

"ABC"-models for subgrain structure evolution in MatCalc 6

(MatCalc 6.00.0258)

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Outlook

- Few words on substructure
- Dislocation density evolution
- Subgrain size evolution
- Model demonstration



Introduction to dislocations

MatCalc Engineering

Dislocations

- Two geometries:
 - Edge
 - Screw



http://www.geology.um.maine.edu/geodynamics/AnalogWebsite/UndergradProjects2010/PatrickRyan/Content/dislocationdiagram.jpg

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Dislocations

Intrinsic dislocations



Wall dislocations





Dislocation density

- Impact:
 - Diffusion (pipe-diffusion)
 - Nucleation rate (number of nucleation sites)
 - Subgrain size (through similitude principle)
 - Recrystallization onset
 - Yield strength
 - Directly work hardening
 - Indirectly subgrain size, precipitate size





MatCalc models

- Sherstnev-Lang-Kozeschnik (SLK) models
 - 1 parameter model (a.k.a. "1ABC")
 - 2 parameters model (a.k.a. "2ABC")
- 1 parameter model: global dislocation density evolution
- 2 parameters model: separate dynamics for intrinsic and wall dislocations



💱 Precipitation domains							? ×
Precipitation domains	General	Mech. Props	MS Ev	olution Tra	apping Specia	I	
Precipitation domains	General Grainstruct	Mech. Props	MS Ev ostructure model no 1-7 1-7 2-1	Solute drag Solute drag substructure e substructure e baram - Sherst baram - Kreyca baram - Sherst	apping Specia y Vacancies evolution evolution nev-Lang-Kozesch -Kozeschnik - 'sig nev-Lang-Kozesch	I Heat generation nnik - 'ABC' ma-theta' nnik - '2-ABC'	
New Remove Set active Rename	No sub	structure evol	ution				
						Cancel	OK



$$\dot{o} = \dot{\rho_1} - \dot{\rho_2} - \dot{\rho_3}$$

- Dislocation generation
 - Deformation $\rightarrow \dot{\rho_1}$
- Dislocation annihilation
 - Dynamic recovery (dislocations with antiparallel Burgers vectors hit each other) $\rightarrow \dot{\rho_2}$
 - Static recovery (dislocation climb) $\rightarrow \dot{\rho_3}$



$$\dot{\rho_1} = \frac{M\dot{\varepsilon}}{bA}\sqrt{\rho}$$

- ρ Dislocation density
- A A-parameter (constant)

- M Taylor factor
- $\dot{\varepsilon}$ Strain rate
- *b* Burgers vector



💱 Prec

Precip

 $\dot{\rho_1} = \frac{M\dot{\varepsilon}}{hA}\sqrt{\rho}$

- ρ Dislocation density
- A A-parameter (constant)

recipitation domains	?					
ecipitation domains	General Mech. Props MS Evolution Trapping Special					
matrix*	Grainstructure Substructure Solute drag Vacancies Heat generation					
	Substructure evolution model 1-param - Sherstnev-Lang-Kozeschnik - 'ABC'					
	Excess dislocations					
	Rho_total [m-2] 0					
	Equilibrium wall dislocation density					
	✓ from Read-Shockley / manual 1e14 Misorientation [deg] 3					
	SGB pinning force					
	✓ include disl. pinning cell width [m] 1e-8					
	Dislocation generation and annihilation					
	Parameter Value Description					
	A 50 Mean free path for dislocation generation					
	B 5 Dislocation annihilation coefficient (DRV)					
	C 1e-3 Dislocation annihilation coefficient (SRV)					
New Remove	A' 30 Similitude parameter. Similar to A. but not totally					
Set active Rename						
	Cancel OK					



 $\dot{\rho_1} = \frac{M\dot{\varepsilon}}{hA}\sqrt{\rho}$

- M Taylor factor
- $\dot{\varepsilon}$ Strain rate
- *b* Burgers vector

Precipitation domains	?
Precipitation domains	General Mech. Props MS Evolution Trapping Special
matrix*	General Solid Solution Segregation CC Diffusion Precipitation Mechanical properties Young's Modulus [Pa] (69220-40.1*T\$C)*1e6
	Taylor factor (2.5-3.1) 3.06 Poisson's ratio 0.3
	Speed of sound 5100.0
	Basic strength [Pa] 20.0e6
	Hall-Petch coeff (gb/sgb) 0.04e6 / 0.0e6 Disl. strengt. coeff. (a1/a2) 0.5 / 0.0
	Dynamic strength
	delta_F_lt_fact 1.0 delta_F_ht +127200 couplexp 3.0 eps_dot_fact 1.0 exp_ht 1.0/3.0 <t< td=""></t<>
	Total strength coupling coefficients
New Remove Set active Rename	Coeff. thermal + athermal (1.0) 1.0
	Cancel OK



ċ	$\underline{M\dot{\varepsilon}}$
p_1	bA

- M Taylor factor
- $\dot{\varepsilon}$ Strain rate
- *b* Burgers vector

Precipitation domains		? 🗙
Precipitation domains	General Mech. Props MS Evolution Tr	rapping Special
matrix*	Thermodynamic matrix phase	
	FCC_A1	
	Microstructure parameters	
	equilibrium dislocation density [m-2]	1e13
	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	e-10
New Remove		
Set active Rename		





- *M* Taylor factor
- $\dot{\varepsilon}$ Strain rate
- *b* Burgers vector

### Edit t/m treatment segment General MS Evolution	Alternatively, use console command: set-simulation-parameter global-defo	rmation-rate=1
deformation mode axisymmetric compression eps-dot 1 Options reset excess vacancies break of the set o	u(forging) n z (up/down) up particles e gb precipitates	
Comment Pre-Segment Script Post-Seg	ment Script Cancel OK	





- d_{ann} Annihilation distance
 - *G* Shear modulus
 - ν Poisson ratio

 E_{Va} - Vacancy formation energy

(from thermodynamic database)

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Engineering

 N_A - Avogadro constant



- d_{ann} Annihilation distance
 - *G* Shear modulus
 - ν Poisson ratio

rix*	Ceneral Solid Solution Segregation CC Diffusion Dracinitation
	Mechanical properties
	Young's Modulus [Pa] (69220-40.1*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) 0.04e6 / 0.0e6
	Disl. strengt. coeff. (a1/a2) 0.5 / 0.0
	Dynamic strength
	delta_F_lt_fact 1.0 delta_F_ht +127200 couplexp 3.0
	eps_dot_fact 1.0 exp_ht 1.0/3.0
	Total strength coupling coefficients
lew Remove	Coeff. thermal + athermal (1.0) 1.0

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- d_{ann} Annihilation distance
 - G Shear modulus
 - ν Poisson ratio

tation domains	General Mech. Props MS Evolution Trapping Special
x*	General Solid Solution Segregation CC Diffusion Precipitation
	Mechanical properties
	Young's Modulus [Pa] (69220-40.1*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) 0.04e6 / 0.0e6
	Disl. strengt. coeff. (a1/a2) 0.5 / 0.0
	Dynamic strength
	delta_F_lt_fact 1.0 delta_F_ht +127200 couplexp 3.0
	eps_dot_fact 1.0 exp_ht 1.0/3.0
	Total strength coupling coefficients
ew Remove	Coeff. thermal + athermal (1.0) 1.0
Rename	

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2Mėd_{ann}B ρ_2 h

B - B-parameter (constant)

tation domains	General Mech. Props MS Evolution Trapping Special					
ix*	Grainstructure Substructure Solute drag Vacancies Heat generation					
	Substructure Substructure Solution and I according Characteria Kasaschrik (ADC)	_				
	Substructure evolution model 1-param - Sherstnev-Lang-Kozeschnik - AbC					
	Excess dislocations					
	Rho_total [m-2] 0					
	Equilibrium wall dislocation density					
	From Read-Shockley / manual 1e14 Misorientation [deg] 3					
	SGB pinning force					
	✓ include disl. pinning cell width [m] 1e-8					
	Dislocation generation and annihilation					
	Parameter Value Description					
	A 50 Mean free path for dislocation generation					
	B 5 Dislocation annihilation coefficient (DRV)					
	C 1e-3 Dislocation annihilation coefficient (SRV)					
w Remove	A 30 Similitude barameter. Similar to A. but not totally					
active Rename						
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$$\dot{\rho_3} = \frac{2Gb^3 D_{eff}C}{k_B T} \left(\rho^2 - \rho_{eq}^2\right)$$

 D_{eff} - Diffusion, incl. enhancement factors like pipe diffusion, excess vacancies, etc.

- k_B Boltzmann constant
- T Temperature

- C C-parameter (constant)
- ρ_{eq} Equilibrium dislocation density

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- C C-parameter (constant)
- ρ_{eq} Equilibrium dislocation density (sum of intrinsic

and wall dislocations)

Precipitation domains	General Mech. P	rops	MS Evolution	Trapping	Special		
matrix*	Graiostructure	Substru	ucture Solute	drag Va	acancies	Heat genera	ation
	Substructure evolu	ution mo	del 1-param - Sh	ierstnev-Lan	g-Kozeschr	ik - 'ABC'	-
	Excess dislocation	tions					
	Rho_total [m-:	2] 0					
	Equilibrium wal	l dislocat	ion density				
	✓ from Read-Shockley / manual 1e14 Misorientation [deg] 3						
	SGB pinning fo	rce					
	✓ include disl	. pinning	cell width [m]	1e-8			
	Dislocation ger	neration	and annihilation .				
	Parameter	Value		Descrip	otion		<u>^</u>
	А	50	Mean free path	n for disloca	tion gene	ation	=
	В	5	Dislocation an	nihilation c	oefficient (DRV)	-
	с	1e-3	Dislocation an	nihilation c	oefficient (SRV)	
New Remove	Α'	30	Similitude para	ameter. Sim	ilar to A. b	ut not totallv	-
Set active Rename							

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- C C-parameter (constant)
- ρ_{eq} Equilibrium dislocation

density (sum of intrinsic

and wall dislocations)

Precipitation domains				? 🗙
Precipitation domains Precipitation domains matrix*	General Mech. Props Thermodynamic matrix ph FCC_A1 Microstructure parameter equilibrium dislocation der initial grain diameter [m] initial subgrain diameter [m]	MS Evolution ase s sity [m-2] 100.0e-6 m] 100.0e-6	Trapping Special 1e11 elongation factor 1 elongation factor 1	
New Remove	Burger's vector	anual value [m] 2.	.5e-10	
			Cance	і ок

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- C C-parameter (constant)
- ρ_{eq} Equilibrium dislocation density (sum of intrinsic

and wall dislocations)

cipitation domains	General Mech. P	rops	MS Evolution Trapping Special
natrix*	Grainstructure	Substru	icture Solute drag Vacancies Heat generation
	Substructure evolu	ution mod	del 1-param - Sherstnev-Lang-Kozeschnik - 'ABC'
	Rho_total [m-2	2] 0	
	Equilibrium wal	dislocat	ion density
	✓ from Read	-Shockle	y / manual 1e14 lisorientation [deg] 3
		rce . pinning	cell width [m] 1e-8
	Dislocation ger	eration a	and annihilation
	Parameter	Value	Description
	A	50	Mean free path for dislocation generation
	В	5	Dislocation annihilation coefficient (DRV)
	С	1e-3	Dislocation annihilation coefficient (SRV)
New Remove	Α'	30	Similitude parameter. Similar to A. but not totally

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Read-Shockley dislocation density



Read-Shockley dislocation density → necessary amount to fulfill geometrical constraint

 $\rho_{RS} = \frac{tan\theta}{\delta b}$

 θ - Misorientation angle



Burgers, J.M., Proc. Phys. Soc. 52 (1940) 23-33

Read-Shockley dislocation density

 Read-Shockley dislocation density → necessary amount to fulfill geometrical constraint

$$\rho_{RS} = \frac{tar\theta}{\delta b}$$

 $\theta~$ - Misorientation angle

Precipitation domains			? 🗙	
Precipitation domains	General Mech. Props	MS Evolution Trapping Special		
matrix*	Grainstructure Subs Substructure evolution m Excess dislocations .	ructure Solute drag Vacancies Heat ge odel 1-param - Sherstnev-Lang-Kozeschnik - 'ABC'	eneration 🗸	
	Rho_total [m-2] 0 Equilibrium wall disloc I from Read-Shock SGB pinning force I include disl. pinni	ation density ley / manual <u>1e14</u> Misorientation [deg] 3 ng cell width [m] <u>1e-8</u>		
	Dislocation generatio	n and annihilation		
	Parameter Valu	e Description	A	
	A 50	Mean free path for dislocation generation	=	
	B 5	Dislocation annihilation coefficient (DRV)		
	C 1e-3	Dislocation annihilation coefficient (SRV)		
New Remove Set active Rename	A' 30	Similitude parameter. Similar to A. but not to	otally	
		Cancel	ОК	

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Subgrain size evolution

Subgrain size evolution



$$\dot{\delta} = \dot{\delta_1} - \dot{\delta_2}$$

- Subgrains grow to minimize the subgrain boundary area (minimize the boundary energy) $\rightarrow \dot{\delta_1}$
- Subgrain walls shrink with increasing dislocation density (more wall dislocations available) $\rightarrow \dot{\delta_2}$



$$\delta_1 = MP_D$$

- Subgrain growth model same as for grain growth → product of mobility and driving force
- Same models for as for grain boundary mobility → same effects for precipitate pinning and solute drag

0.55





 Same models as for grain boundary mobility → same effects for precipitate pinning and solute drag

recipitation domains				? <mark>×</mark>
recipitation domains	General Mech. F	Props MS Evolution Trappin	g Special	
matrix*	Diffusion control	Energies Mobilities		
	Grain boundarie	s (HAGB)		
	intrinsic M0	0.01*MOB_HAGB\$@	Q 0.0	
	solute drag M0	1000.0*GB_MOB_INT\$@	Q 0.0	
	pinned M0	0.01*GB_MOB_INT\$@	Q 0.0	
	-Subgrain bound	aries (LAGB)		
	intrinsic M0	1.0*MOB_LAGB\$@	Q 0.0	
		👿 use same solute drag factor tha	an HA grain boundaries	
	solute drag M0	1000.0*SGB_MOB_INT\$@	Q 0.0	
		use same pinning factor than H	A grain boundaries	
	pinned M0	0.01*SGB_MOB_INT\$@	Q 0.0	
New Remove				
Set active Rename				
			Cancel	ок



Driving force – balance between Laplace pressure and

dislocation pinning of subgrain walls

$$P_D = \frac{4\gamma_{sgb}}{\delta} - \frac{Gb^2}{\sqrt{w\rho}}\sqrt{\rho - \rho_{RS}}$$

- $\gamma_{s,gb}$ Subgrain boundary energy
 - δ Subgrain size

- *w* Cell width for dislocation pinning
- ρ_{RS} Read-Shockley dislocation density



 Driving force – balance betwo dislocation pinning of subgra

$$P_D = \frac{4\gamma_{sgb}}{\delta} - \frac{Gb^2}{\sqrt{w\rho}}\sqrt{\rho - \rho_{RS}}$$

- γ_{sgb} Subgrain boundary energy
 - δ Subgrain size

Precipitation domains General Mech. Props MS Evolution Trapping Special Imatrix* Diffusion control Energies Mobilities Defects Grain boundary [J/m2] 0.5 Subgrain boundary [J/m2] 0.3 Dislocations [J/m] 0.0 Stacking fault energy I automatic SFE manual [J/m2] 0.0 New Remove Set active Rename	Precipitation domains		? ×
Set active Rename Cancel OK	Precipitation domains matrix* New Remove	General Mech. Props MS Evolution Trapping Special Diffusion control Energies Mobilities Defects Grain boundary [J/m2] 0.5 Subgrain boundary [J/m2] 0.3 Dislocations [J/m] 0.0 Stacking fault energy ✓ automatic SFE manual [J/m2] 0.0	
	Set active Rename	Cancel	ОК



 Driving force – balance betv dislocation pinning of subgr

$$P_D = \frac{4\gamma_{sgb}}{\delta} - \frac{Gb^2}{\sqrt{w\rho}}\sqrt{\rho - \rho_{RS}}$$

w - Cell width for

dislocation pinning

						_	6
bitation domains	General Mech. P	rops	MS Evolution	Trapping	Special		
trix*	Grainstructure	Substru	ucture Solute	drag V	acancies	Heat generat	ion
	Substructure evolu	ution mo	del 1-param - Sł	nerstnev-La	ng-Kozeschr	nik - 'ABC'	-
	Excess dislocat	tions					
	Rho_total [m-2	2] 0					
	Equilibrium wal	dislocat	ion density –				
	📝 from Read	-Shockle	y/manual 1e1	.4 M	isorientatior	1 [deg] 3	
	SGB pinning for	rce . pinning	cell width [m]	1e-8			
	-SGB pinning for include disl Dislocation gen	rce . pinning neration	cell width [m]	1e-8			
	-SGB pinning for include disl Dislocation gen Parameter	rce . pinning neration Value	cell width [m] and annihilation .	1e-8 Descri	ption		^
	-SGB pinning for include disl Dislocation gen Parameter A	rce pinning eration Value 50	cell width [m] and annihilation Mean free patl	1e-8 Descri	ption ation gene	ration	
	SGB pinning for include disl Dislocation gen Parameter A B	value value	cell width [m] and annihilation Mean free pat Dislocation an	1e-8 Descri h for disloc	ption ation gene coefficient	ration (DRV)	• III
	-SGB pinning for include disl -Dislocation gen Parameter A B C	value 50 1e-3	cell width [m] and annihilation Mean free path Dislocation an Dislocation an	1e-8 Descri h for disloc nihilation o nihilation o	ption ation gene coefficient coefficient	ration (DRV) (SRV)	
lew Remove	SGB pinning for include disl Dislocation gen Parameter A B C A'	value 50 5 1e-3 30	cell width [m] and annihilation Mean free path Dislocation an Dislocation an Similitude para	1e-8 h for disloc nihilation o nihilation o ameter. Sin	ption ation gene coefficient coefficient nilar to A. b	ration (DRV) (SRV) out not totally	
ew Remove	SGB pinning for include disl Dislocation gen Parameter A B C A'	value value value value value value value value value value	cell width [m] and annihilation Mean free path Dislocation an Dislocation an Similitude para	1e-8 h for disloc nihilation o ameter. Sin	ption ation gene coefficient coefficient nilar to A. b	ration (DRV) (SRV) out not totally	

Subgrain shrinkage





A' - A'-parameter (constant)

ecipitation domains	General Mech. Pr	ops	MS Evolution	Trapping Sp	ecial		
matrix*	Grainstructure	Substru	ucture Solute	e drag Vacanci	es Heat generati	on	
	Substructure evolut	tion mod	del 1-param - Sł	herstnev-Lang-Koz	eschnik - 'ABC'	-	
	Excess dislocations						
	Rho_total [m-2] 0						
	Equilibrium wall	dislocati	ion density –				
	from Read-Shockley / manual 1e14 Misorientation [deg] 3						
	SGB pinning for	ce –					
	M include disi.	pinning	cell width [m]	1e-8			
	Dislocation gene	eration a	and annihilation .				
	Parameter	Value	e Description				
	A	50	Mean free pat	generation	=		
	B	5 1e-3	Dislocation an	nihilation coeffic	ient (DRV)		
New Remove	A'	30	Similitude para	ameter. Similar to	A. but not totally	-	
Set active Rename							



Model demonstration

1-parameter model





Al, 400°C isothermal, A=50, B=5, C=1e-3 (default values)

1-parameter model





Al, 400°C isothermal, A=50, B=5, C=1e-3 (default values)

2-parameters model





Al, 400°C isothermal, A=50, B=5, C=1e-3, Aw=250, Bw=2e-1, Cw=0 (default values)

2-parameters model





Al, 400°C isothermal, A=50, B=5, C=1e-3, Aw=250, Bw=2e-1, Cw=0 (default values)

2-parameters model





Al, 400°C isothermal, A=50, B=5, C=1e-3, Aw=250, Bw=2e-1, Cw=0 (default values)

Acknowledgments



- Yao Shan
- Heinrich Buken