

Precipitate shape factors

(MatCalc 6.00.0200)

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Outline

- Introduction, definition
- Precipitate growth
- Precipitation strengthening

Introduction

- Usual assumption: spherical precipitates

$$G = \underbrace{\sum_i N_{0,i} \mu_{0,i}}_{\text{Matrix contribution}} + \underbrace{\sum_k \frac{4}{3} \pi \rho_k^3 \left(\lambda_k + \sum_i c_{k,i} \mu_{k,i} \right)}_{\text{Precipitate contribution}} + \underbrace{\sum_k 4\pi \gamma_k \rho_k^2}_{\text{Precipitate/matrix interface contribution}}$$

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

Definition

- Shape parameter
 - Spherical \rightarrow cylindrical
 - Cylinder aspect ratio

$$h = H / D$$

h - Shape parameter

H - Cylinder height

D - Cylinder diameter

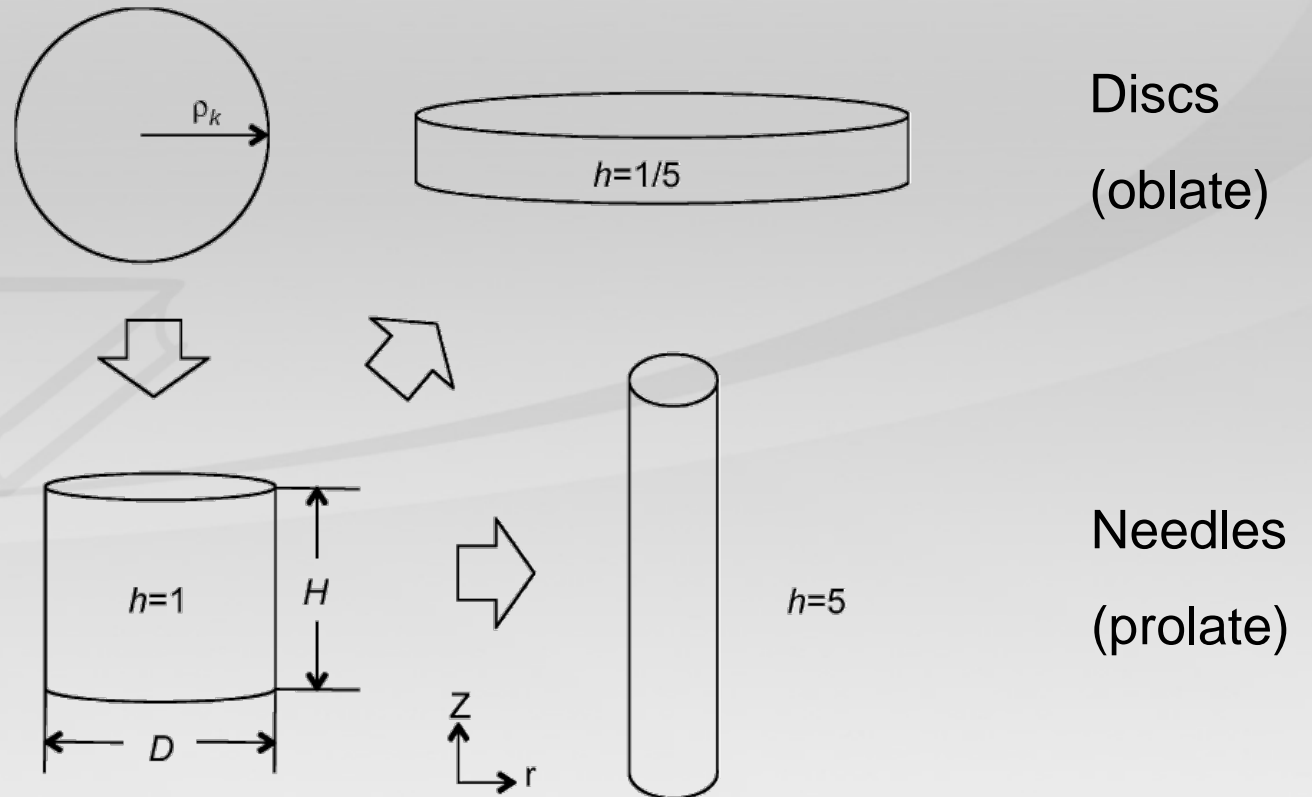


Fig. 1. Illustration of the shape parameter $h = H/D$.

Definition

Phase status ...

Phases ...

- BCC_A2
- BCC_A2#01
- BCC_A2#01_P0

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 1.0

Interfacial energy [J/m²]

- auto planar sharp interface from planar sharp ie
- interfacial energy size effect
- volume energy size effect
- diffuse interface effect

regular solution T_crit / K 0.0

Interface mobility [m⁴/Js] 1e100

Driving force model for growth size class based - SFFK

Create ... Remove

Help Cancel OK

Effects

- Shape modification → interface area changed

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

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

$$\text{For } h = 1 \rightarrow S_k = 1.1447 !$$

Effects

- Influence on Gibbs energy dissipation contributions Q

$Q_1 = \sum_k \frac{4\pi\rho_k^2 \dot{\rho}_k^2}{M_k^{IF}} K_k$	<p>Interface migration</p>	$K_k = 0.2912h^{2/3} + 0.5824h^{-1/3}$
$Q_2 = \sum_k \frac{4\pi RT \rho_k^5 \dot{c}_{k,i}^2}{45c_{k,i} D_{k,i}} I_k$	<p>Precipitate diffusion</p>	$I_k = 0.4239h^{4/3} + 0.6453h^{-2/3}$
$Q_3 = \sum_k \sum_i \frac{4\pi RT \rho_k^3 \left(\dot{\rho}_k (c_{k,i} - c_{0,i}) + \rho_k \dot{c}_{k,i} / 3 \right)^2}{c_{0,i} D_{0,i}} O_k$	<p>Matrix diffusion</p>	$O_k = 1.0692h^{2/3}$

Precipitate growth

- Evolution equations affected

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

$$Q = Q_1 + Q_2 + Q_3$$

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

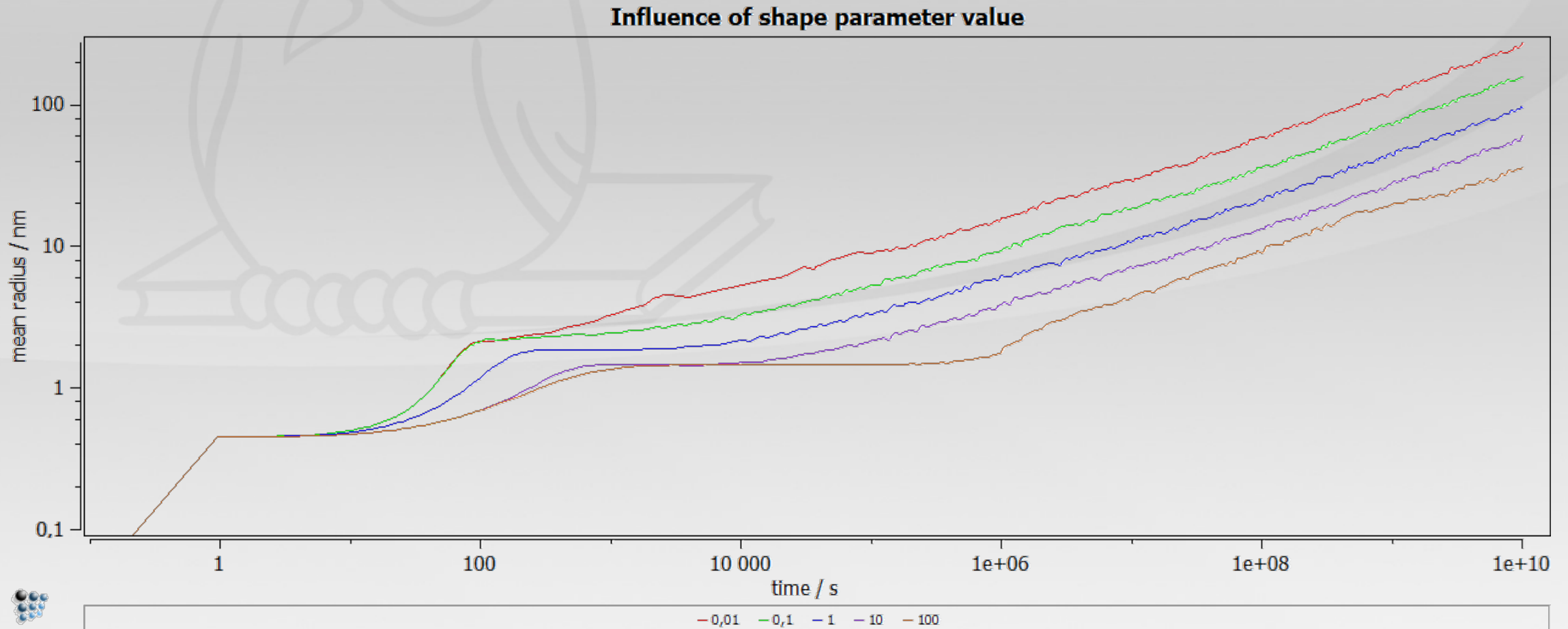
$$G = \sum_i N_{0,i} \mu_{0,i} + \sum_k \frac{4}{3} \pi \rho_k^3 \left(\lambda_k + \sum_i c_{k,i} \mu_{k,i} \right) + \sum_k 4\pi \gamma_k \rho_k^2 S_k$$

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

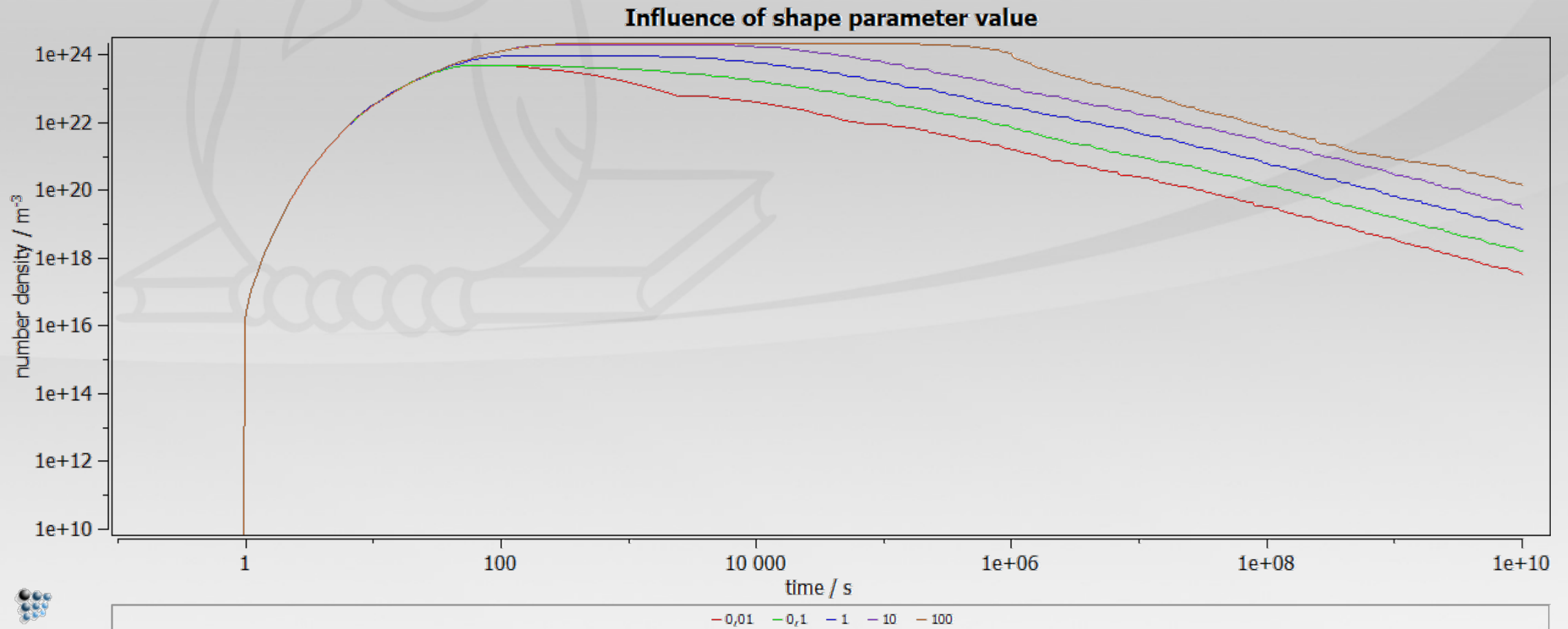
$$Q_2 = \sum_k \frac{4\pi RT \rho_k^5 \dot{c}_{k,i}^2}{45 c_{k,i} D_{k,i}} I_k$$

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

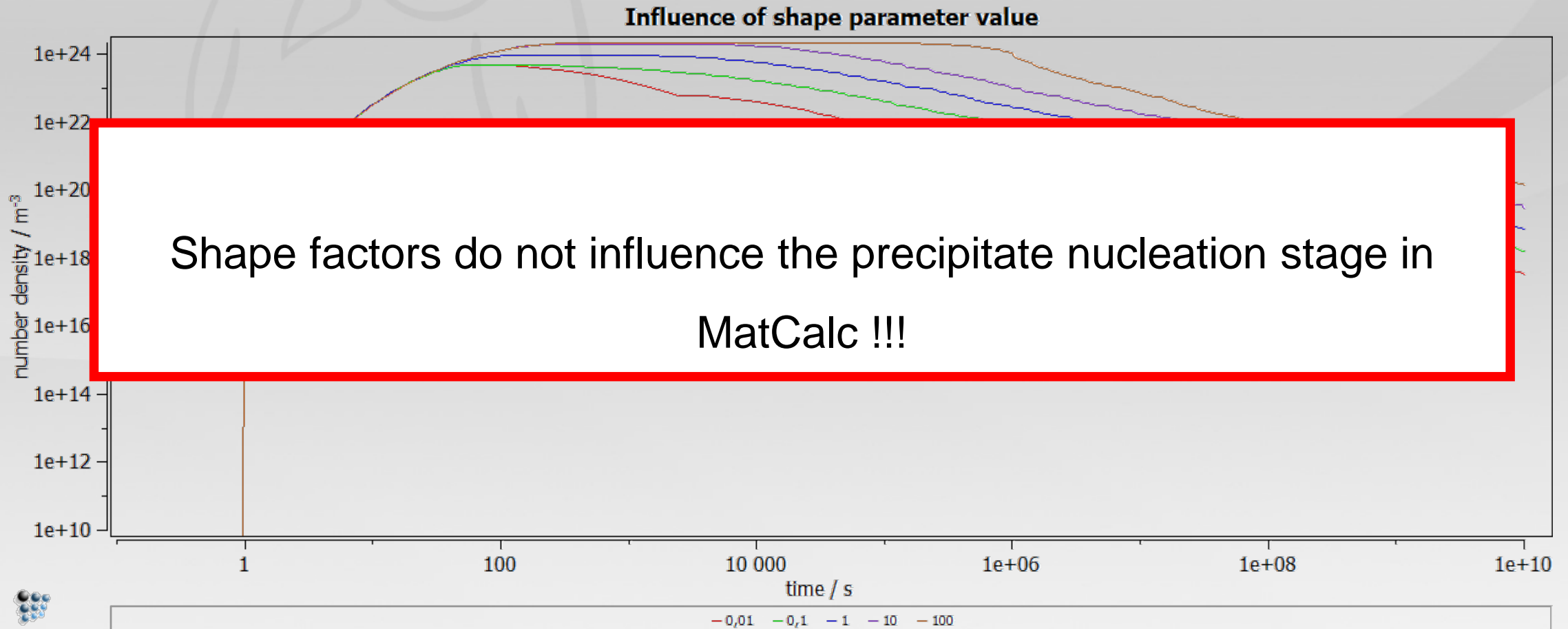
Precipitate growth



Precipitate growth



Precipitate growth



Precipitate growth

- Growth rates
(Anisotropy effects neglected!)
- Minimal diffusion distances for disc growth

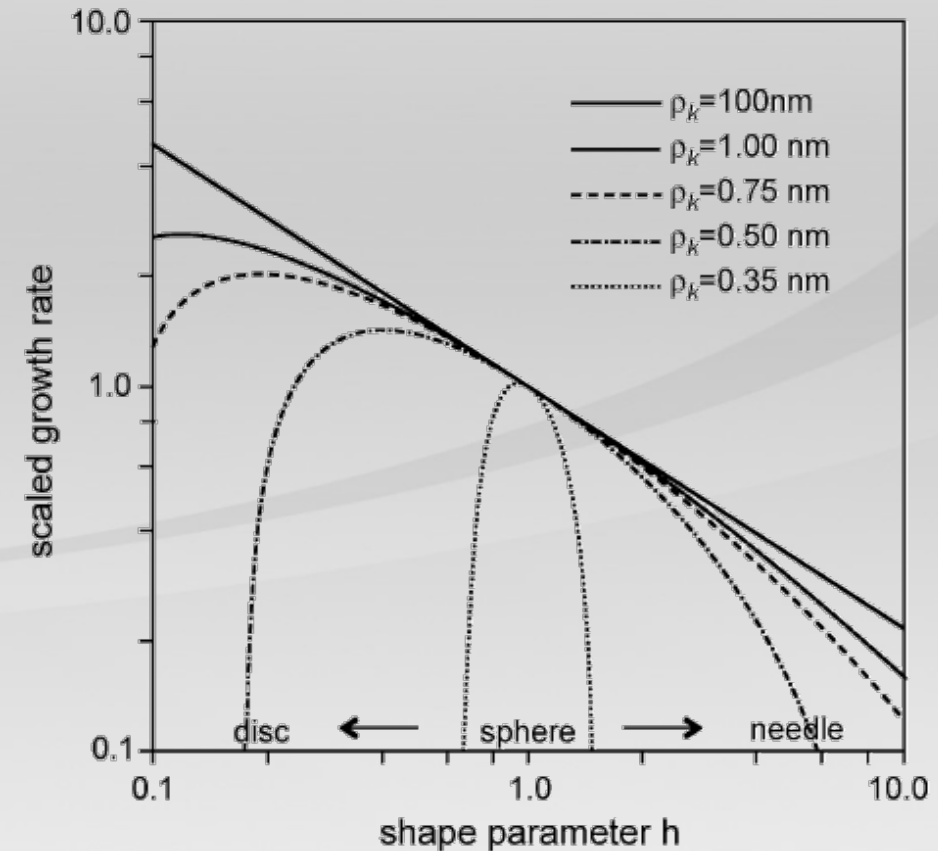


Fig. 3. Scaled growth rate as a function of the shape parameter $h = H/D$ and the equivalent precipitate radius ρ_k .

Precipitation strengthening

- Surface-surface precipitate distance

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

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

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

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

Precipitation strengthening

- Surface-surface precipitate distance

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

$$L_p = KL_{sph}$$

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

τ - Shear stress

L_p - Distance between the precipitates

L_{sph} - Distance between the spherical precipitates

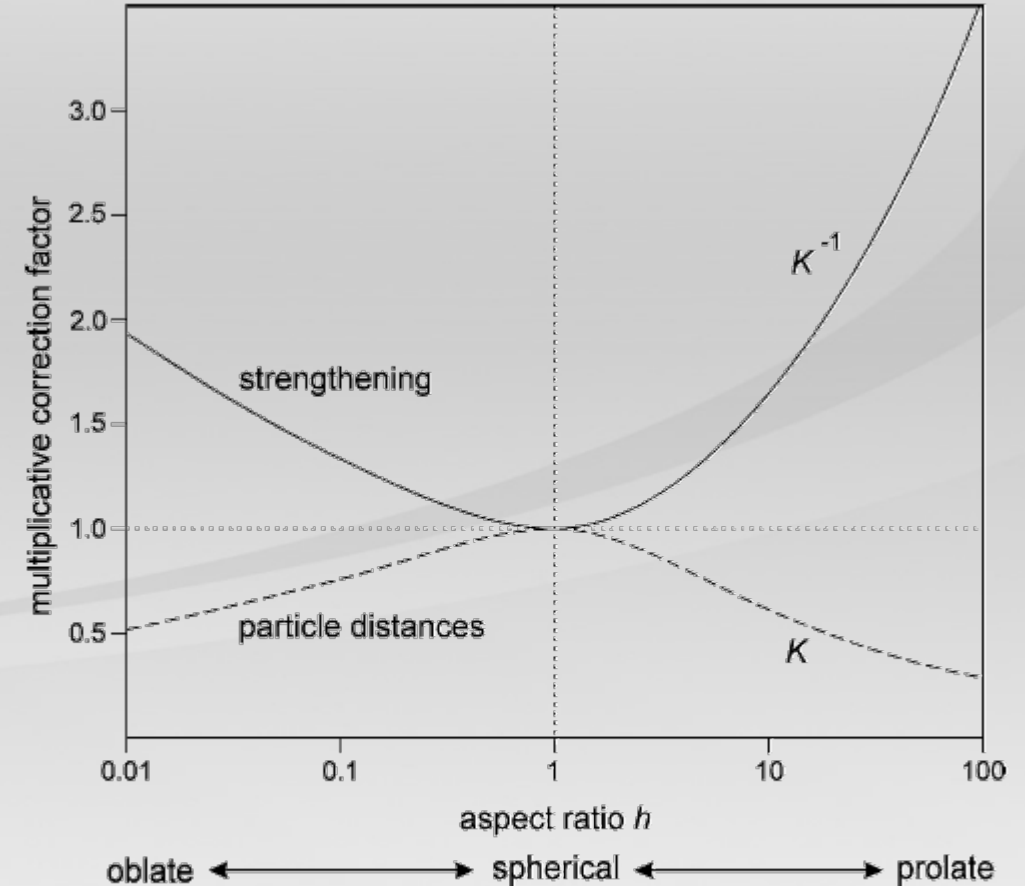


Figure 2. Variation in particle distances and strengthening for prolate and oblate precipitates relative to spherical particles.

Precipitation strengthening

- Equivalent radius - Shearable precipitate

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

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

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

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

$r_{eq,edge}$ - 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.

Precipitation strengthening

- Equivalent radius - Shearable precipitate

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

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

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

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

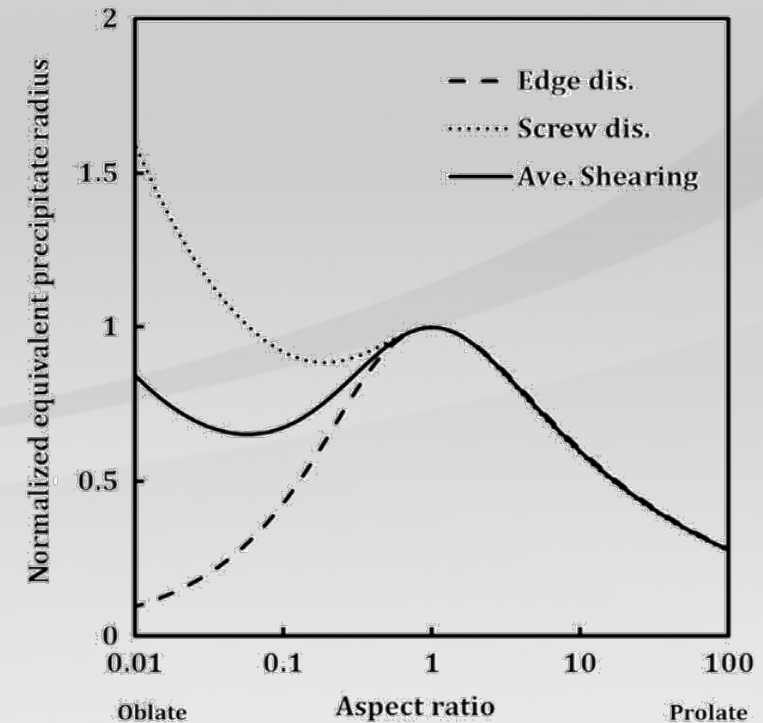


Fig. 3. Normalized equivalent precipitate radius for edge and screw dislocations in the shearing mechanism.

Precipitation strengthening

- Outer cut-off radius – Orowan mechanism

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

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

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

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

$R_{eq,edge}$ - 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.

Precipitation strengthening

- Outer cut-off radius – Orowan mechanism

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

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

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

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

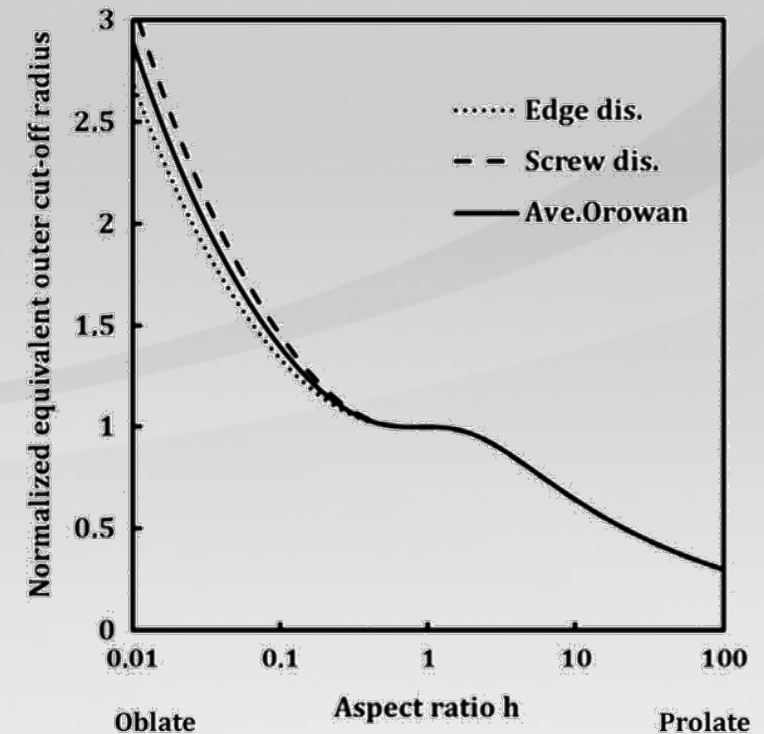


Fig. 4. Normalized equivalent outer cut-off radius for edge and screw dislocations for the non-shearing mechanism.

Precipitation strengthening

- Dislocation characterization

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

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

