\boxed{m_{nsh}}}} \right]^{\frac{1}{\boxed{m_{sum}}}}$$



Summation of $\tau_{i,regime}$

- Precipitation strengthening, σ_{prec} (derived from τ_{prec})
  - Evaluation of τ_{prec}

$$\boxed{\tau_{prec}} = \left[\left(\boxed{\left(\sum_i \tau_{i,sh}^{m_{sh}} \right)^{\frac{1}{m_{sh}}}} \right)^{m_{sum}} + \left(\boxed{\left(\sum_i \tau_{i,nsh}^{m_{nsh}} \right)^{\frac{1}{m_{nsh}}}} \right)^{m_{sum}} \right]^{\frac{1}{m_{sum}}}$$

variables	value
kinetics: pd strength	
TTAO_NON_SHEAR$*	
TTAO_NON_SHEAR$nickelmatrix	4.47201e+08
TTAO_SHEAR$*	
TTAO_SHEAR$nickelmatrix	1.81568e+08
TTAO_PREC$*	
TTAO_PREC$nickelmatrix	5.34359e+08

category: kinetics: pd strength
expression: TTAO_NON_SHEAR$nickelmatrix
legal unit qualifiers: *none*
-> total shear stress from non-shearable precipitates

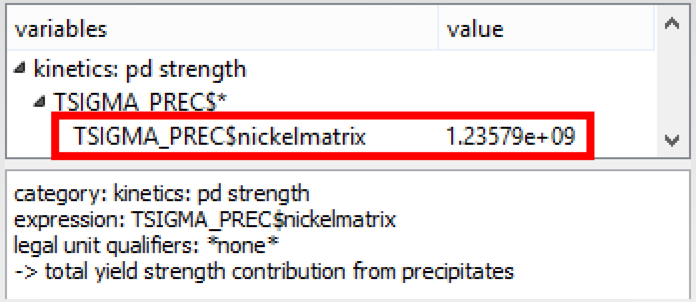
Precipitation strengthening, σ_{prec}

- Evaluation
  - Identifying the regime for each precipitate separately
  - Summation of the calculated $\tau_{i,regime}$ of each precipitate
  - Conversion of τ_{prec} to σ_{prec}

Precipitation strengthening, σ_{prec}

- Evaluation
  - Identifying the regime for each precipitate separately
  - Summation of the calculated $\tau_{i,regime}$ of each precipitate
  - Conversion of τ_{prec} to σ_{prec}

$$\boxed{\sigma_{prec}} = \alpha \tau_{prec}$$



α - Taylor factor

Total yield strength, σ_{YS}

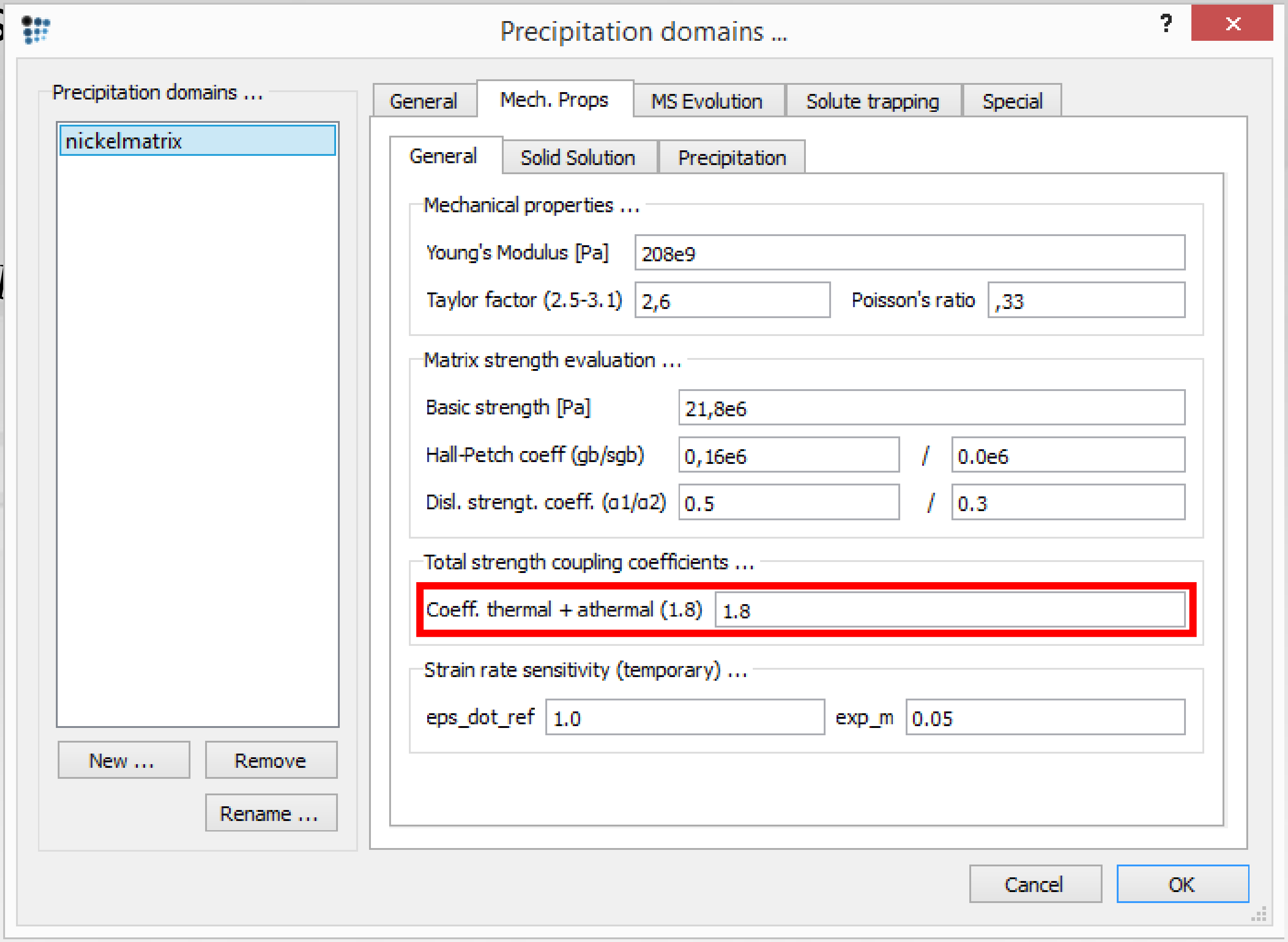
- Summation of contributions

$$\sigma_{YS} = \left[\sigma_{disl}^{m_{sig}} + \left(\sigma_i + \sigma_{gb} + \sigma_{sgb} + \sigma_{ss} + \sigma_{prec}\right)^{m_{sig}}\right]^{1/m_{sig}}$$

Total yield strength, σ_{YS}

- Summation of contributions

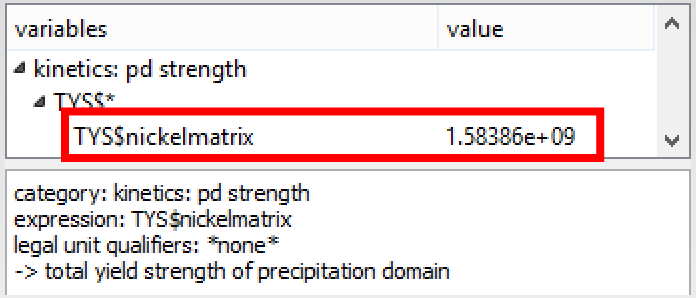
$$\sigma_{YS} = \left[\sigma_{disl}^{\boxed{m_{sig}}} + \left(\sigma_i + \sigma_{gl}\right.\right.$$



Total yield strength, σ_{YS}

- Summation of contributions

$$\sigma_{YS} = \left[\sigma_{disl}^{m_{sig}} + \left(\sigma_i + \sigma_{gb} + \sigma_{sgb} + \sigma_{ss} + \sigma_{prec} \right)^{m_{sig}} \right]^{1/m_{sig}}$$



Thank you for your attention !

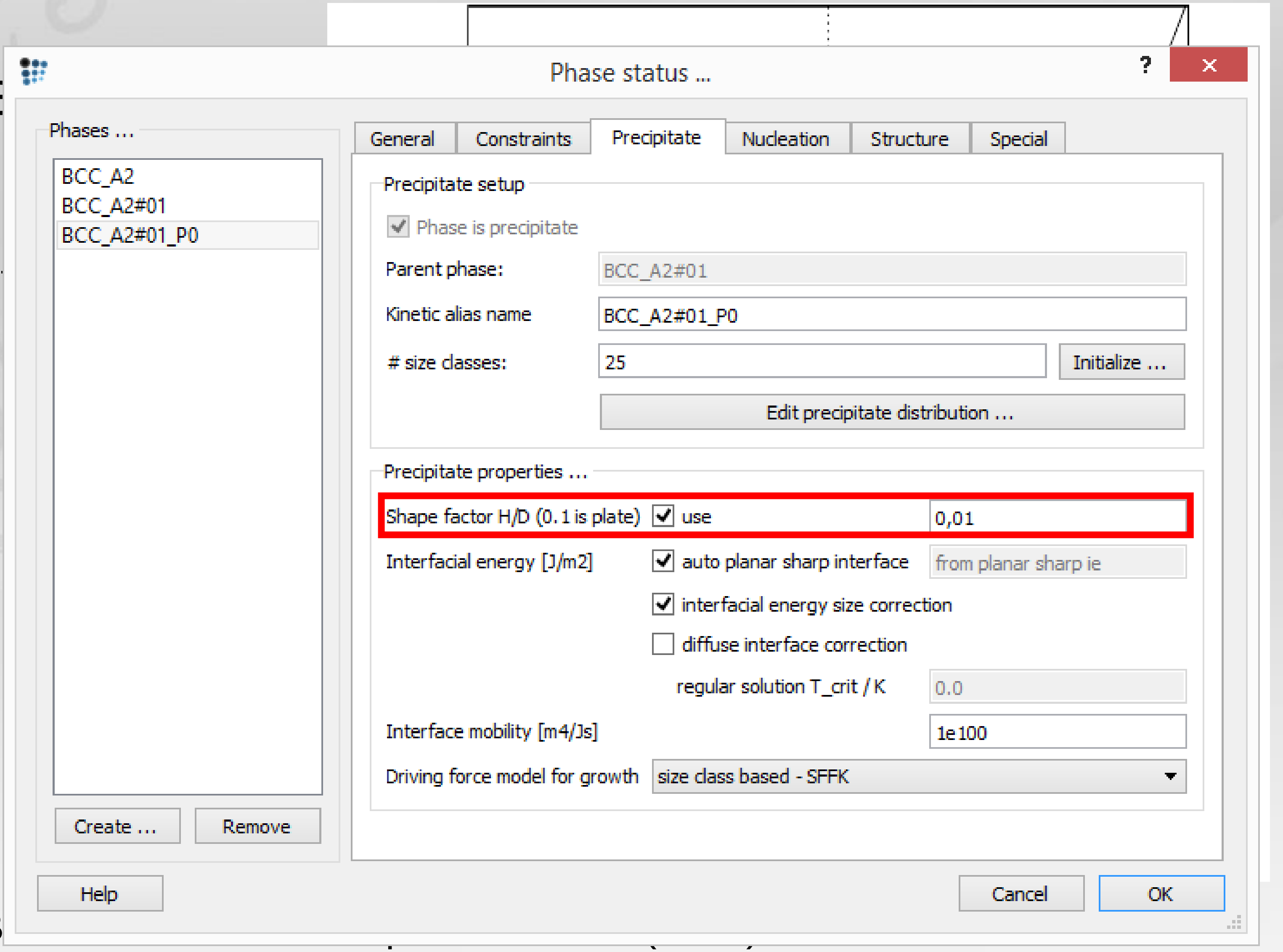
Precipitation hardening

Shape factor influence

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

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

h - Shape factor



Sonderegger B

Precipitation hardening

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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

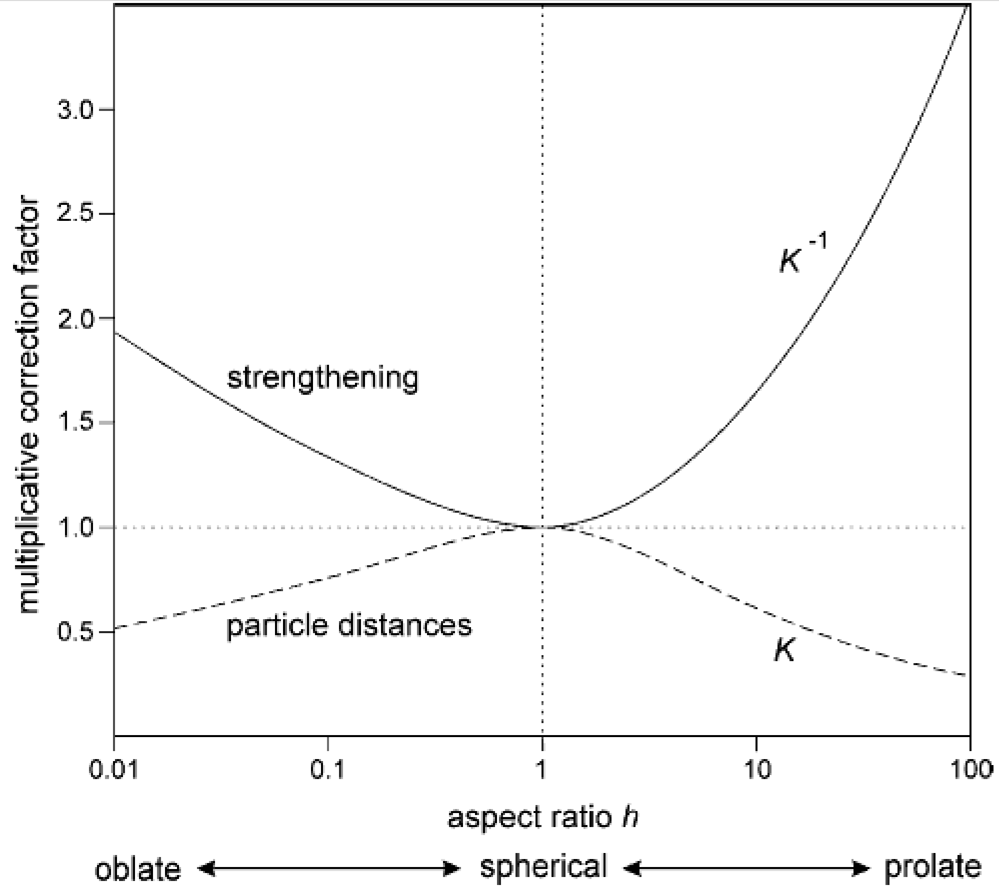


Figure 2. Variation in particle distances and strengthening for prolate and oblate precipitates relative to spherical particles.

Sonderegger B., Kozeschnik E., Scripta Mater., 66 (2012) 52-55

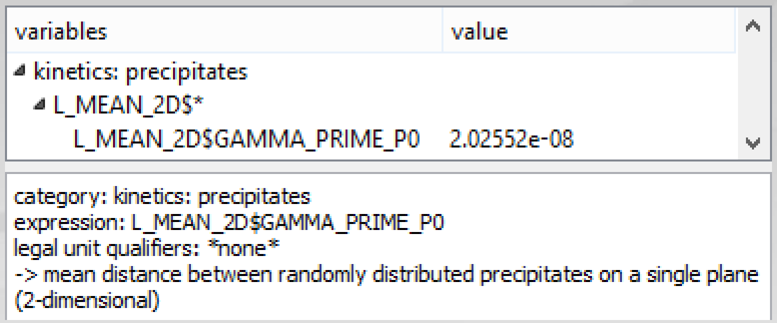
Precipitation hardening

Shape factor influence on L_S

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

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

h - Shape factor



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Precipitation hardening

- Non-shearable particles (Orowan mechanism)

$$\tau_{Orowan} = \frac{JGb}{2\pi\sqrt{1-\upsilon}L_s}\ln\left(\frac{2r_{eq}}{r_i}\right)$$

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

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

$$r_{eq,screw,ns} = \left[\frac{2h^{2/3}}{3}\left(\frac{1}{h} + \sqrt{\frac{1}{h^2} + \frac{9}{2+h^2}}\right)\right]\frac{\pi}{4}r_m$$

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

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

P_{edge} - Fraction of edge disl.

P_{screw} - Fraction of screw disl.

Precipitation hardening

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

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

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

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

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

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

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

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

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

Summing up…

- Total yield strength, σ_{YS}
  - Summation of contributions

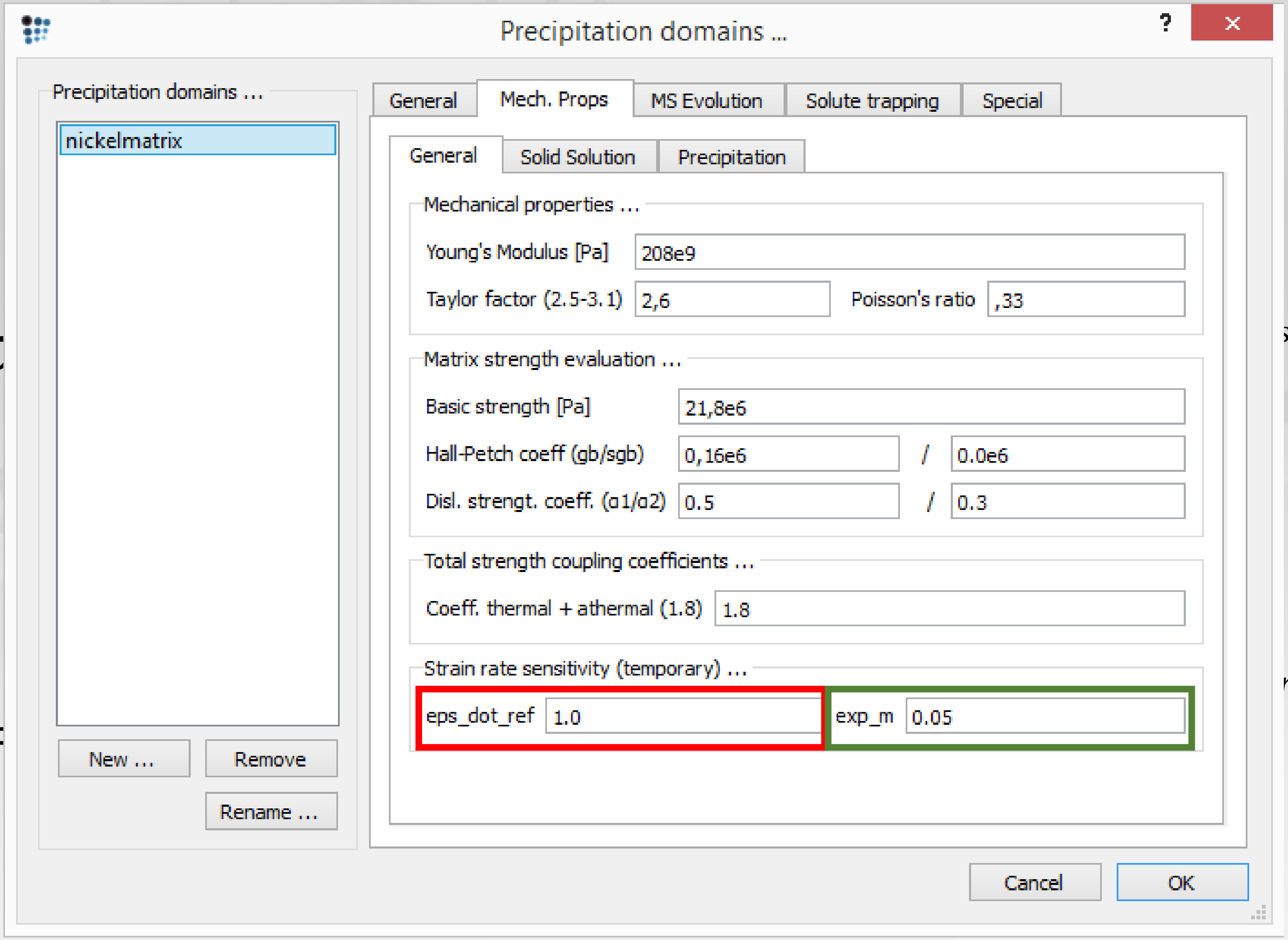
$$\sigma_{YS} = \left[\sigma_{disl}^{m_{sig}} + \left(\sigma_i + \sigma_{gb} + \sigma_{sgb} + \sigma_{ss} + \sigma_{prec}\right)^{m_{sig}}\right]^{1/m_{sig}}$$

  - Influence of strain rate, $\dot{\varphi}$

$$\sigma_{YS} = \left[\sigma_{disl}^{m_{sig}} + \left(\sigma_i + \sigma_{gb} + \sigma_{sgb} + \sigma_{ss} + \sigma_{prec}\right)^{m_{sig}}\right]^{1/m_{sig}} \left(1 + \frac{\dot{\varphi}}{C_1}\right)^{C_2}$$

Summing up...

• Tot



$$\ldots_{sig} \Big]^{1/m_{sig}}$$

$$\sigma_{YS} = \ldots m_{sig} \left(1+\frac{\dot{\varphi}}{\boxed{C_1}}\right)^{\boxed{C_2}}$$

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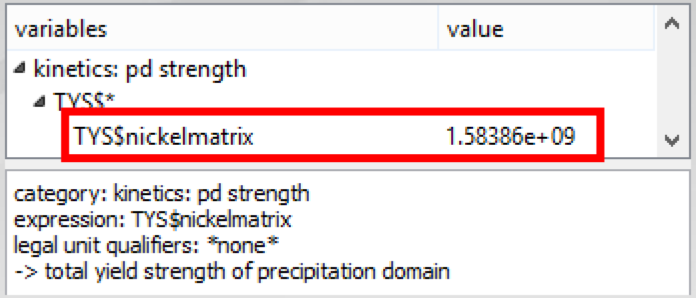
Summing up...

- Total yield strength, σ_{YS}
    - Summation of contributions

$$\sigma_{YS} = \left[\sigma_{disl}^{m_{sig}} + \left(\sigma_i + \sigma_{gb} + \sigma_{sgb} + \sigma_{ss} + \sigma_{prec}\right)^{m_{sig}}\right]^{1/m_{sig}}$$



- Influence of strain rate, $\dot{\varphi}$

$$\boxed{\sigma_{YS}} = \left[\sigma_{disl}^{m_{sig}} + \left(\sigma_i + \sigma_{gb} + \sigma_{sgb} + \sigma_{ss} + \sigma_{prec}\right)^{m_{sig}}\right]^{1/m_{sig}} \left(1 + \frac{\dot{\varphi}}{C_1}\right)^{C_2}$$