MatCalc
Engineering

Precipitate shape factors

(MatCalc 5.61.0027)

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Outline

- Introduction, definition
- Precipitate growth
- Precipitation strengthening

Introduction

- Usual assumption: spherical precipitates

$$G = \boxed{\sum_i N_{0,i}\mu_{0,i}} + \boxed{\sum_k \tfrac{4}{3}\pi\rho_k^3\left(\lambda_k + \sum_i c_{k,i}\mu_{k,i}\right)} + \boxed{\sum_k 4\pi\gamma_k\rho_k^2}$$

Matrix contribution

Precipitate contribution

Precipitate/matrix interface contribution

i - element

0 - matrix

k - precipitate class

G - Gibbs energy of the system

$N_{0,i}$ - Number of i moles in the matrix

$\mu_{0,i}$ - Chemical potential of i in the matrix

ρ_k - Radius of k

λ_k - Mechanical contribution of k

$c_{k,i}$ - i content in k

$\mu_{k,i}$ - Chemical potential of I in k

γ_k - Interfacial energy of k

Svoboda et. al., Mater. Sci. Eng. A., 385 (2004) 166-174

Definition

- Shape parameter
  - Spherical → cylindrical
  - Cylinder aspect ratio

$$h = H / D$$

h - Shape parameter

H - Cylinder height

D - Cylinder diameter

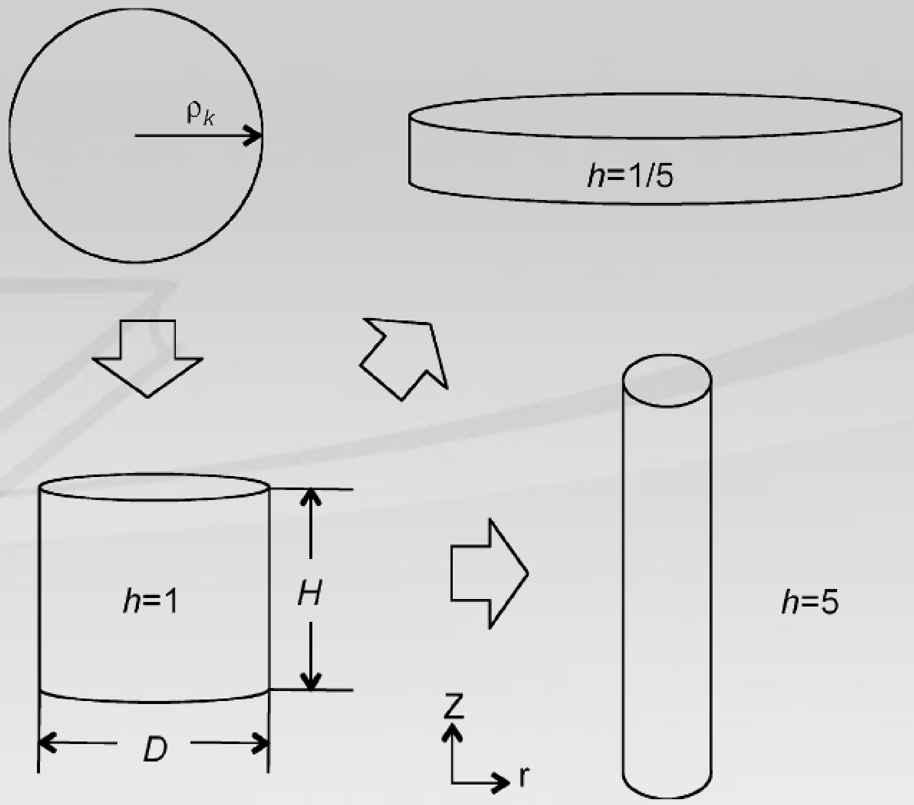


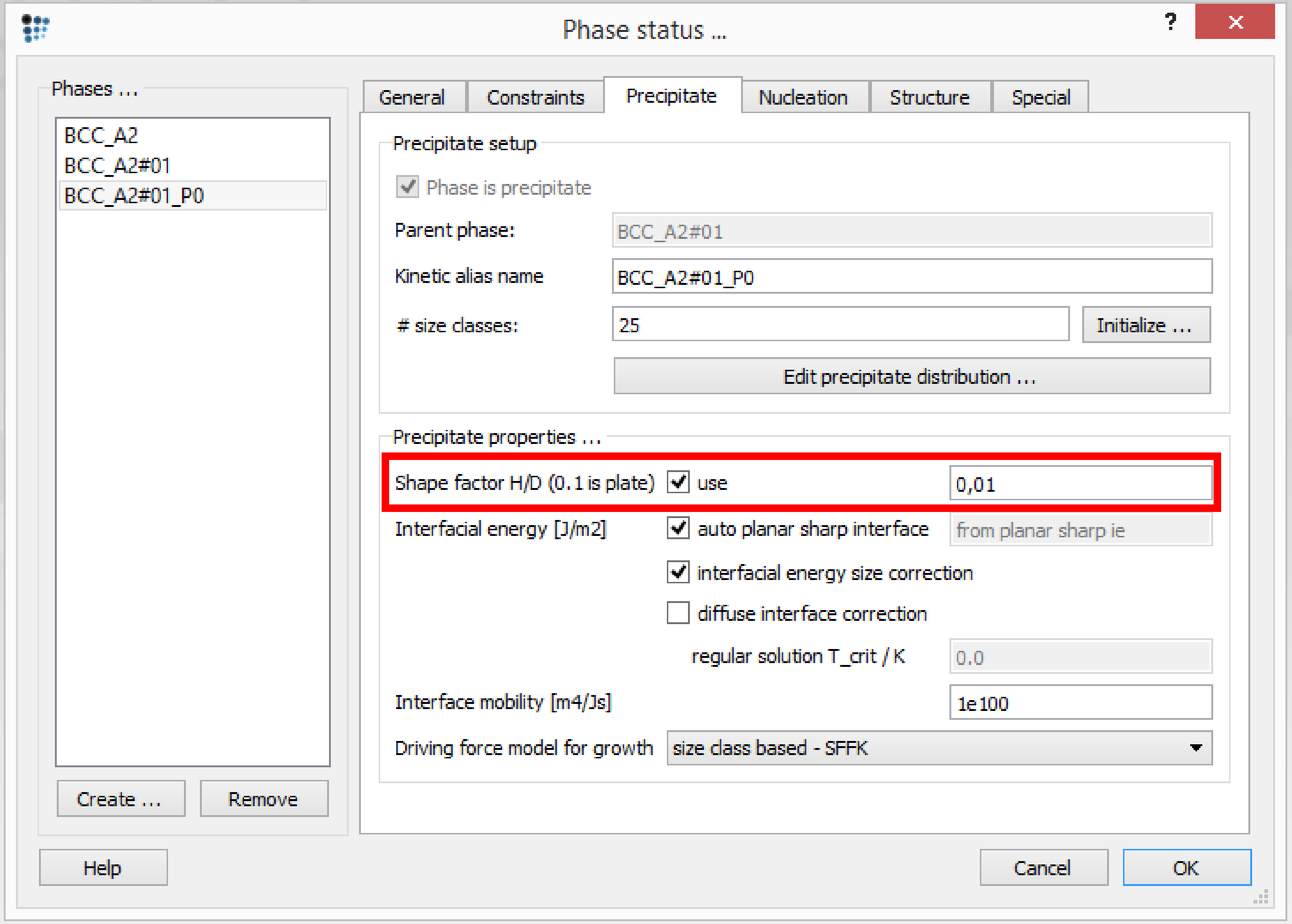
Fig. 1. Illustration of the shape parameter $h = H/D$.

Discs (oblate)

Needles (prolate)

Kozeschnik et. al., Mater. Sci. Eng. A., 441 (2006) 68-72

Definition


Phase status ...
?
Phases ...
BCC_A2
BCC_A2#01
BCC_A2#01_P0
Create ...
Remove
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 precipitate distribution ...
Precipitate properties ...
Shape factor H/D (0.1 is plate)
use
0,01
Interfacial energy [J/m2]
auto planar sharp interface
from planar sharp ie
interfacial energy size correction
diffuse interface correction
regular solution T_crit / K
0.0
Interface mobility [m4/Js]
1e100
Driving force model for growth
size class based - SFFK
Help
Cancel
OK

Effects

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- Shape modification → interface area changed

$$G=\sum_i N_{0,i}\mu_{0,i}+\sum_k \frac{4}{3}\pi\rho_k^3\left(\lambda_k+\sum_i c_{k,i}\mu_{k,i}\right)+\sum_k 4\pi\gamma_k\rho_k^2 \boxed{S_k}$$

$$S_k=0.7631h^{1/3}+0.3816h^{-2/3}$$

For h = 1 ➔ S_k = 1.1447 !

Kozeschnik et. al., Mater. Sci. Eng. A., 441 (2006) 68-72

Effects

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- Influence on Gibbs energy dissipation contributions Q

$$Q_1 = \sum_k \frac{4\pi\rho_k^2\dot{\rho}_k^2}{M_k^{IF}} K_k$$

Interface migration

$$K_k = 0.2912\,h^{2/3} + 0.5824\,h^{-1/3}$$

$$Q_2 = \sum_k \frac{4\pi RT\rho_k^5\dot{c}_{k,i}^2}{45c_{k,i}D_{k,i}} I_k$$

Precipitate diffusion

$$I_k = 0.4239\,h^{4/3} + 0.6453\,h^{-2/3}$$

$$Q_3 = \sum_k \sum_i \frac{4\pi RT\rho_k^3\left(\dot{\rho}_k\left(c_{k,i} - c_{0,i}\right) + \rho_k\dot{c}_{k,i}/3\right)^2}{c_{0,i}D_{0,i}} O_k$$

Matrix diffusion

$$O_k = 1.0692\,h^{2/3}$$

Kozeschnik et. al., Mater. Sci. Eng. A., 441 (2006) 68-72

Precipitate growth

- Evolution equations affected

$$\frac{\partial G}{\partial q_i} = -\frac{1}{2}\frac{\partial Q}{\partial \dot{q}_i}$$

$$Q = Q_1 + Q_2 + Q_3$$

$$q_i \leftarrow \rho_k, c_{k,i}$$

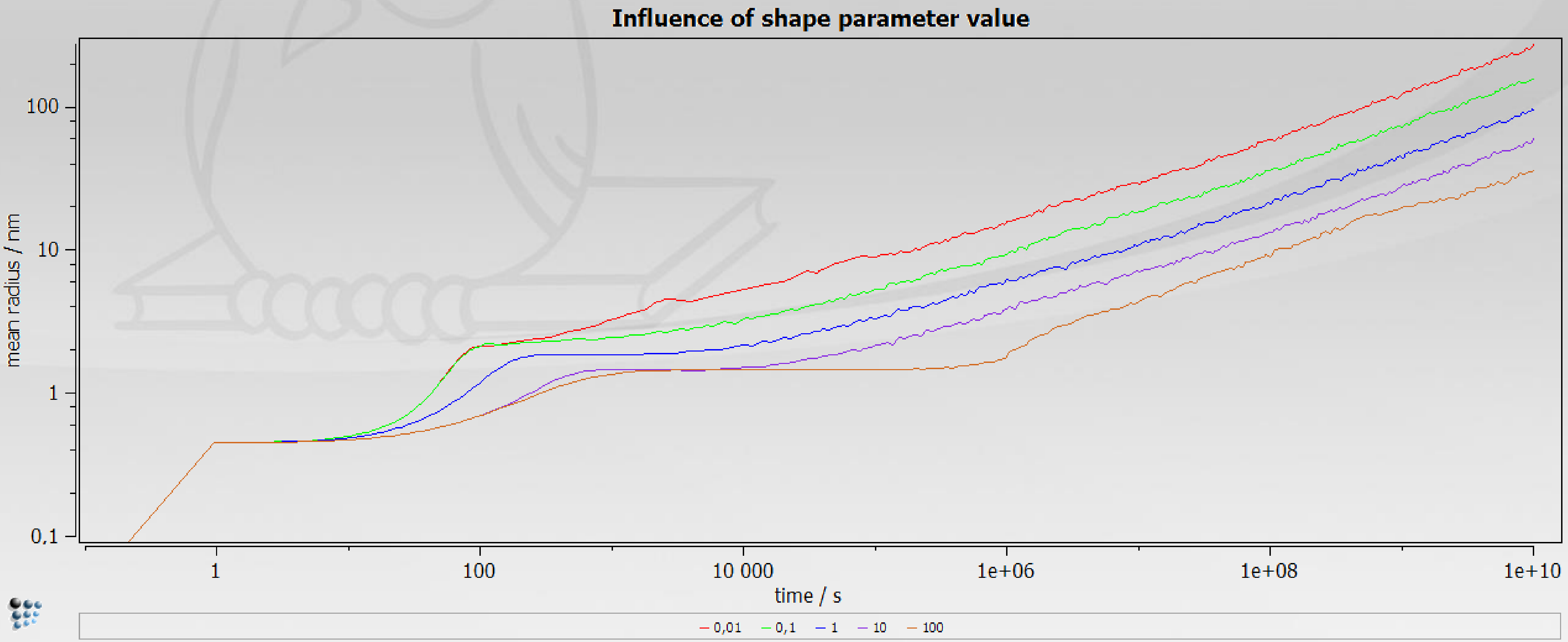
$$G = \sum_i N_{0,i}\mu_{0,i} + \sum_k \tfrac{4}{3}\pi\rho_k^3\left(\lambda_k + \sum_i c_{k,i}\mu_{k,i}\right) + \sum_k 4\pi\gamma_k\rho_k^2 S_k$$

$$Q_1 = \sum_k \frac{4\pi\rho_k^2\dot{\rho}_k^2}{M_k^{IF}} K_k$$

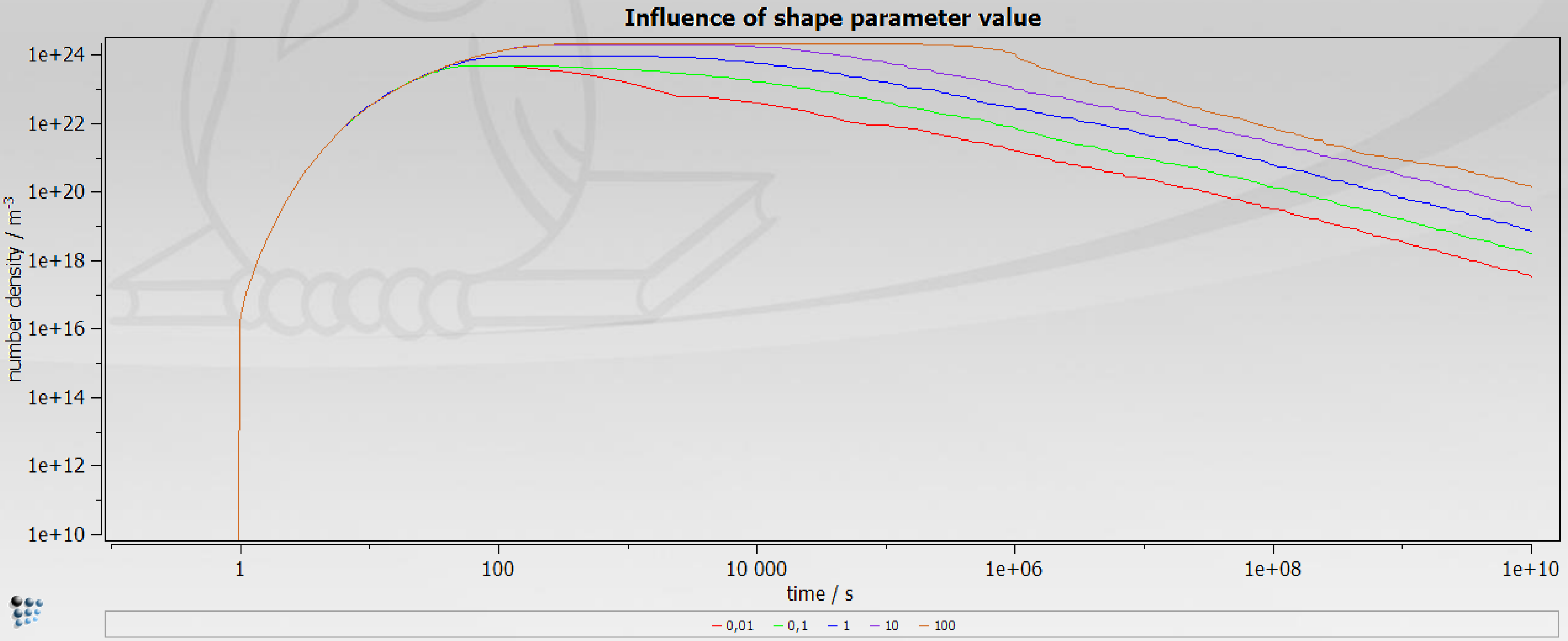
$$Q_2 = \sum_k \frac{4\pi RT\rho_k^5\dot{c}_{k,i}^2}{45 c_{k,i} D_{k,i}} I_k$$

$$Q_3 = \sum_k \sum_i \frac{4\pi RT\rho_k^3\left(\dot{\rho}_k\left(c_{k,i} - c_{0,i}\right) + \rho_k\dot{c}_{k,i}/3\right)^2}{c_{0,i}D_{0,i}} O_k$$

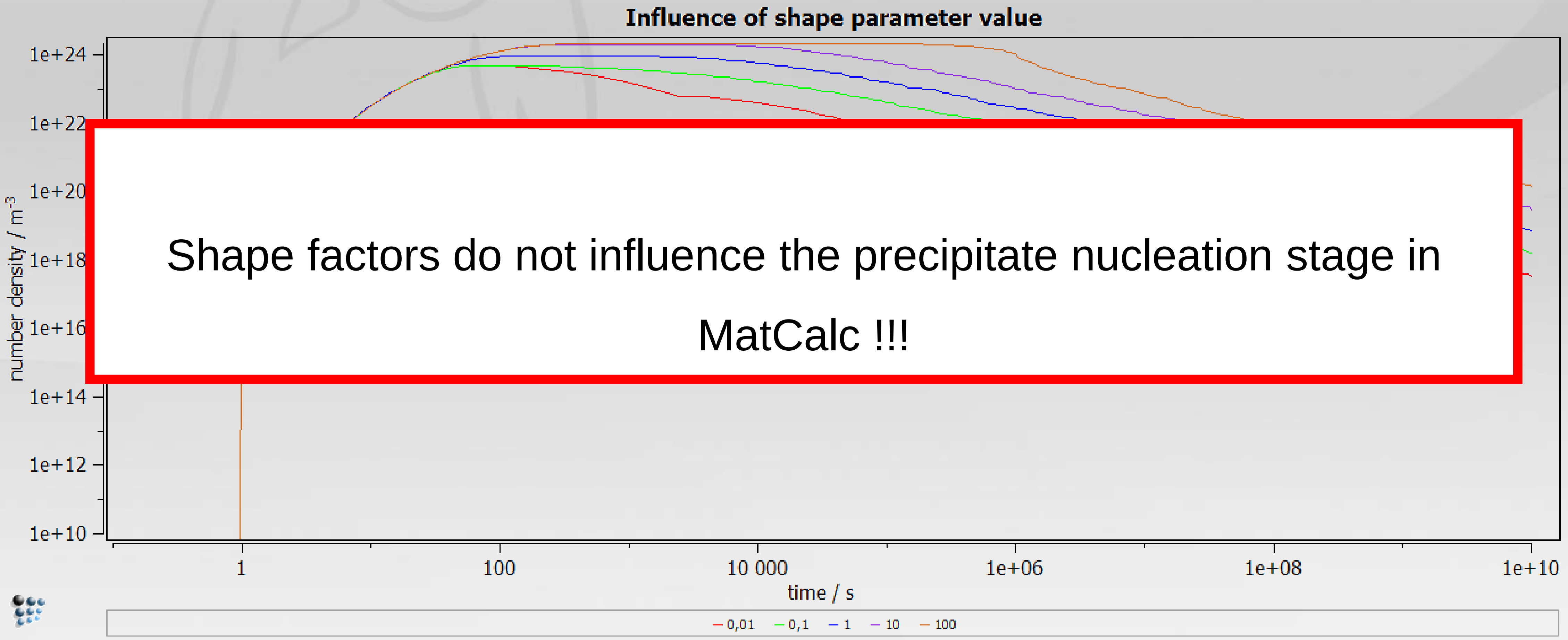
Precipitate growth



Precipitate growth



Precipitate growth



Shape factors do not influence the precipitate nucleation stage in MatCalc !!!

Precipitate growth

•Growth rates

(Anisotropy effects neglected!)

•Minimal diffusion distances for disc growth

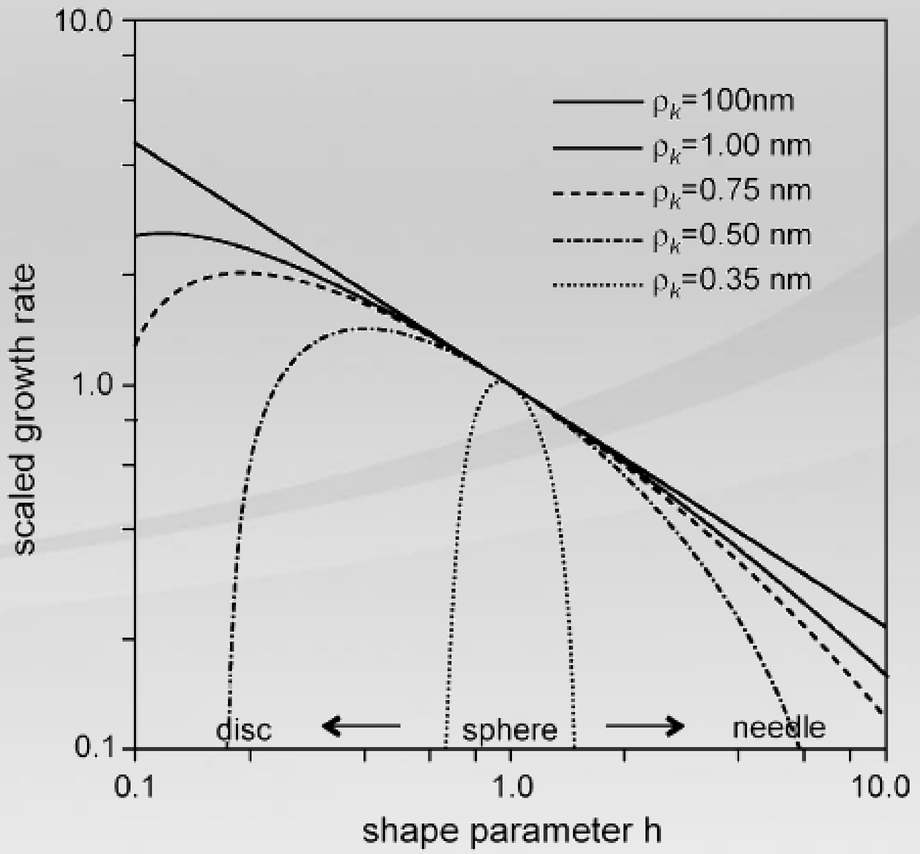


Fig. 3. Scaled growth rate as a function of the shape parameter $h = H/D$ and the equivalent precipitate radius ρ_k.

Kozeschnik et. al., Mater. Sci. Eng. A., 441 (2006) 68-72

Precipitation strengthening

- Surface-surface precipitate distance

$$\tau \sim L_p^{-1} f(r)$$

$$\tau_{Orowan} \sim L_p^{-1} \ln\left(R_{eq}\right)$$

$$\tau_{shear} \sim L_p^{-1} \left(r_{eq}\right)^m$$

τ - Shear stress

τ_{Orowan} - Shear stress for Orowan mechanism

τ_{shear} - Shear stress for shearable precipitates

L_p - Distance between the precipitates

r - Precipitate radius

R_{eq} - Outer cut-off radius

r_{eq} - Equivalent radius

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

Precipitation strengthening

- Surface-surface precipitate distance

$$\tau \sim \boxed{L_p^{-1}} f(r)$$

$$L_p = K L_{sph}$$

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

τ - Shear stress

L_p - Distance between the precipitates

L_{sph} - Distance between the spherical precipitates

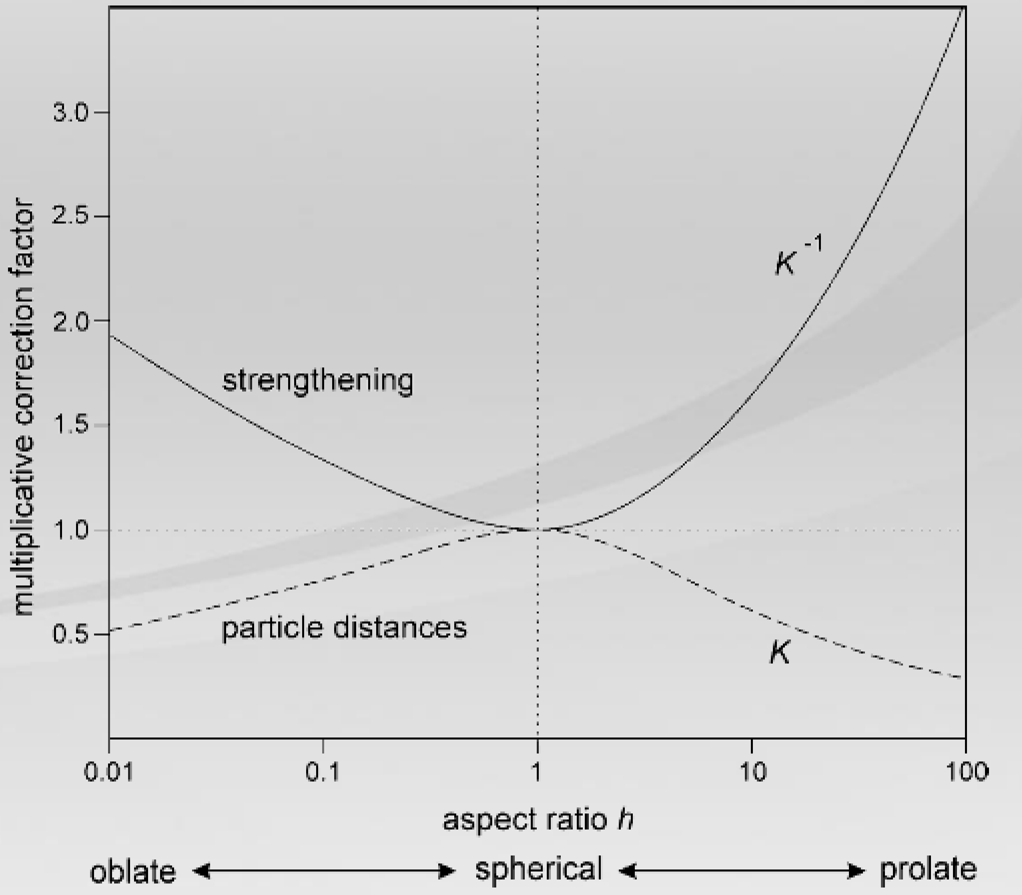


Figure 2. Variation in particle distances and strengthening for prolate and oblate precipitates relative to spherical particles.

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

Precipitation strengthening

- Equivalent radius - Shearable precipitate

$$\tau \sim L_p^{-1} f\boxed{\left(r_{eq}\right)}$$

$$r_{eq} = P_{edge} r_{edge} + P_{screw} r_{screw}$$

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

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

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

$r_{sph,edge}$ - Sphere radius for edge disl.

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

$r_{sph,screw}$ - Sphere radius for screw disl.

P_{edge} - Fraction of edge disl.

P_{screw} - Fraction of screw disl.

Ahmadi M.R. et al., Mater. Sci. Eng. A, 590 (2014) 262-266

Precipitation strengthening

- Equivalent radius - Shearable precipitate

$$\tau \sim L_p^{-1} f\boxed{\left(r_{eq}\right)}$$

$$r_{eq} = P_{edge} r_{edge} + P_{screw} r_{screw}$$

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

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

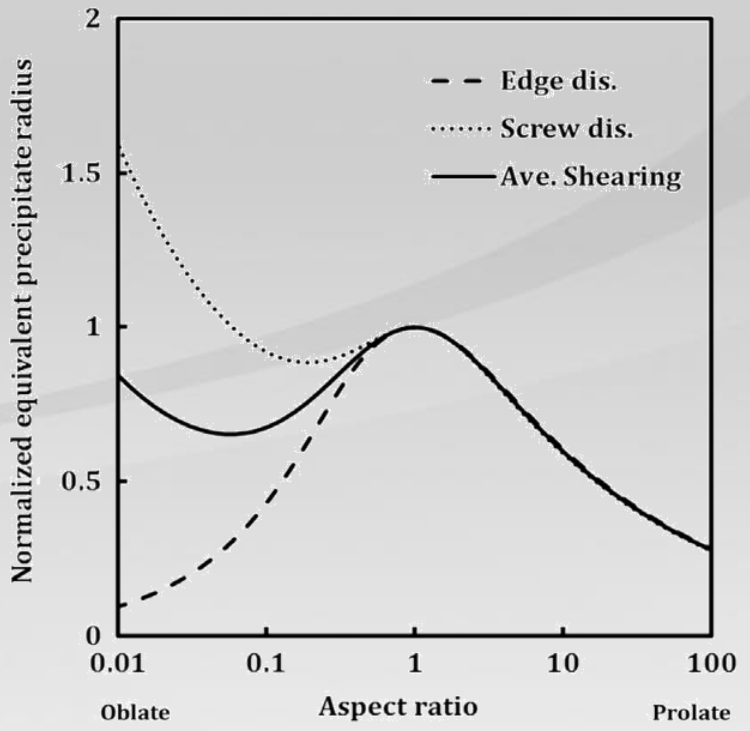


Fig. 3. Normalized equivalent precipitate radius for edge and screw dislocations in the shearing mechanism.

Ahmadi M.R. et al., Mater. Sci. Eng. A, 590 (2014) 262-266

Precipitation strengthening

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- Outer cut-off radius – Orowan mechanism

$$\tau \sim L_p^{-1} f\boxed{\left(R_{eq}\right)}$$

$$R_{eq} = P_{edge} R_{edge} + P_{screw} R_{screw}$$

$$R_{eq,edge} = R_{sph,edge}\left[\frac{2h^{2/3}}{3}\left(\sqrt{\frac{3}{2+h^2}} + \sqrt{\frac{3}{h^2} + \frac{3}{2+h^2}}\right)\right]$$

$$R_{eq,screw} = R_{sph,screw}\left[\frac{2h^{2/3}}{3}\left(\frac{1}{h} + \sqrt{\frac{1}{h^2} + \frac{9}{2+h^2}}\right)\right]$$

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

$R_{sph,edge}$ - Sphere radius for edge disl.

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

$R_{sph,screw}$ - Sphere radius for screw disl.

P_{edge} - Fraction of edge disl.

P_{screw} - Fraction of screw disl.

Ahmadi M.R. et al., Mater. Sci. Eng. A, 590 (2014) 262-266

Precipitation strengthening

• Outer cut-off radius – Orowan mechanism

$$\tau \sim L_p^{-1} f\left(\boxed{R_{eq}}\right)$$

$$R_{eq} = P_{edge} R_{edge} + P_{screw} R_{screw}$$

$$R_{eq,edge} = R_{sph,edge}\left[\frac{2h^{2/3}}{3}\left(\sqrt{\frac{3}{2+h^2}} + \sqrt{\frac{3}{h^2} + \frac{3}{2+h^2}}\right)\right]$$

$$R_{eq,screw} = R_{sph,screw}\left[\frac{2h^{2/3}}{3}\left(\frac{1}{h} + \sqrt{\frac{1}{h^2} + \frac{9}{2+h^2}}\right)\right]$$

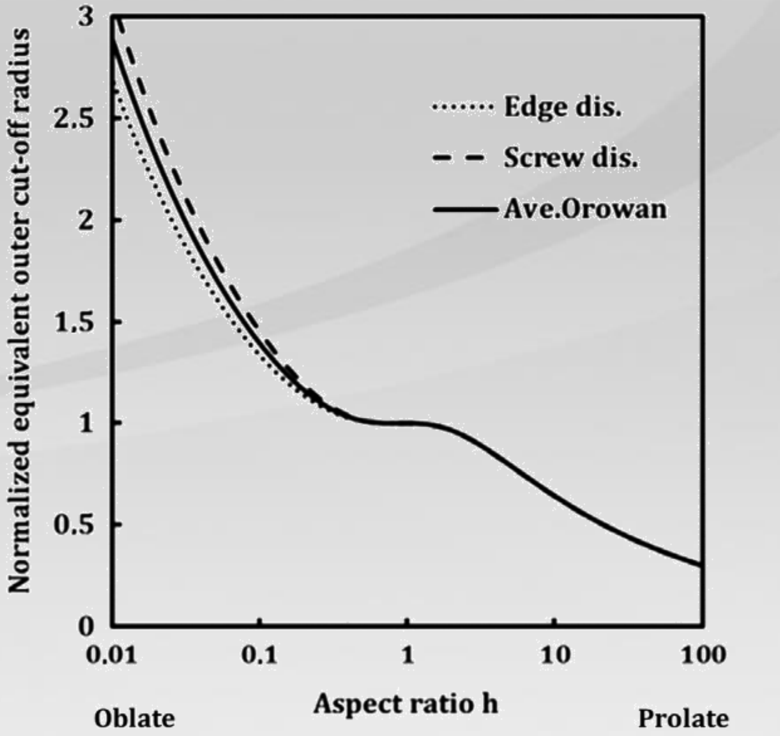

Fig. 4. Normalized equivalent outer cut-off radius for edge and screw dislocations for the non-shearing mechanism.

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Precipitation strengthening

- Dislocation characterization

$$r_{eq} = \boxed{P_{edge}}\, r_{edge} + \boxed{P_{screw}}\, r_{screw}$$

$$R_{eq} = \boxed{P_{edge}}\, R_{edge} + \boxed{P_{screw}}\, R_{screw}$$