

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

P. Warczok



Mechanical threshold

- Yield stress at temperature 0 K
- Microstructure dependent

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

Thermal & athermal contributions

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



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

 σ_{ath} - Athermal contribution [Pa]

 σ_{th} - Thermal contribution [Pa]



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}

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



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



Intrinsic strength, σ_i

f	Precipitation domains	?
Precipitation domains	General Mech. Props MS Evolution Trapping Special	
Ni_matrix*	General Solid Solution Segregation CC Diffusion Precipitation Mechanical properties Young's Modulus [Pa] (222750-83.6*T\$C)*1e6 Taylor factor (2.5-3.1) 3.06 Poisson's ratio 0.3 Speed of sound 5100.0 Matrix strength evaluation Basic strength [Pa] 20.0e6	
	Hall-Petch coeff (gb/sgb) 0.74e6 / 0.0e6 Disl. strengt. coeff. (a1/a2) 0.5 / 0.0	
	Dynamic strength delta_F_lt_fact 1.0 delta_F_ht 0.0 couplexp 3.0 eps_dot_fact 1.0 exp_ht 1.0/3.0	
New Remove Set active Rename	Coeff. thermal + athermal (1.0) 1.0	<u>Ок</u>

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Model overview

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



Taylor equation

 $\sigma_{disl} = \alpha MGb\sqrt{\rho}$

- M Taylor factor
- G Shear modulus
- b Burger's vector
- $ho\,$ Dislocation density
- lpha Strengthening coefficient



Taylor equation

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

- M Taylor factor
- $G\,$ Shear modulus
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- ho Dislocation density
- $lpha\,$ Strengthening coefficient



660 657 657	Precipitation domains	? ×
Precipitation domains	General Mech. Props MS Evolution Trapping Special	
Ni_matrix*	General Solid Solution Segregation CC Diffusion Precipitation	
	Mechanical properties	
	Young's Modulus [Pa] (222750-83.6*T\$C)*1e6	
	Taylor factor (2.5-3.1) 3.06 Poisson's ratio 0.3	
	Speed of sound 5100.0	
	Matrix strength evaluation	
	Basic strength [Pa] 20.0e6	
	Hall-Petch coeff (gb/sgb) 0.74e6 / 0.0e6	
	Disl. strengt. coeff. (a1/a2) 0.5 / 0.0	
	Dynamic strength	
	delta_F_lt_fact 1.0 delta_F_ht 0.0 couplexp 3.0	
	eps_dot_fact 1.0 exp_ht 1.0/3.0	
	Total strength coupling coefficients	
New Remove	Coeff. thermal + athermal (1.0) 1.0	
Set active Rename		
	Cancel	<u>O</u> K



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- Taylor equation
 - $\sigma_{disl} = \alpha MGb\sqrt{\rho}$
 - M Taylor factor
 - G Shear modulus
 - b Burger's vector
 - $ho\,$ Dislocation density
 - ${\boldsymbol {\mathcal C}}$ Strengthening coefficient

	Precipitation domains	? ×
ecipitation domains	General Mech. Props MS Evolution Tr	rapping Special
Ni_matrix*	Thermodynamic matrix phase	
	FCC_A1	▼
	Microstructure parameters	
	equilibrium dislocation density [m-2]	1.0e11
	initial grain diameter [m] 100.0e-6	elongation factor 1
	initial subgrain diameter [m] 100.0e-6	elongation factor 1
	Burger's vector	
	✓ automatic manual value [m] 2.5€	2-10
New Remove		
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		<u>C</u> ancel <u>O</u> K



Cancel

<u>O</u>K

Work hardening, σ_{disl}

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- Taylor equation
 - Two parameter model

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

 ρ_1 - Internal dislocation density ho_2 - Wall dislocation density

	Precipitation domains ?
Precipitation domains	General Mech. Props MS Evolution Trapping Special
Ni_matrix*	General Solid Solution Segregation CC Diffusion Precipitation Mechanical properties Young's Modulus [Pa] (222750-83.6*T\$C)*1e6 Taylor factor (2.5-3.1) 3.06 Poisson's ratio 0.3 Speed of sound 5100.0 Speed of sound 5100.0 Matrix strength evaluation Basic strength [Pa] 20.0e6 10.0e6 10.0e6 10.0e6 Disl. strengt. coeff. (gb/sgb) 0.74e6 10.0e6 10.0e6 Dynamic strength delta_F_lt fact 1.0 delta_F_ht 0.0 Dynamic strength delta_F_ht 0.0 couplexp 3.0 eps_dot_fact 1.0 exp_ht 1.0/3.0 Total strength coupling coefficients Coeff. thermal + athermal (1.0) 1.0 1.0 1.0 1.0



- Taylor equation
 - Two parameter model

$$\sigma_{disl} = \alpha_1 M G b \sqrt{\rho_1} + \alpha_2 M G b \sqrt{\rho_2}$$

 ρ_1 - Internal dislocation density ρ_2 - Wall dislocation density

variables	value	
A kinetics: pd strength A TDS\$*		
TDS\$nickelmatrix	7.1404e+06	~
category: kinetics: pd streng expression: TDS\$nickelmatri legal unit qualifiers: *none* -> dislocation vield strength	jth x contribution in precipitation domain	



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- Contributions to yield strength, σ_{YS}
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 - Work hardening, σ_{disl}

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

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



• Hall-Petch equation

 k_{gb} k_{sgb} $\sigma_{_{gb}}$ σ_{sgb}

- D Grain diameter
- δ Subgrain diameter
- k_n Constant

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Precipita

Hall-Petch equation



- Grain diameter
- Subgrain diameter
- k_n Constant

Ni_matrix* General Solid Solution Segregation CC Diffusion Precipitation Mechanical properties Young's Modulus [Pa] (222750-83.6*T\$C)*1e6 Taylor factor (2.5-3.1) 3.06 Poisson's ratio 0.3 Speed of sound 5100.0 Matrix strength evaluation Matrix strength evaluation Basic strength [Pa] 20.0e6 Hall-Petch coeff (gb/sgb) 0.74e6 / 0.0e6 Disl. strengt. coeff. (a1/a2) 0.5 / 0.0 Dynamic strength delta_F_ht 0.0 couplexp 3.0 eps_dot_fact 1.0 exp_ht 1.0/3.0 Total strength coupling coefficients New Remove Coeff. thermal + athermal (1.0) 1.0	cipitation domains	General Mech. Props MS Evolution Trapping Special
Dynamic strength delta_F_lt_fact 1.0 delta_F_lt_fact 1.0 eps_dot_fact 1.0 exp_ht 1.0/3.0 Total strength coupling coefficients Coeff. thermal + athermal (1.0) 1.0	li_matrix*	General Solid Solution Segregation CC Diffusion Precipitation Mechanical properties Young's Modulus [Pa] (222750-83.6*T\$C)*1e6 Taylor factor (2.5-3.1) 3.06 Poisson's ratio 0.3 Speed of sound 5100.0 Matrix strength evaluation Basic strength [Pa] 20.0e6 Hall-Petch coeff (gb/sgb) 0.74e6 / 0.0e6 Disl. strengt. coeff. (a1/a2) 0.5 / 0.0
occocore include in	New Remove	Dynamic strength delta_F_lt_fact 1.0 delta_F_ht 0.0 couplexp eps_dot_fact 1.0 exp_ht 1.0/3.0 Total strength coupling coefficients Coeff. thermal + athermal (1.0) 1.0



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Precip

Hall-Petch equation



Grain diameter - Subgrain diameter

- Constant k_n

	Precipitation domains	? ×
Precipitation domains Ni_matrix*	General Mech. Props MS Evolution Trapping Special Thermodynamic matrix phase FCC_A1 FCC_A1 Microstructure parameters equilibrium dislocation density [m-2] 1.0e11 initial grain diameter [m] 100.0e-6 elongation factor 1 initial subgrain diameter [m] 100.0e-6 elongation factor 1 Burger's vector ✓ automatic manual value [m] 2.5e-10	
Set active Rename		
	Cancel	<u>O</u> K



• Hall-Petch equation



D - Grain diameter δ - Subgrain diameter k_n - Constant

		<u> </u>
variables	value	^
4 kinetics: pd strength 4 TGS\$*		
TGS\$nickelmatrix	3.57771e+07	~
category: kinetics: pd streng expression: TGS\$* legal unit qualifiers: *none* -> fine grain yield strength co	th ontribution 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 con	tribution in precipitation domain		



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





- 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
- $m_{\rm int}$ Exponent for interstitial elements
- m_{tot} Global exponent



••••	Precipitation domains	? × $\frac{m_{tot}}{m_{sub}}$ $\frac{m_{tot}}{m_{int}}$
Precipitation domains	General Mech. Props MS Evolution Solute trapping Special	$\left(\sum \left(1 - n_{1} \right) m_{sub} \right)^{sub} \left(\sum \left(1 - n_{1} \right) m_{int} \right)^{sub}$
nickelmatrix	General Solid Solution Precipitation	$\sigma_{ss} = \sum (k_i c_i^{n_i}) + \sum (k_i c_i^n) + \sum (k_i c_i^n) + $
	Strengthening coefficients	$\left(\begin{array}{c} \hline i \end{array} \right)_{sub} \left(\begin{array}{c} \hline i \end{array} \right)_{int}$
	Element Coefficient Exponent	
	AL 225.0e6 1/2	
	C 1061.0e6 1/2 CO 39.4e6 1/2	
	CR 337e6 1/2	1
	FE 153.0e6 1/2	K_i - Coefficient for element <i>i</i>
	MO 1015.0e6 1/2 NB 1183.0e6 1/2	l
	NI 0.0 1/2	C - Element i content in the prec domain
	TI 775.0e6 1/2	c_i Element represe domain
	W 977.0e6 1/2	11 Expanse for element i
		n_i - Exponent for element /
	SSS coupling coefficients	
	substitutional (1.8) 1.8 interstitial (1.8) 1.8	M_{sub} - Exponent for substitutional elements
New Remove	total SS strength (1.8) 1.8	540
Rename		$m_{\rm int}$ - Exponent for interstitial elements
	Cancel	m_{μ} - Global exponent
Page = 19		tot Crobal oxponent





variables	value	^
4 kinetics: pd strength 4 TSSS\$*		
TSSS\$nickelmatrix	2.82649e+08	\checkmark
category: kinetics: pd strength expression: TSSS\$*		

-> solid solution yield strength contribution in precipitation domain

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• Solid solution strengthening, σ_{ss}



variables	value	^
kinetics: pd strength		
TSSS_EL\$*\$*		
TSSS_EL\$nickelmatrix\$*		
TSSS_EL\$nickeImatrix\$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



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



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}

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

🗱 Phase status								?	×
Phases	General	Constraints	Precipitate	Nucleation	Structure	Special			
FCC_A1 AL B DP	Propertie	es Strength	ening MS E	Evolution					
CL_MGSI CL_MGSI_P0	Setup .		Desa alternativ						
AL_B_DP_P0	Streng	thening model	Ignore contrib	ution					
	A	PB energy [J/m	Prec. strengtr Prec. strengtr Prec. strengtr	n mean (number- n mean (volume-v n multi-class	weighted) weighted)				
	A V a	PB: disl. repulsi uto SF enerav	ion strong	2.8	APB: disl. rep	o. weak (0-1)	0.0		
		dislocation chara	acter angle: cu	rrent value = 45	screw	-	edge		
		se linear misfit i Iodulus strengti	instead of vol. hening model	Nembach 🗸	linear misfit [dL/L]	0.0		
	Multi	size classes	_		1				
	coup	ling coefficient	1.4						
Create Remove									
Help						Cance	ł	OK	:



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



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- 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

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- 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, $r_{m,v}$

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

Precipitate size distribution

Size class index <i>i</i>	Size class radius r_i	Size class number density <i>N_i</i>
0	r_0	N ₀
1	r_1	N ₁
2	<i>r</i> ₂	N ₂
3	r_3	N ₃

• Size class radius, r_i



- 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)

👯 Phase status		?	×
Phases	General Constraints Precipitate Nucleation Structure Special		
FCC_A1 AL_B_DP CL_MGSL	Properties Strengthening MS Evolution		
CL_MGSI_P0 AL_B_DP_P0	Strengthening model Prec. strength multi-class	~	
	Ignore contribution Precipitation streng Prec. strength mean (number-weighted) Prec. strength mean (volume-weighted) APB energy [J/r Prec. strength multi-dass		
	APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0		
	dislocation character angle: current value = 45 screw edge	2	
	□ use linear misfit instead of vol. linear misfit [dL/L] 0.0 Modulus strengthening model Nembach ∨		
	Multi size dasses		
	coupling coefficient 1.4		
Create Remove			
Help	Cancel	OK	



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

(edge/screw ratio; $\theta = 0$ for pure screw; $\theta = \pi/2$ for pure edge)

- Equivalent radius, r_{eq} (describes precipitate-dislocation interference area)
- Mean distance between the precipitate surfaces, L_S



- Some general parameters/settings
 - Angle between dislocation line and Burger's vector $\boldsymbol{\theta}$

(edge/screw ratio; $\theta = 0$ for pure screw; $\theta = \pi/2$ for pure edge)

1 7	Phase status ?
Phases FCC_A1 GAMMA_PRIME GAMMA_PRIME_P0	General Constraints Precipitate Nucleation Structure Special Properties Strengthening MS Evolution Setup Strengthening model Precipitation strengthening Size dasses
	coupling coefficient 1.8 Precipitation strengthening APB energy [J/m2] 0,111 number of pair disl. 3 APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 1 Image: Interview of the strong 0.0 0.0
	dislocation character angle: current value = 45 screw edge Image: screw edg
Create Remove	Cancel OK



- 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



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

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

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

		~
4 kinetics: precipitates 4 L_MEAN_2D\$*		
L_MEAN_2D\$GAMMA_PRIME_P0	2.02552e-08	~

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

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

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- Precipitate size dependence
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Non-shearable particles

$$\tau_{nsh} = \frac{JGb}{2\pi L_S} ln\left(\frac{\pi}{2}\frac{r_{eq}}{r_i}f(\theta,h)\right)$$
$$J = \frac{1-\upsilon\left[cos^2\left(\frac{\pi}{2}-\theta\right)\right]}{1-\upsilon}$$



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

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Non-shearable particles

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

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

- au_{nsh} Critical stress for a dislocation to by-pass the precipitate
 - G Shear modulus
 - *b* Burgers vector
 - v Poisson's ratio
- r_{eq} Equivalent radius θ - ∠(*b*; dislocation line) r_i – dislocation core radius
 - h Shape factor

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



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

Non-shearable particles

Descripte tion domains	Precipitation domains ? ×	G - Shear modulus	r_{eq} – Equivalent radius
Precipitation domains	General Mech. Props MS Evolution Solute trapping Special General Solid Solution Precipitation Precipitate retarding force Image: Construction of the system of	 b - Burgers vector v - Poisson's ratio 	θ - \angle (<i>b</i> ; dislocation line) r_i – dislocation core radius <i>h</i> - Shape factor
New Remove Rename	inner cut off=2,0xb 1xb 4xb Precipitation strengthening coupling coefficients (1-2) shearing (1.8) 1.8 non-shearing (1.8) 1.8 1.8 total (1.4) 1.4 Cancel	$\left(\frac{1}{\sqrt{2}}\right)sin^2\theta + \left(\sqrt{\frac{1}{h^2}}\right)$	$+\sqrt{\frac{9}{2+h^2}+\frac{1}{h^2}}\right)\cos^2\theta$



Non-shearable particles

		Phase	e status				
hases	General	Constraints	Precipitate	Nucleation	Structure	Special	
FCC_A1 GAMMA_PRIME GAMMA_PRIME_P0	Precipita Phas Parent p Kinetic a # size d	te setup e is precipitate hase: lias name asses:	SAMMA_PRIM SAMMA_PRIM 50	E E_P0 Edit precis	pitate distributi	on	Initialize
	Shape fa	te properties – actor H/D (0.1 is pl ial energy [J/m2]	ate) 🗌 use 🔽 auto ✔ inter ✔ diffu regul	planar sharp in facial energy si se interface cor ar solution T_cr	1.0 terface from ze correction rection it / K 235	n planar sh 0	arp ie
	Interfac Driving f	e mobility [m4/Js] force model for gro	wth size clas	ss based - SFFK	1e1	00	•
Create Remove							

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

- G Shear modulus
- *b* Burgers vector
- v Poisson's ratio

 r_{eq} – Equivalent radius

- θ \angle (*b*; dislocation line)
- r_i dislocation core radius

h - Shape factor

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

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Non-shearable particles

$$\tau_{nsh} = \frac{JGb}{2\pi L_S} ln\left(\frac{\pi r_{eq}}{2r_i}f(\theta,h)\right)$$
$$J = \frac{1 - v\left[cos^2\left(\frac{\pi}{2} - \theta\right)\right]}{1 - v}$$

variables	value	^
kinetics: prec. strength		
A TAO_OROWAN\$*		
TAO_OROWAN\$GAMMA_PRIME_P0	7.74823e+08	¥
category: kinetics: prec. strength expression: TAO_OROWAN\$GAMMA_PRIME_P(legal unit gualifiers: *none*	0	

-> Ashby-Orowan shear stress for impenetrable precipitates of individual phase

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



Size distribution dependent strengthening

- Precipitate size dependence
- Some general parameters/settings
- 2 scenarios for dislocation behavior:
 - Non-shearable particles (Orowan mechanism) \rightarrow bypassing precipitate
 - Shearable particles (weak or strong) \rightarrow 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

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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

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



 $0^{\circ} - \psi \rightarrow$ "strong" particles

 ψ - 180° \rightarrow "weak" particles

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

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"Weak" vs. "strong" particles

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

·	Precipitation domains ? ×	
Precipitation domains Gen	meral Mech. Props MS Evolution Solute trapping Special Solid Solution Precipitate retarding force Image: auto value obtained from internal calculation pinned mobility M0' 0.0 Q' 0.0 Dislocation line tension Image: simple (1/2Gb2) dislocation character Image: simple (1/2Gb2)	$0^{\circ} - \psi \rightarrow$ "strong" particles $\psi - 180^{\circ} \rightarrow$ "weak" particles



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



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

Strong particles



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.

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- Criterion: Dislocation bending angle ψ threshold
 - Strong resistance of particles \rightarrow High curvature of dislocation line \rightarrow 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.

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- Dislocation line tension, T
 - Simple model

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

- G Shear modulus
- *b* Burgers vector
- v Poisson's ratio
- r_i dislocation core radius
- Advanced model (different values for "weak" and "strong" particles)

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

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



- Dislocation line tension, T
 - Simple model

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

varia	ables	value	<u>^</u>
⊿ kir ⊿ (netics: prec. strength		
4	DLT_SIMPLE\$GAMMA_PRIME_P0	1.92907e-09	
4	DLT_WEAK\$GAMMA_PRIME_P0	1.6019e-09	
	DLT_STRONG\$GAMMA_PRIME_P0	1.46929e-09	~
cate expr legal -> di	gory: kinetics: prec. strength ession: DLT_SIMPLE\$* unit qualifiers: *none* islocation line tension from simple description	on (1/2Gb^2)	

• Advanced model (different values for "weak" and "strong" particles)

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

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



.

- Dislocation line tension, T
 - Simple
 - Advanced

	Precipitation domains ? ×
recipitation domains	General Mech. Props MS Evolution Solute trapping Special
nickelmatrix	General Solid Solution Precipitation
	Precipitate retarding force Image: auto walue obtained from internal calculation pinned mobility M0' 0.0 Q' 0.0
	Dislocation line tension Image: Simple (1/2Gb2) dislocation character Image: Image: Image: Simple (1/2Gb2) dislocation character Image: Image
	Precipitation strengthening coupling coefficients (1-2) shearing (1.8) 1.8 non-shearing (1.8) 1.8 total (1.4) 1.4
New Remove	Cancel OK



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

Page
52



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

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

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

• Weak particles

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

$$\Delta_{lin}$$
 - Linear misfit Δ_{vol} - Volumetric misfit

au



Phases	General Constraints Precipitate Nucleation Structure Special
FCC_A1 GAMMA_PRIME GAMMA_PRIME_PO	General Constraints Precipitate Nucleation Structure Special Properties Strengthening MS Evolution Mechanical properties use same values as matrix young's modulus [Pa] 202e9 Poisson's ratio 0.3 Structure auto vol. misfit (dV/V) 0,004*3 V auto Burger's vector [m] 2.5e-10 Coherency rad. [m] 0.0 Breakable above rad. [m] 1.0
Create Remove	Cancel OK

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

?

×

 Δ_{lin} - Linear misfit



Page 54



• • • • • • • • • • • • • • • • • • •	Phase status ? ×
Phases	General Constraints Precipitate Nucleation Structure Special
FCC_A1 GAMMA_PRIME GAMMA_PRIME_P0	Properties Strengthening MS Evolution Setup Strengthening model Precipitation strengthening Size dasses coupling coefficient 1.8 Precipitation strengthening APB energy [J/m2] 0,111 number of pair disl. 3 APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 1 Image: Precipitation strengy [J/m2] 0.0 0.0
	dislocation character angle: current value = 45 screw edge
	Modulus strengthening model Nembach
Create Remove	
Help	Cancel OK

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



MCE-ppt-M04E-V1

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

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

• Weak particles

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

varia	ables	value	^	
⊿ kir ⊿]	netics: prec. strength TAO_COHER_WEAK\$*			
4	TAO_COHER_WEAK\$GAMMA_PRIME_P0	8.9264e+07		
	TAO_COHER_STRONG\$GAMMA_PRIME_P0	4.92374e+08	~	
categ expr legal -> co indivi	gory: kinetics: prec. strength ession: TAO_COHER_WEAK\$GAMMA_PRIME_P0 unit qualifiers: *none* oherency hardening shear stress for shearable wea idual phase	ak precipitates of		



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



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



а.

Modulus effect

- Elastic properties of pr
 - energy inside and outs
- 2 models
 - NembachSiems

	Phase status
hases	General Constraints Precipitate Nucleation Structure Special
FCC_A1 GAMMA_PRIME	Properties Strengthening MS Evolution
GAMMA_PRIME_P0	Setup Strengthening model Precipitation strengthening
	Size classes coupling coefficient 1.8
	Precipitation strengthening
	APB energy [J/m2] 0,111 number of pair disl. 3
	APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 1
	✓ auto SF energy [J/m2] 0.0 dislocation character angle: current value = 45 screw edge
	✓ use linear misfit instead of vol. linear misfit [dL/L] 0,004
	Modulus strengthening model Nembach 💌
Create Remove	
Help	Cancel OK



- Nembach model
 - Strong particles

$$\tau_{\text{mod},\text{strong}} = \frac{F_{\text{mod}}}{bL_{s}}$$

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

• Weak particles

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

 G_p - Particle shear modulus

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• Siems model











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

$ au_{\mathrm{mod},\mathit{weak}}$
$ au_{\mathrm{mod}, strong}$

varia		value	
⊿ kin	etics: prec. strength		
⊿ T/	AO MOD WEAK\$*		
	TAO_MOD_WEAK\$GAMMA_PRIME_P0	1.80848e+06	
⊿ T	AO_MOD_STRONGS*		
	TAO_MOD_STRONG\$GAMMA_PRIME_P0	1.32552e+07	~

-> modulus mismatch hardening shear stress for weak shearable precipitates of individual phase



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

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

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65

MCE-ppt-M04E-V1

 γ_{APB} - APB energy

 w, β - Interaction parameter between

the leading and trailing dislocation

 $_{S}$ - Number of pair dislocations



Anti-phase boundary (APB) effect

Phases Ger	roperties Strengthening MS Evolution	cipitate increases the energy
GAMMA_PRIME GAMMA_PRIME_PO	Strengthening model Precipitation strengthening Size classes coupling coefficient 1.8 Precipitation strengthening APB energy [J/m2] 0,111 number of pair disl. 3 APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 1 I auto SF energy [J/m2] 0.0 dislocation character angle: current value = 45 screw edge I use linear misfit instead of vol. Inear misfit [dL/L] 0,004	γ_{APB} - APB energy W, β - Interaction parameter between
Create Remove	Cancel OK	the leading and trailing dislocatio



Anti-phase boundary (APB) effect

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

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

• Weak particles

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

variables value A kinetics: prec. strength
 A TAO_APB_WEAK\$*
 TAO_APB_WEAK\$GAMMA_PRIME_P0
 2.2558e+08
 AO_APB_STRONG\$GAMMA_PRIME_P0
 7.78014e+08

category: kinetics: prec. strength

expression: TAO_APB_WEAK\$GAMMA_PRIME_P0

legal unit qualifiers: *none*

-> anti-phase boundary hardening shear stress for weak shearable precipitates of individual phase

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67



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



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

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

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

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

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- b_p Burger's vector of particle
- $\gamma_{\rm SFP}$ Stacking fault energy of particle
- γ_{SFM} Stacking fault energy of matrix



• Passing dislocation creates a stacking fault – energy difference

between the SF in the precipitate and matrix

• Strong particles

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

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

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

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

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



• • • • • • •	Precipitation domains	[?] – energy difference
Precipitation domains nickelmatrix New Remove	Precipitation domains General Mech. Props MS Evolution Solute trapping Special Diffusion control Energies	, where p_{a} = energy difference rix b_{p} - Burger's vector of particle γ_{SFP} - Stacking fault energy of particle γ_{SFM} - Stacking fault energy of matrix
Rename	Cancel	ок

0



Phase status	? ×
Phases General Constraints Precipitate Nucleation Structure Special FCC_A1 Properties Strengthening MS Evolution GAMMA_PRIME Setup GAMMA_PRIME Strengthening model Precipitation strengthening Size classes coupling coefficient 1.8 Precipitation strengthening APB energy [J/m2] 0,111 APB energy [J/m2] 0,0 dislocation character angle: current value = 45 screw Image: Work Strengthening model Nembach Image: Market Nucleation Modulus strengthening model Nembach Image: Caracel	It – 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



variables ... variables value
Valu

category: kinetics: prec. strength expression: TAO_SFE_WEAK\$GAMMA_PRIME_P0 legal unit qualifiers: *none* -> stacking fault energy hardening shear stress for weak shearable precipitates of individual phase

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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

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Interfacial effect

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

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

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

• Weak particles

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

 γ_{PM} - Precipitate/matrix interface energy

Interfacial effect

- Passing dislocation increases
 - Strong particles

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

• Weak particles

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

	Phas	se status				?
hases	General Constraints	Precipitate	Nucleation	Structure	Specia	
FCC_A1 GAMMA_PRIME	Precipitate setup Phase is precipitate					
	Parent phase:	GAMMA_PRIM	1E			
	Kinetic alias name GAMMA_PRIME_P0					
	# size classes:	50				Initialize
		ution				
	Precipitate properties Shape factor H/D (0.1 is p	olate) 🗌 use		1.	0	
	Interfacial energy [J/m2]	✓ auto ✓ inter ✓ diffu) planar sharp int facial energy size ise interface corr	erface fro	om planar s	harp ie
		regul	ar solution T_crit	:/K 23	350	
	Interface mobility [m4/Js] Driving force model for gr	owth size cla	ss based - SFFK	16	100	•
Create Remove						
Help					Cance	ОК

MatCalc

 γ_{PM} - Precipitate/matrix interface energy



Interfacial effect

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



• Weak particles





legal unit qualifiers: *none* -> chemical hardening shear stress for shearable weak 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) \rightarrow bypassing precipitate
 - Shearable particles (weak or strong) \rightarrow cutting precipitate

• Critical stresses for both scenarios are evaluated



lsh

Identifying the strengthening regime

• Values of τ evaluated for each of three regimes (Non-shearable, shearable weak, shearable strong)

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

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

$$\tau_{i,nsh}$$

$$i - \left\{ \begin{array}{c} \text{Precipitate phase (for "mean radius" models)} \\ \text{Size class (for "multi-class" model)} \end{array} \right.$$



×

?

Identifying the strengthening regime

- Values of τ evaluated f
 - shearable weak, sheara



Precipitate retarding force Image: auto image	elmatrix	General Solid Solution Precipitation
Precipitation strengthening coupling coefficients (1-2) shearing (1.8) 1.8 non-shearing (1.8) 1.8 total (1.4) 1.4		Precipitate retarding force Image: auto value obtained from internal calculation pinned mobility M0' 0.0 Q' 0.0 Dislocation line tension Image: simple (1/2Gb2) dislocation character Image: outer cut off=120° 120 Image: inner cut off=2,0xb 1xb
shearing (1.8) 1.8 non-shearing (1.8) 1.8 total (1.4) 1.4		Precipitation strengthening coupling coefficients (1-2)
non-shearing (1.8) 1.8 total (1.4) 1.4		shearing (1.8) 1.8
		non-shearing (1.8) 1.8 total (1.4) 1.4

Precipitation domains





Evaluation of au_{prec}

• Summation of $\tau_{i,regime}$



 $au_{i,sh}$ -Shearable particles contribution (weak or strong regime)

 $\boldsymbol{\mathcal{T}}_{i,nsh}$ -Non-shearable particles contribution

 $i - \begin{cases} Precipitate phase (for "mean radius" models) \\ Size class (for "multi-class" model) \end{cases}$

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Evaluation of au_{prec}

.

• Summation of $\tau_{i,regime}$

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

- $au_{i,sh}$ -Shearable particles contribution (weak or s
- $\tau_{i,nsh}$ -Non-shearable particles contribution

	Precipitation domains
pitation domains	General Mech. Props MS Evolution Solute trapping Special
kelmatrix	General Solid Solution Precipitation
	Precipitate retarding force
	✓ auto value obtained from internal calculation
	pinned mobility M0' 0.0 Q' 0.0
	Dislocation line tension
	Simple (1/2Gb2) dislocation character
	advanced form outer cut off=120° 120
	inner cut off=2,0xb 1xb 4xb
	Precipitation strengthening coupling coefficients (1-2)
	shearing (1.8) 1.8
	non-shearing (1.8) 1.8
	total (1.4) 1.4
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Evaluation of au_{prec}

• Summation of $\tau_{i,regime}$





Precipitation strengthening, σ_{prec}

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

Phases General Constraints Precipitate Nucleation Structure Special FCC_A1 AL_B_P_CL_MGSI CL_MGSI Properties Strengthening MS Evolution Setup Strengthening model Prec. strength multi-class Ignore contribution Precipitation strengt Prec. strength mean (number-weighted) APB energy []/m?Prec. strength mean (number-weighted) APB energy []/m?Prec. strength mean (number-weighted) APB energy []/m?Prec. strength mean (number-weighted) APB: disl. repulsion strong 2.8 APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. rep. weak (0-1) 0.0 Image: APB: disl. rep. weak (0-1) 0.0	Phase status		?	×
FCC_A1 AL.B. DP CL_MGSI CL_MGSI CL_MGSI Strengthening model Prec.strength multi-class Impore contribution Precipitation strengt Prec.strength mean (volume-weighted) prec.strength mean (volume-weighted) prec.streng	Phases	General Constraints Precipitate Nucleation Structure Special		
Create Remove	Phases FCC_A1 AL_B_DP CL_MGSI CL_MGSI CL_MGSI_P0 AL_B_DP_P0	General Constraints Precipitate Nucleation Structure Special Properties Strengthening MS Evolution Strengthening MS Evolution Strengthening model Prec. strength multi-class Ignore contribution Precipitation strengt Prec. strength mean (number-weighted) Precipitation strengt Prec. strength multi-class Co-Cluster strengthening (Wang&Starink) APB energy [J/m Prec. strength multi-class Co-Cluster strengthening (Wang&Starink) APB: disl. repulsion strong 2.8 APB: disl. rep. weak (0-1) 0.0 ✓ auto SF energy [J/m2] 0.0 edge edge ☐ use linear misfit instead of vol. linear misfit [dL/L] 0.0 Modulus strengthening model Nembach ✓ Multi size classes	~	
Help Cancel OK	Create Remove	coupling coefficient 1.4		

Co-cluster strengthening

Related to binding enthalpy of co-cluster elements

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

 ΔH_{ccl} - Enthalpy of binding between elements

A and B in co-cluster

- *b* Burgers vector
- \mathcal{Y}_i Content of element *i* in co-cluster
- x_i Content of element *i* in matrix

 f_{ccl} - Co-cluster phase fraction

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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.







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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Precipitation strengthening, σ_{prec}

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

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

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

۱	variables	value	^
1	I kinetics: pd strength I SIGMA PREC\$*		
L	TSIGMA_PREC\$nickelmatrix	1.23579e+09	~
e	ategory: kinetics: pd strength expression: TSIGMA_PREC\$nickelmatrix egal unit gualifiers: *none*		

-> total yield strength contribution from precipitates

M_T - Taylor factor

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Mechanical threshold, σ_0



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

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

$$\begin{aligned} \sigma_{th} &= \sigma_{disl} \\ \sigma_0 &= f(\sigma_i, \ \sigma_{disl}, \sigma_{gb}, \sigma_{sgb}, \ \sigma_{ss}, \sigma_{prec}) \\ \sigma_0 &= \sigma_{ath} + \sigma_{th} \end{aligned}$$

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Thank you for your attention !

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Shape factor influence



Create

Help

Sonderegger B

Pha	se status				· · · ·
General Constraints	Precipitate	Nucleation	Structure	Special	
Precipitate setup					
 Phase is precipitate 					
Parent phase:	BCC_A2#01				
Kinetic alias name	BCC_A2#01_	P0			
# size classes:	25				Initialize .
		Edit precipit	ate distribu	ution	
Shape factor H/D (0.1 is	plate) 🗹 use		0,	01	
Shape factor H/D (0.1 is Interfacial energy [J/m2]	plate) 🔽 use	planar sharp inte	0, erface fro	01 om planar sh	arp ie
Shape factor H/D (0.1 is Interfacial energy [J/m2]	plate) 🗹 use] 🗹 auto ✔ inter	planar sharp inte facial energy size	0, erface fro correction	01 om planar sh	arp ie
Shape factor H/D (0.1 is Interfacial energy [J/m2	plate) 🗹 use] 🗹 auto ✔ inter 🗌 diffu	planar sharp inte facial energy size se interface corre	0, erface fro correction ection	01 om planar sh	arp ie
Shape factor H/D (0.1 is Interfacial energy [J/m2	plate) 🗹 use] 🗹 auto ✔ inter 🗌 diffu regul	planar sharp inte facial energy size se interface corre ar solution T_crit	0, erface fro correction ection / K 0.	01 om planar sh 0	arp ie
Shape factor H/D (0.1 is Interfacial energy [J/m2] Interface mobility [m4/Js	plate) 🗹 use] 🔽 auto 🔽 inter 🗌 diffu regul	planar sharp inte facial energy size se interface corre ar solution T_crit	0, erface from correction ection / K 0, 16	01 om planar sh 0 :100	arp ie
Shape factor H/D (0.1 is Interfacial energy [J/m2] Interface mobility [m4/Js Driving force model for g	plate) 🗹 use]	planar sharp inte facial energy size se interface corre ar solution T_crit ss based - SFFK	0, erface from correction ection / K 0. 16	01 om planar sh 0 :100	arp ie
Shape factor H/D (0.1 is Interfacial energy [J/m2] Interface mobility [m4/Js Driving force model for g	plate) 🗹 use] v auto v inter diffu regul s] rowth size dat	planar sharp inte facial energy size se interface corre ar solution T_crit ss based - SFFK	0, erface from ection / K 0, 1e	01 om planar sh 0 2100	arp ie



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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Shape factor influence on L_S

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

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

variables	value	^
kinetics: precipitates		
L_MEAN_2D\$*		
L_MEAN_2D\$GAMMA_PRIME_P0	2.02552e-08	Y
ategory: kinetics: precipitates		

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)

h - Shape factor

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Shearable particles – (e.g. coherency effect)

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

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

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

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

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

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- Shearable particles Coherency effect for non-spherical particles
 - Strong particles

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

• Weak particles

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

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- Yao Shan





Thank you for

your attention!

