

# MatCalc approach for the modelling of the vacancy concentration evolution

(MatCalc 5.60.0005)

P. Warczok





# What is it all about?

<b>#</b>	Phase status .	
Phases	General Constraints Precipitate	Nucleation Structure Special
BCC_A2 CEMENTITE CEMENTITE_P0	General       Constraints       Precipitate         General       Sites <ul> <li>bulk (homogeneous)</li> <li>dislocations</li> <li>grain boundary (diff. geom.!)</li> <li>grain boundary edge</li> <li>grain boundary edge</li> <li>grain boundary corner</li> <li>subgrain boundary edge</li> <li>subgrain boundary corner</li> <li>### warning ### no nucleation sites defined !!!!</li> </ul>	Nucleation       Structure       Special         Image: structure       other precipitates       Add         Image: structure       Add       Remove         Image: structure       nucleate at precipitate surface       Remove         Image: structure       0.0       0.0         Image: structure       0.0       max.       3.0e-9         Image: structure       max.       5.0e-9       Image: structure
Create Remove		Nucleation site efficiency 1.0
Help		Cancel O



## What is it all about?

Consequences

Number of available nucleation sites

Interfacial energy model

Precipitate growth & coarsening  $\rightarrow$  nucleation on grain boundaries

Special cases: Nucleation on/within precipitates



Nucleation rate  $\rightarrow J \sim N_x$ 

Available nucleation sites – bulk

 $N_{bulk} = NA/Vm$ 

Available nucleation sites – dislocations

$$N_{disl} = \rho (N_A / V_m)^{1/3}$$

J – Nucleation rate  $N_x$  – Number of nucleation sites on x position  $N_A$  – Avogadro number  $V_m$  – Molar volume  $\rho$  – Dislocation density



а

## Number of available nucleation sites

#### Grain&subgrain boundaries – tetra(kai)decahedron concept

Strictly: Truncated octahedron

$$V_{tdh} = 8\sqrt{2}a^3$$
$$S_{tdh} = 6(1+2\sqrt{3})a^3$$

$$L_{tdh} = 36a$$

 $V_{tdh}$  – Volume of the polygon

 $S_{tdh}$  – Total surface of the polygon

 $L_{tdh}$  – Total edge length of the polygon Page = 5



http://mathworld.wolfram.com/TruncatedOctahedron.html



Grain&subgrain boundaries – tetra(kai)decahedron concept

Strictly: Truncated octahedron

$$V_{tdh} = 8\sqrt{2}a^3$$
  
 $S_{tdh} = 6(1 + 2\sqrt{3})a^2$   
 $L_{tdh} = 36a$   
 $V_{tdh}$  – Volume of the polygon  
 $S_{tdh}$  – Total surface of the polygon  
 $L_{tdh}$  – Total edge length of the polygon

 $a = \frac{d_{gr/sgr}}{\sqrt{10}}$ 

 $d_{gr}$  – Grain diameter  $d_{sgr}$  – Subgrain diameter



#### Grain&subgrain boundaries – tetra(kai)decahedron concept

 $a = \frac{d_{gr/sgr}}{\sqrt{10}}$ 

Strictly: Truncated octahedron

$$V_{tdh} = 8\sqrt{2}a^3 + 6a^2H$$

 $S_{tdh} = 6(1 + 2\sqrt{3})a^2 + 2a(2H + a)$ 

 $d_{gr}$  – Grain diameter

 $d_{sgr}$  – Subgrain diameter

 $D_{gr}$  – Elongation factor for grains

 $D_{gr}$  – Elongation factor for subgrains

 $L_{tdh} = 36a + 8H$ 

 $V_{tdh}$  – Volume of the polygon  $S_{tdh}$  – Total surface of the polygon  $L_{tdh}$  – Total edge length of the polygon

$$H = \sqrt{\left(D_{gr/sgr}^2 - \frac{d_{gr/sgr}^2}{5}\right) - 2\sqrt{\frac{d_{gr/sgr}^2}{5}}}$$



<b>\$</b> #7	Precipitation domains	<sup>?</sup> × hedron concent
Precipitation domains	Precipitation domains         General       Mech. Props       MS Evolution       Solute trapping       Special         Thermodynamic matrix phase       Image: Comparison of the system of t	hedron concept $gr$ $d_{gr}$ – Grain diameter $d_{sgr}$ – Subgrain diameter $D_{gr}$ – Elongation factor for grains $D_{gr}$ – Elongation factor for subgrains
New Remove Rename	Cancel	$r - \frac{d_{gr/sgr}^2}{5} - 2\sqrt{\frac{d_{gr/sgr}^2}{5}}$



Available nucleation sites – grain&subgrain boundaries

$$N_{gb/sgb} = \frac{S_{tdh}}{2V_{tdh}} \left(\frac{N_A}{V_m}\right)^{2/3}$$

Available nucleation sites – grain&subgrain boundary edges

$$N_{gbe/sgbe} = \frac{L_{tdh}}{3V_{tdh}} \left(\frac{N_A}{V_m}\right)^{1/3}$$

Available nucleation sites – grain&subgrain boundary corners

$$N_{gbc/sgbc} = \frac{6}{V_{tdh}}$$



"Nucleation site efficiency"

scales linearly the number

of available nucleation sites

9 <b>9</b> 9 9 • *	Phase status ? ×		
Phases FCC_A1 FCC_A1#01 FCC_A1#02 FCC_A1#01_P0 FCC_A1#02_P0	Phase status         General       Constraints       Precipitate       Nucleation       Structure       Special         General       Sites         Bulk (homogeneous)       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary (diff. geom.!)       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations       Image: dislocations       Image: dislocations         Image: grain boundary edge       Image: dislocations		
Create Remove	Cancel OK		



Bulk & dislocations  $\rightarrow$  standard interfacial energy evaluation

Grain & subgrains (surface, edges, corners)  $\rightarrow$  Clemm-Fisher model



energy Page = 11

Clemm P.J., Fisher J.C., Acta Metall. 3 (1955) 70-73



Preci

Bulk & dislocations  $\rightarrow$  stan

Grain & subgrains (surface,



energy Page ■ 12

	Precipitation domains ? ×
pitation domains	General Mech. Props MS Evolution Solute trapping Special
ite	Diffusion control Energies Defects Grain boundary [1/m2] 0.5
	Subgrain boundary [J/m2] 0.3
	Dislocations [J/m] 0.0
	Stacking fault energy automatic SFE manual [J/m2] 0.0
Remove Rename	
	Cancel OK



Grain & subgrains surfaces



Clemm P.J., Fisher J.C., Acta Metall. 3 (1955) 70-73

![](_page_13_Picture_0.jpeg)

Grain & subgrains edges

![](_page_13_Picture_3.jpeg)

$$a = 3\beta(1 - \cos^2\theta) - \cos\theta\sqrt{(3 - 4\cos^2\theta)}$$

$$b = 12\left(\frac{\pi}{2} - \alpha - \beta \cos\theta\right)$$

$$c = 2\left(\pi - 2\alpha + \cos^2\theta \sqrt{(3 - 4\cos^2\theta)} - \beta\cos\theta(3 - \cos^2\theta)\right)$$

$$\alpha = \arcsin \frac{1}{2\sqrt{(1 - \cos^2 \theta)}} \qquad \qquad \beta = \arccos \frac{\cos \theta}{\sqrt{3(1 - \cos^2 \theta)}}$$

Clemm P.J., Fisher J.C., Acta Metall. 3 (1955) 70-73

![](_page_14_Picture_0.jpeg)

Grain & subgrains corners

$$a = 3\left\{2\phi(1-\cos^2\theta) - K\left[\sqrt{1-\cos^2\theta} - \frac{K^2}{4} - \frac{K^2}{\sqrt{8}}\right]\right\}$$
$$b = 24\left(\frac{\pi}{3} - \phi\cos\theta - \delta\right)$$
$$c = 2\left\{4\left(\frac{\pi}{3} - \delta\right) + K\cos\theta\left[\sqrt{1-\cos^2\theta} - \frac{K^2}{4} - \frac{K^2}{\sqrt{8}}\right] - 2\phi\cos\theta(3-\cos^2\theta)\right\}$$

$$K = \frac{4}{3}\sqrt{\left(\frac{3}{2} - 2\cos^2\theta\right)} - \frac{3}{2}\cos\theta \qquad \phi = \arcsin\frac{K}{2\sqrt{(1 - \cos^2\theta)}} \qquad \delta = \arccos\frac{\sqrt{2 - \cos^2\theta}}{K\sqrt{(1 - \cos^2\theta)}}$$

Clemm P.J., Fisher J.C., Acta Metall. 3 (1955) 70-73

Page ■ 15

![](_page_15_Picture_0.jpeg)

#### **Clemm-Fisher model**

#### needs to be activated!

8.	Phase status ? ×
Phases BCC_A2 CEMENTITE CEMENTITE_P0	Phase status ? ×     General Constraints     Precipitate Nucleation     Structure Special     General Sites     Nucleation model Becker/Doering time-dep.     Nucleation model Becker/Doering time-dep.     Nucleation constant: 1.0     Incubation time constant: 1.0     Incubation time constant: 1.0     Minimum nucleation radius [m] 0.35e-9     Incubation for coherent misfit stress Ignore misfit stress during deformation     Itake into account shape factor Image during deformation
Create Remove	account for excess va contribution indeate only with valid major constituents     restrict nucleation to prec domain

Clemm P.J., Fisher J.C., Acta Metall. 3 (1955) 70-73

![](_page_16_Picture_0.jpeg)

•::

e

### Rulk & dislocations -> standard interfacial energy evaluation

•••			
Phases	General Constraints Precipitate	Nucleation Structure Special	
BCC_A2 CEMENTITE	General Sites		Clemm-Fisher mode
CEMENTITE_P0	Nucleation model	Becker/Doering time-dep.	
	Nucleus composition:	ortho-equilibrium   Calc	2/
	Nucleation constant:	1.0	$\cos \theta = \frac{\gamma_{AA}}{\gamma_{AA}}$
	Incubation time constant:	1.0	$2030 = \frac{21}{100}$
	Minimum nucleation radius [m]	0.35e-9	-YAB
	account for coherent misfit stress	ignore misfit stress during deformation	
	account for excess va contribution	account for gb / disl. line energy nucleate only with valid major constituents	$a, b, c = f(cos\theta)$
	restrict nucleation to prec domain		
			$(b\gamma_{AB} - a\gamma_{AA})$
			$F = \frac{3}{3}$
Create Remove			$\sqrt{36\pi c^2}$
Help		Cancel OK	
			55) /0-/3

![](_page_17_Picture_0.jpeg)

#### Difference in diffusion fields

![](_page_17_Figure_3.jpeg)

**Figure 1.** Schematic precipitate distributions and diffusion fields (shaded areas) for random precipitation (left) and heterogeneous precipitation at grain boundaries (right) in 2D.

![](_page_18_Picture_0.jpeg)

# Difference in diffusion fields $\rightarrow$ modification of radius evolution equations derived from thermodynamic extremum principle

![](_page_18_Figure_3.jpeg)

Kozeschnik et al., Modelling Simul. Mater. Sci. Eng. 18 (2010) 015011

![](_page_19_Picture_0.jpeg)

# Difference in diffusion fields $\rightarrow$ modification of radius evolution equations derived from thermodynamic extremum principle

![](_page_19_Figure_3.jpeg)

Precipitation of AIN at austenite at grain boundaries

Kozeschnik et al., Modelling Simul. Mater. Sci. Eng. 18 (2010) 015011

![](_page_20_Picture_0.jpeg)

### Diffei NOTE:

- eq
- The grain boundary diffusion field model is automatically used when "grain boundary" is selected as the nucleation site
- This model is relevant for the system with large grain size and small precipitate phase fractions.
- In other cases, use the random diffusion field model → select other nucleation sites (e.g. "dislocations") and adjust the available number of the nucleation sites using the "nucleation site efficiency"

Kozeschnik et al., Modelling Simul. Mater. Sci. Eng. 18 (2010) 015011

![](_page_21_Picture_0.jpeg)

# Nucleation on the precipitate surface

FCC_A1#01 FCC_A1#02 FCC_A1#01_P0 FCC_A1#02_P0	Imeral Sites     bulk (homogeneous)   dislocations   grain boundary (diff. geom.!)   grain boundary edge   grain boundary corner   subgrain boundary edge   diffusion geometry: random   diffusion geometry: random   distribution     Nucleation site efficiency     1.0
--	---

![](_page_22_Picture_0.jpeg)

## Nucleation on the precipitate surface

#### Available nucleation sites $\rightarrow$ atoms on the surface of the parent phase

$$N_{prec,surf} = 4\pi \left(\frac{N_A}{V_m}\right)^{2/3} \left(\sum_{class} N_j r_j^2\right)$$

 $N_j$  - Number of precipitates in class "j"

 $r_i$  - Radius of precipitates in class "j"

#### Parent phase is not modified by the nucleation of the new phase

![](_page_23_Picture_0.jpeg)

# Nucleation within the precipitate

FCC_A1       General       Sites         General       Sites         CC_A1#02       bulk (homogeneous)         GCC_A1#01_P0       dislocations         Grain boundary (diff. geom.!)       grain boundary edge         grain boundary edge       grain boundary corner         subgrain boundary       outper precipitate surface         Image: subgrain boundary corner       subgrain boundary corner         General       Sites
distribution     inherit parent comp.       Nucleation site efficiency     1.0

![](_page_24_Picture_0.jpeg)

## Nucleation within the precipitate

Available nucleation sites  $\rightarrow$  atoms on the surface of the parent phase (as

in the previous case)

Nucleation 
$$\rightarrow$$
  $d_{new} > d_{parent}$   $d_{nucl,new} = d_{new} - d_{parent}$ 

 $d_{new}$  - Driving force of the new phase  $d_{parent}$  - Driving force of the parent phase

 $d_{nucl,new}$  - Nucleation driving force of the new phase

Interfacial energy defined by user, critical radius from parent prec.

Parent phase transforms gradually into the new one

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![](_page_25_Picture_0.jpeg)

# Transformation of the precipitate

*	Phase status ?
Phases FCC_A1 FCC_A1#01 FCC_A1#02 FCC_A1#01_P0 FCC_A1#02_P0	General       Constraints       Precipitate       Nucleation       Structure       Special         General       Sites         bulk (homogeneous)       Gislocations         grain boundary (diff. geom.!)       grain boundary edge         grain boundary edge       Remove         subgrain boundary       nucleate at precipitate surface         subgrain boundary edge       0.15         subgrain boundary corner       with the energy         diffusion geometry: random       max.         5.0e-9       inherit parent comp.

![](_page_26_Picture_0.jpeg)

## Transformation of the precipitate

"Transformation towards" rather than "nucleation of" the new precipitate

Transformation condition:  $d_{new} > d_{parent}$ ,  $d_{nucl,new} = d_{new} - d_{parent}$ 

New precipitate size taken from the parent phase

Initial precipitate composition might be taken from the parent phase

![](_page_27_Picture_0.jpeg)

## Transformation of the precipitate

Parent phase transforms gradually into the new one

![](_page_27_Figure_3.jpeg)

![](_page_28_Picture_0.jpeg)

?

## Transformation of the precipitate

#### Parent phase transforms gradua

![](_page_28_Figure_3.jpeg)

Phase status ...

![](_page_29_Picture_0.jpeg)

## Direct particle transformation

For the two last cases: (nucleation within and transformation of the precipitate)

Change the nucleation model to "direct particle transformation"!

<b>**</b> *	Phase status	? ×
Phases FCC_A1 FCC_A1#01	General Constraints Precipitate General Sites	Nucleation Structure Special
FCC_A1#02 FCC_A1#01_P0	Nucleation model	direct particle transformation 👻
FCC_A1#02_P0	Nucleus composition:	ortho-equilibrium   Calc
	Nucleation constant:	1.0
	Incubation time constant:	1.0
	Minimum nucleation radius [m]	0.35e-9
	account for coherent misfit stress	ignore misfit stress during deformation
	account for excess va contribution	nucleate only with valid major constituents
	restrict nucleation to prec domain	
Create Remove		
Help		Cancel OK

![](_page_30_Picture_0.jpeg)

# Acknowledgments

• Yao Shan