Macro-, Micro-, and Nanoscale Structures - how to model in a correct manner within Continuum Mechanics

Holm Altenbach

Otto-von-Guericke University Magdeburg, Germany

Institute of Mathematics
Sibirian Federal University
Krasnoyarsk, Russian Federation

OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG

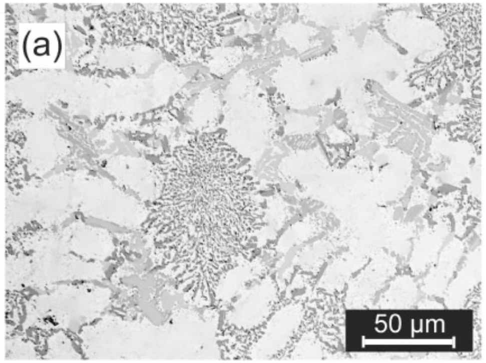
MB FAKULTÄT FÜR MASCHINENBAU

IFME

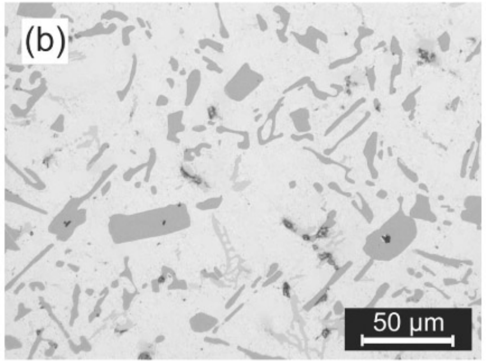
DFG - Graduiertenkolleg
Micro-Macro-Interactions
of Structured Media and Particle Systems

Sr-modified Alloy

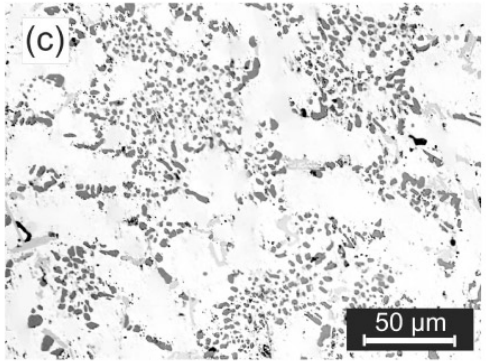
Microstructure (light microscope observation)



M-F alloy (a)



UM-T6 alloy (b)



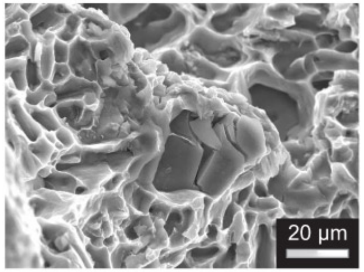
M-T6 alloy (c)

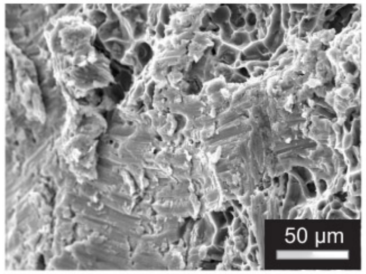
Ultimate tensile strength (UTS), yield strength (YS), and ultimate elongation (UE) for investigated alloys

Alloy code	at 20^0C			at 300^0C		
	YS, MPa	UTS, MPa	UE, %	YS, MPa	UTS, MPa	UE, %
M-F	132	208	1.0	99	110	5.6
UM-T6	350	358	0.3	136	149	2.9
M-T6	341	363	0.8	138	143	4.8

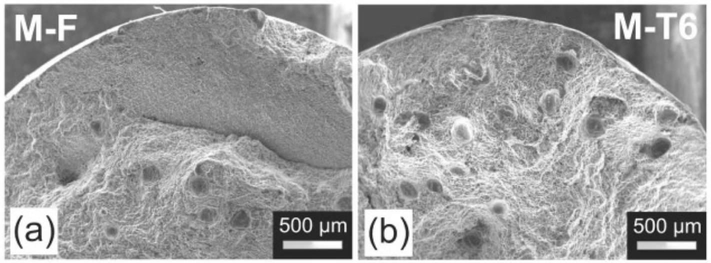
Fractography

UM-T6 alloy

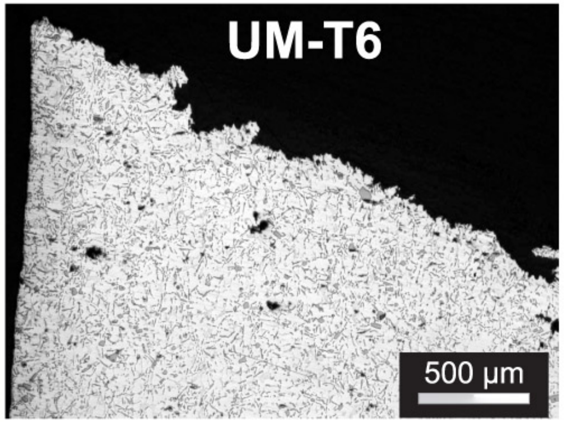


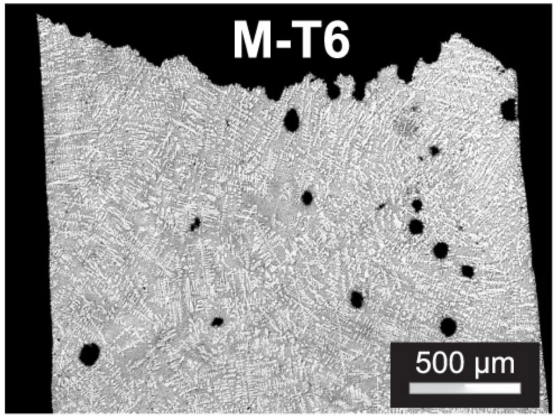


M-F (a) and M-T6 (b) alloys

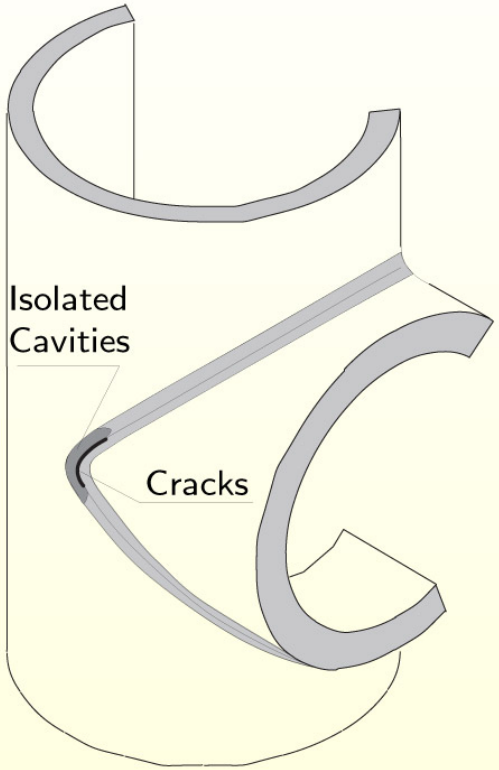


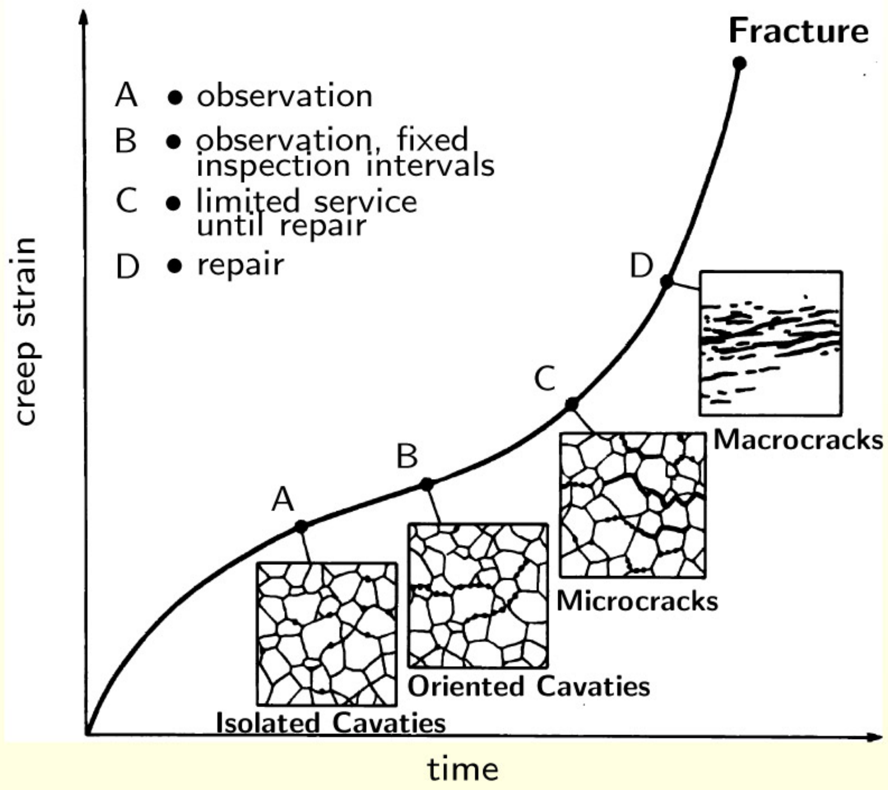
Longitudinal section





Welded Structure and Life Cycle



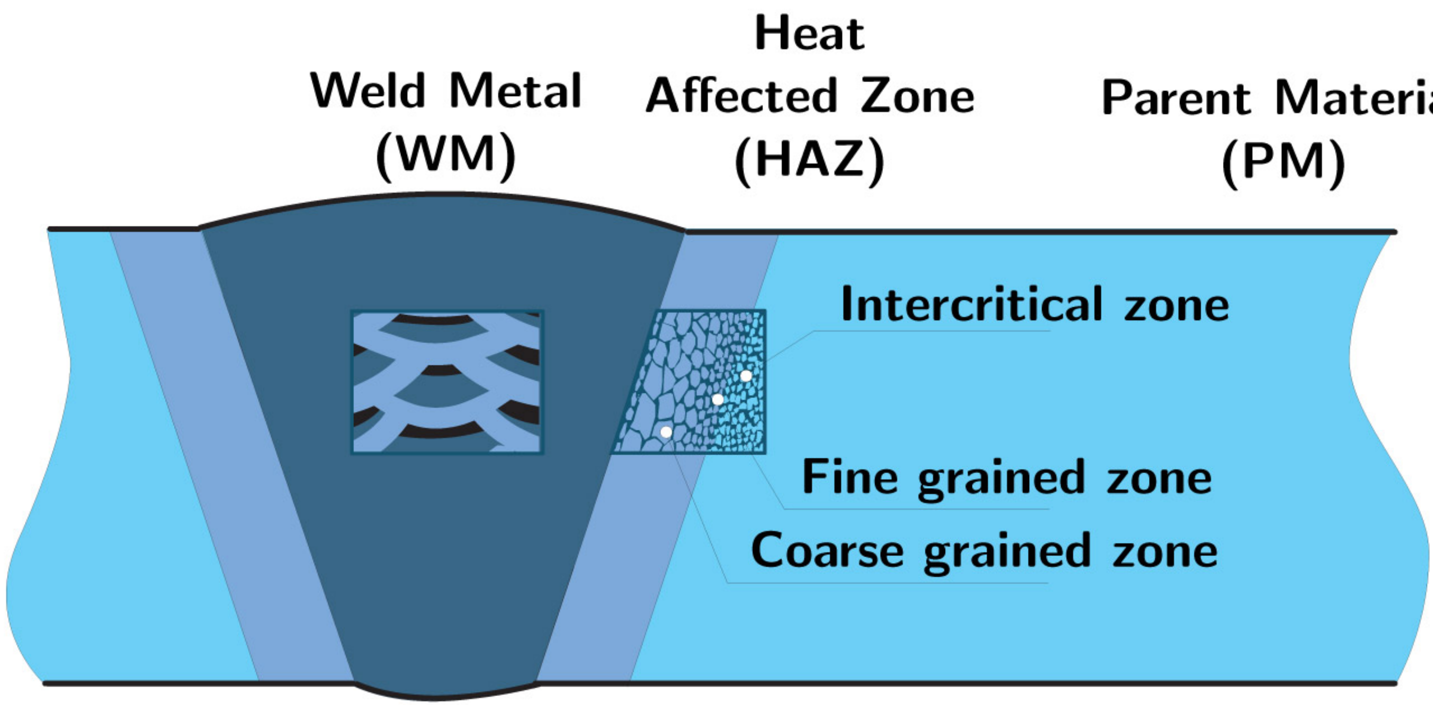


Residual life assessment in a weld region (after *Cella & Fossati*, 1992)

Classification of creep damage and corresponding action (after *Neubauer & Wedel*, 1983)

Microstructure of Welds

after *Easterling* (1992), *Hyde et al.* (2003), *Wohlfahrt et al.* (2001)

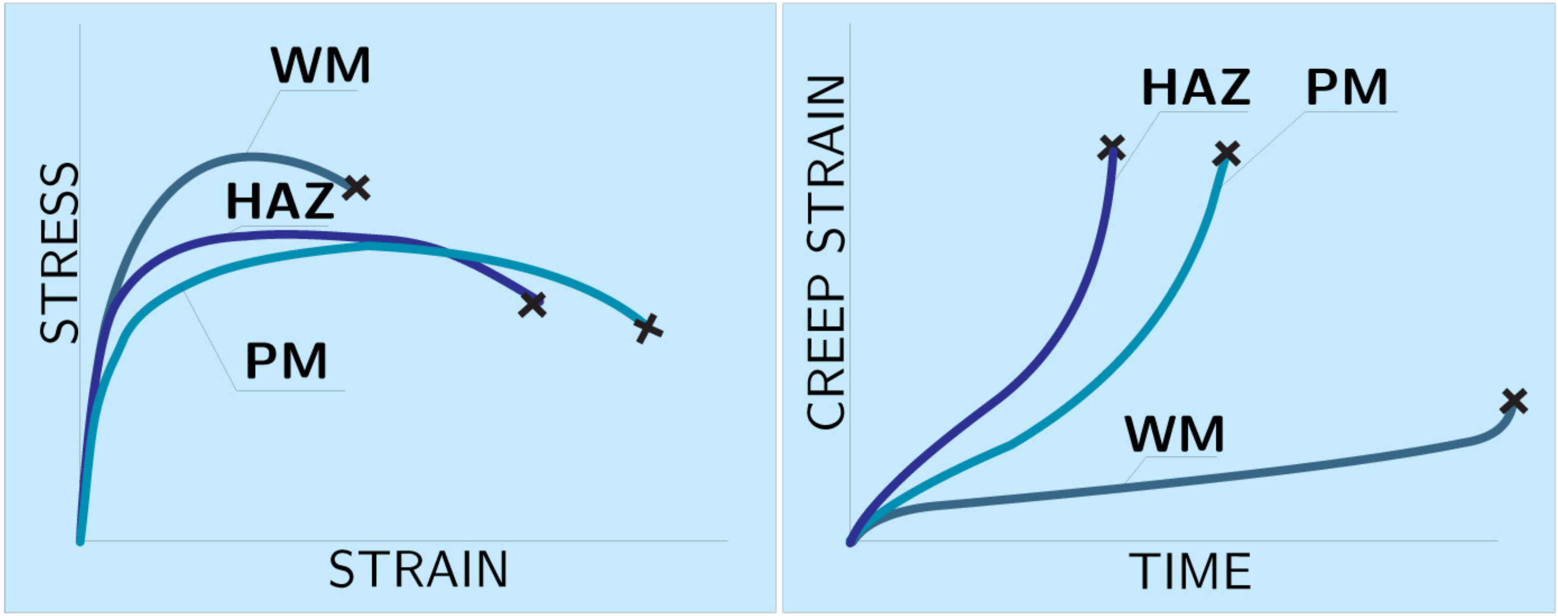


Creep Behavior

after *Easterling* (1992), *Hyde et al.* (2003), *Wohlfahrt et al.* (2001)

Stress-strain behavior
(room temperature)

Creep behavior
($T = 0.5 - 0.7\,T_m$)

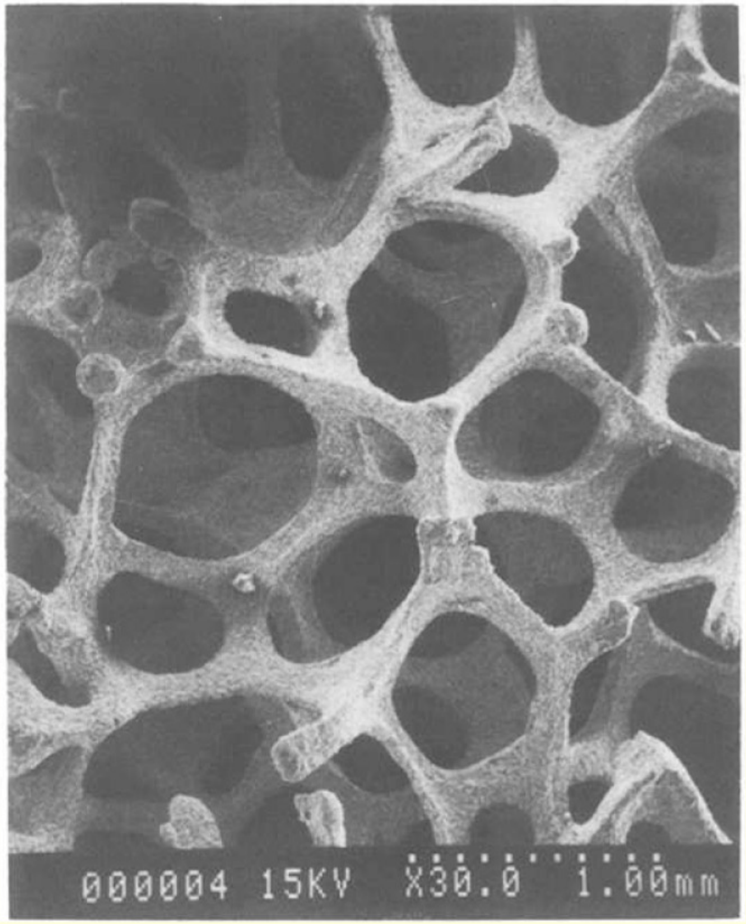


Foams as Nonhomogeneous Materials

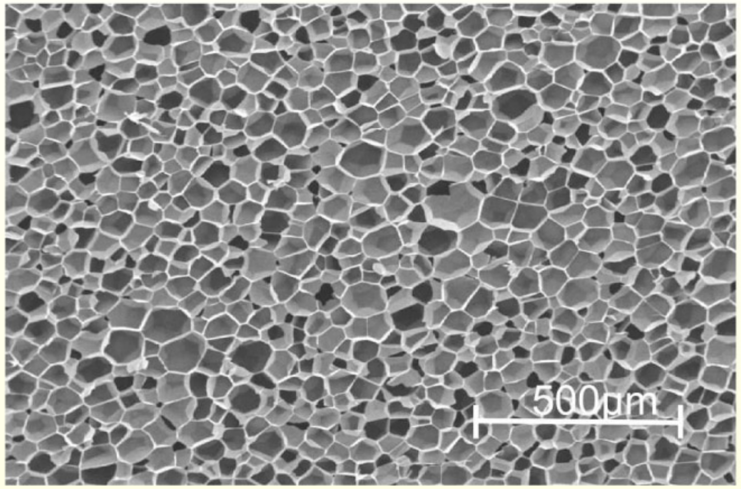
- All materials show a more or less significant microstructure. In many cases the microstructure can be ignored in problems of structural mechanics.
- In the case of foams or porous materials the microstructure must be taken into account. For the first analysis of the microstructure properties can be averaged, e.g. introducing distribution laws.
- Engineering structures made of **foams**, have been used in different applications.[1] **Polymer foam** is a cellular structure consisting of a solid polymer, for example polyurethane, etc., containing a large volume fraction of gas-filled pores. The defining property is the **very high porosity**: typically well over 80%, 90% and even 98% of the volume consists of void spaces.

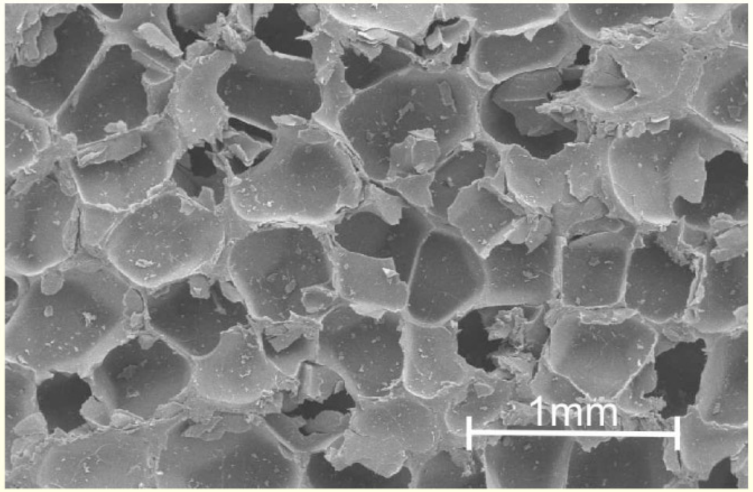
[1] Gibson L J, Ashby M F (1997) Cellular Solids: Structure and Properties; Mills N (2007) Polymer Foams Handbook Engineering and Biomechanics Applications and Design Guide

Copper Foams



Closed-cell Foams[2]

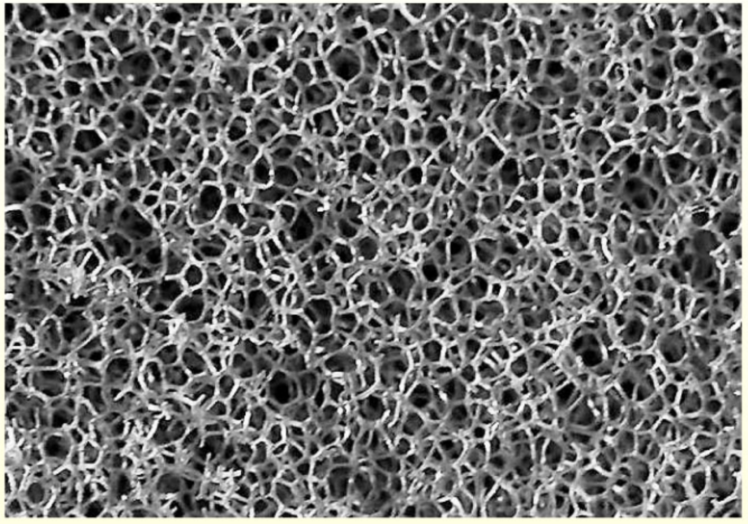


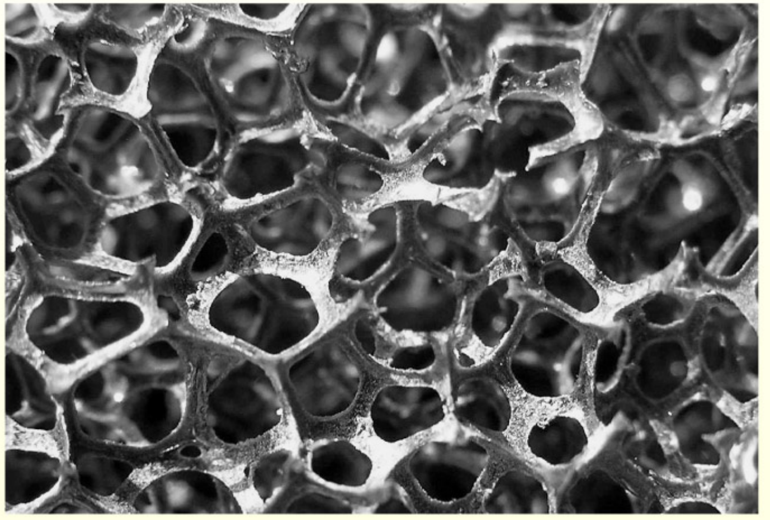


Closed-cell polymeric foams with various densities

[2]Kraatz (2007), DKI, Darmstadt, Germany

Open-cell Foams

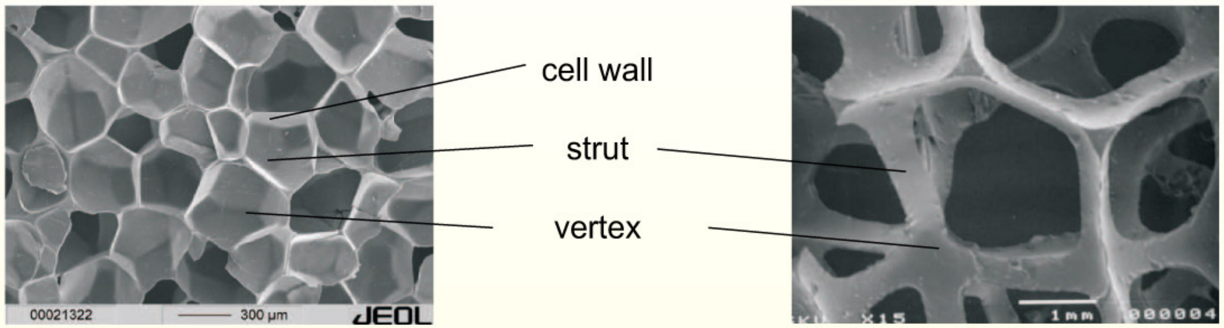




Open-cell foams with various densities

Open and Closed Cell Foams

closed cell foam **open cell foam**

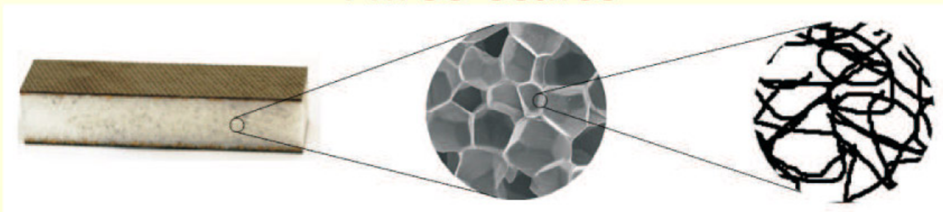


Rohacell 51WF; IWMH

open cell PU-foam; Mills2000

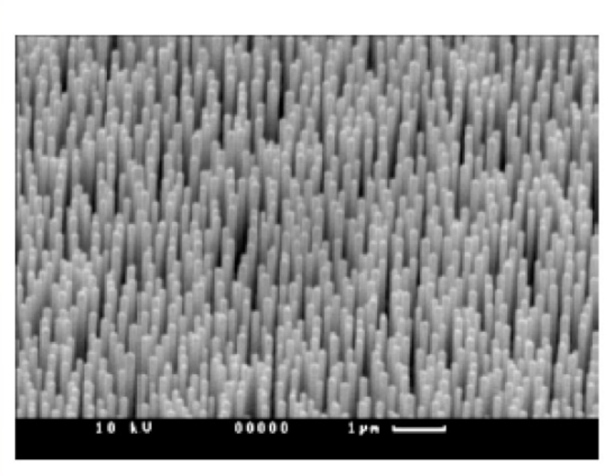
- investigation via microscopy,
- X-ray-tomography,
- geometrical properties in a statistical distribution

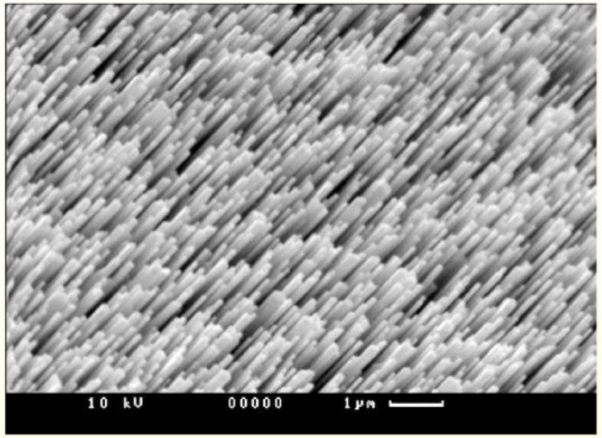
Three scales

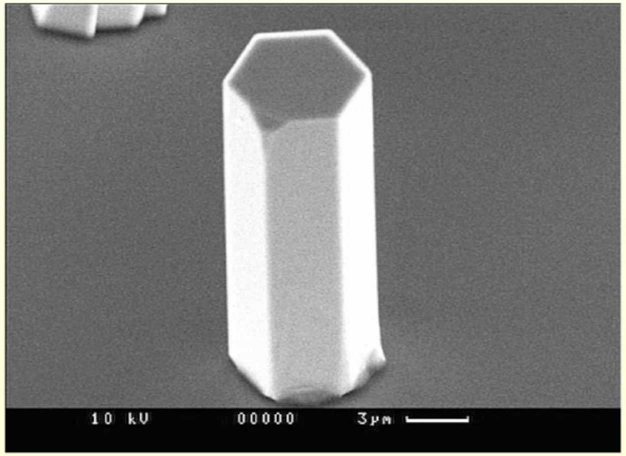


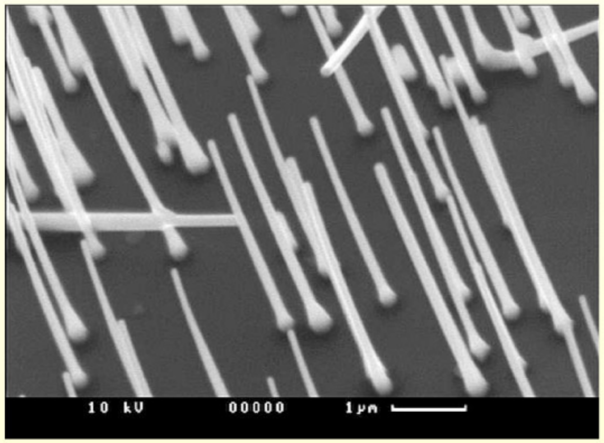
Macroscale Mesoscale Microscale

Nanostructures

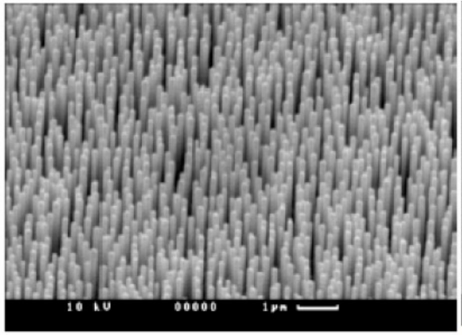


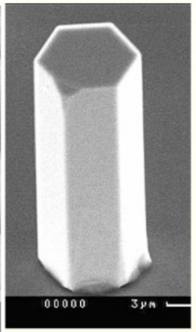


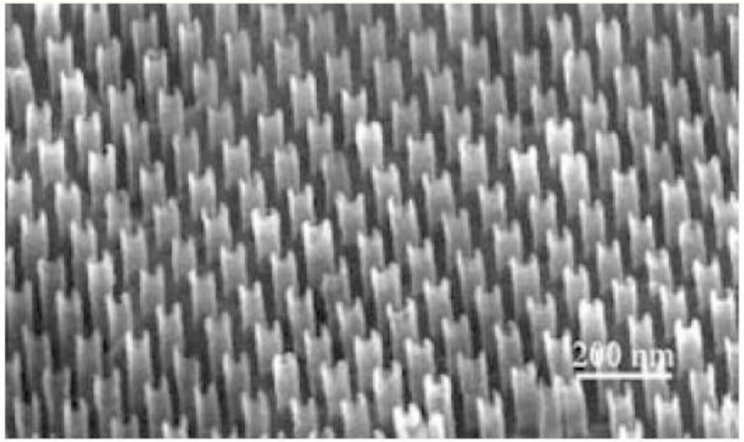


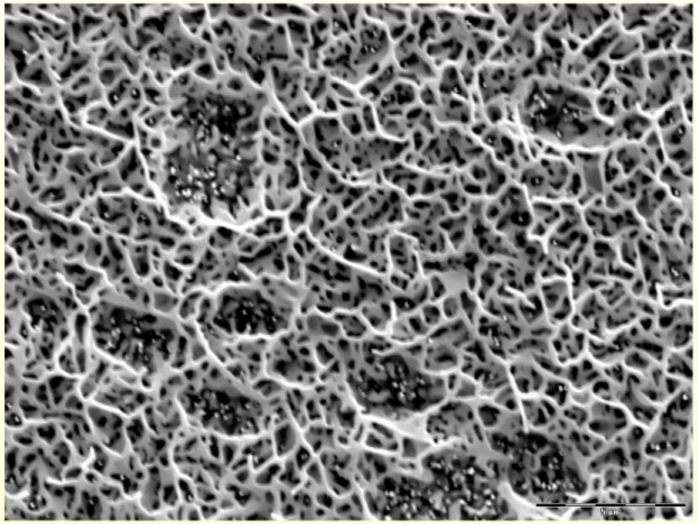
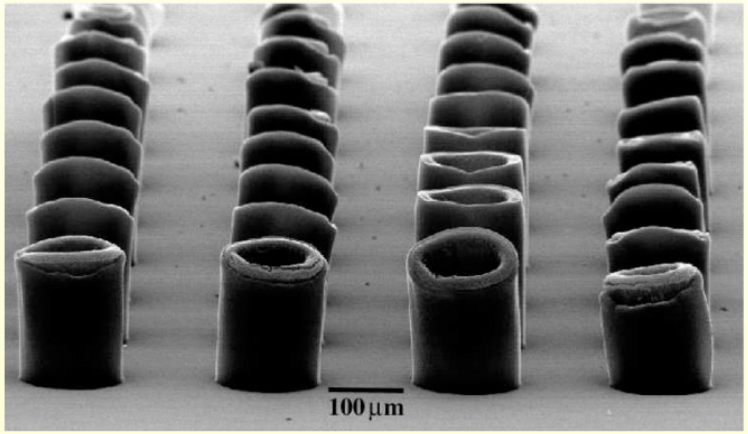


Nanostructures



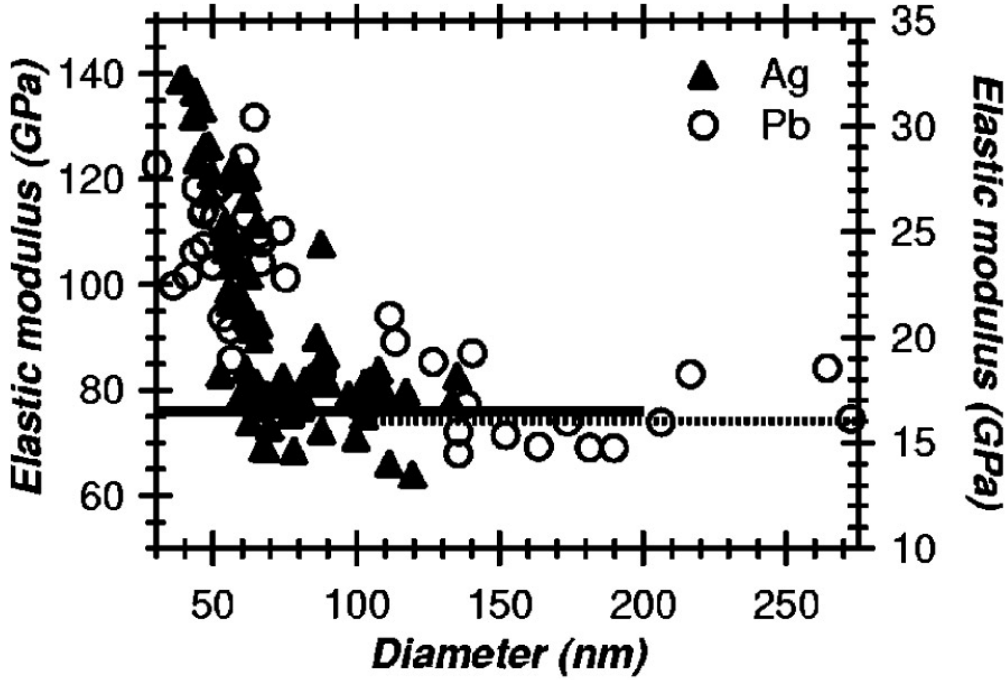




Nano-scale Structure Behavior - Size Dependent[3]

Young's Modulus vs. Nanowire Diameter



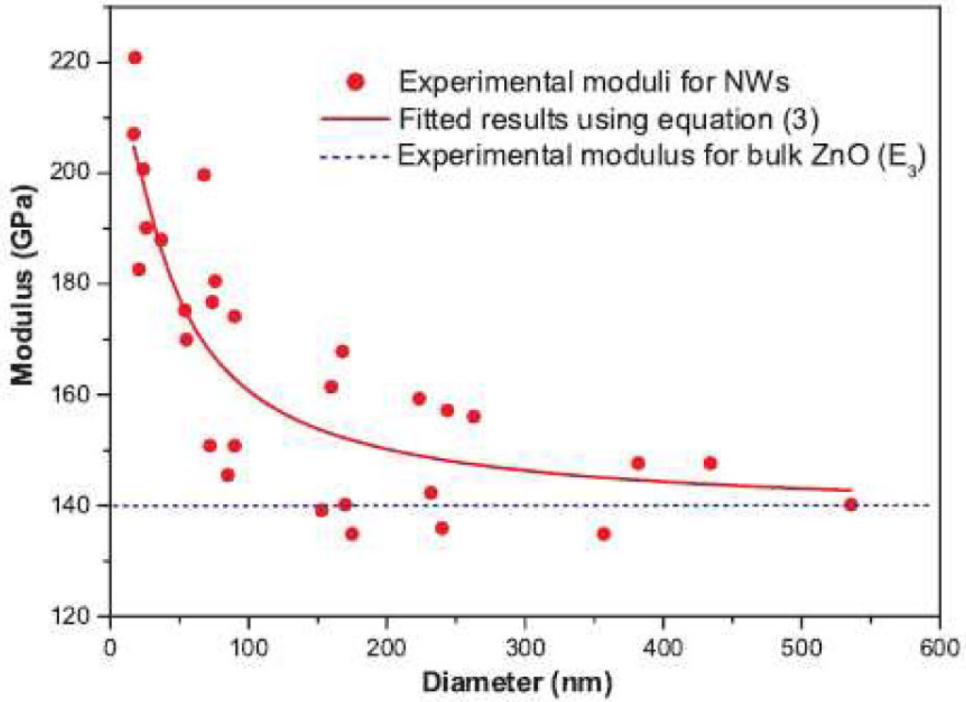
solid line - elastic modulus of bulk silver
dotted line - elastic modulus of bulk lead

[3] S. Cuenot, Physical Review B **69**(2004) 165410 1-5

Experimental Observations

Surface stresses → size effect

Young's modulus, experimental data: eigenfrequencies of nanowires[a]



[a] Chen et al. (2006)

Qualitative Microstructure Prediction

Aim of the modeling

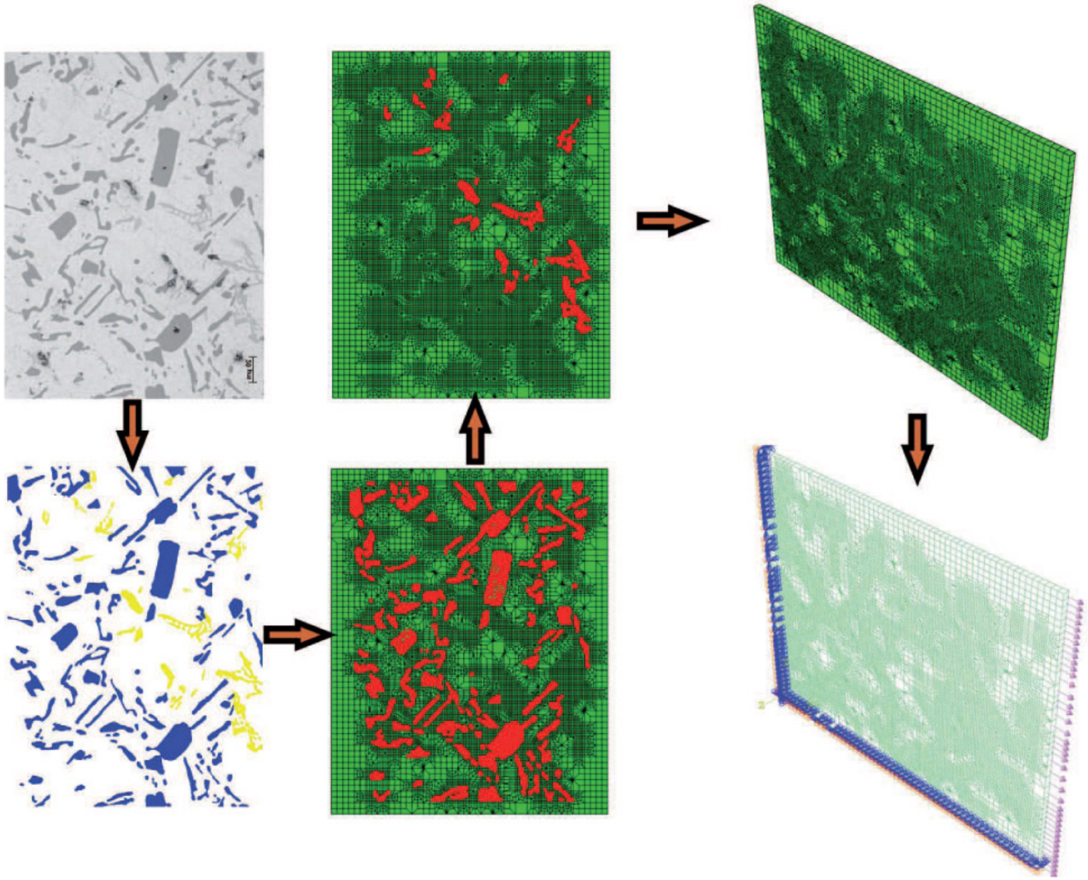
Investigation of the influence of the hard phases and the morphology of silicon on the behavior of the primary material in the original (RT6) and the improved (MT6) state wit the help of micrographs.

Preliminary steps

1. Image analysis using the software *ImageJ*.
2. Image improvement and color coding of the phases using the software *CorelDraw*
3. Image input and FE meshing using of the software *OOF2*
4. Input in the FE software *ABAQUS*
5. Extrusion of the elements for threedimensional model
6. Prescription of the boundary conditions

FE-Modeling

FE model from the RT6 microstructure



FE-Modeling

Material Parameters

		aluminium	intermetallic	silicon
surface fraction/volume fraction [%]	MT6 RT6	85,4 85,7	2,6 2,3	12 12
thermal expansion coefficient	α [K^{-1}]	$2,77 \cdot 10^{-5}$	$1,16 \cdot 10^{-5}$	$0,38 \cdot 10^{-5}$
elastic properties	E [GPa] ν	55 0,34	140 0,31	103 0,215
inelastic properties	$\dot{\varepsilon}^{cr}_{eq} = a\sigma^n_{eq}$	$a = 3,3 \cdot 10^{-7}$ [MPa^{-n}/h] $n = 5$	—	—

Loading Parameters

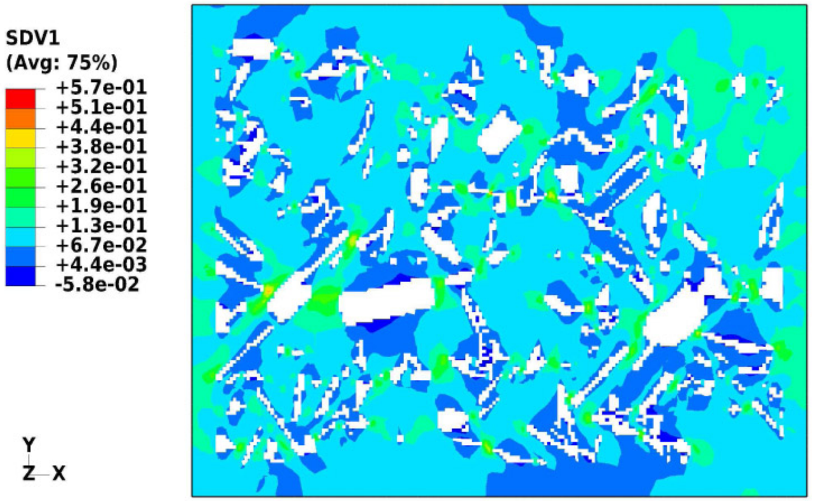
- heating $T_1 = 20^\circ$C; $T_2 = 300^\circ$C
- monotonic creep $\sigma = 10$ MPa
- cyclic creep $\sigma_{max} = 10$ MPa

Modell Parameters

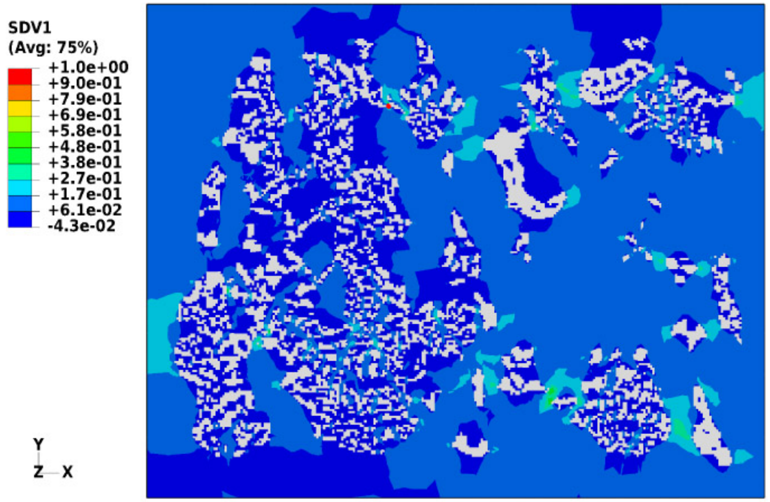
- size 0.295 mm $\times$ 0.236 mm
- hexaedric element C3D8
- number of elements
  16034 – RT6, 19662 – MT6

Results of the FE-Modeling. Monotonic creep

Distribution of the inelastic strain $\varepsilon_{xx}^{\text{in}}$ (SDV1; [m/m]) at static creep



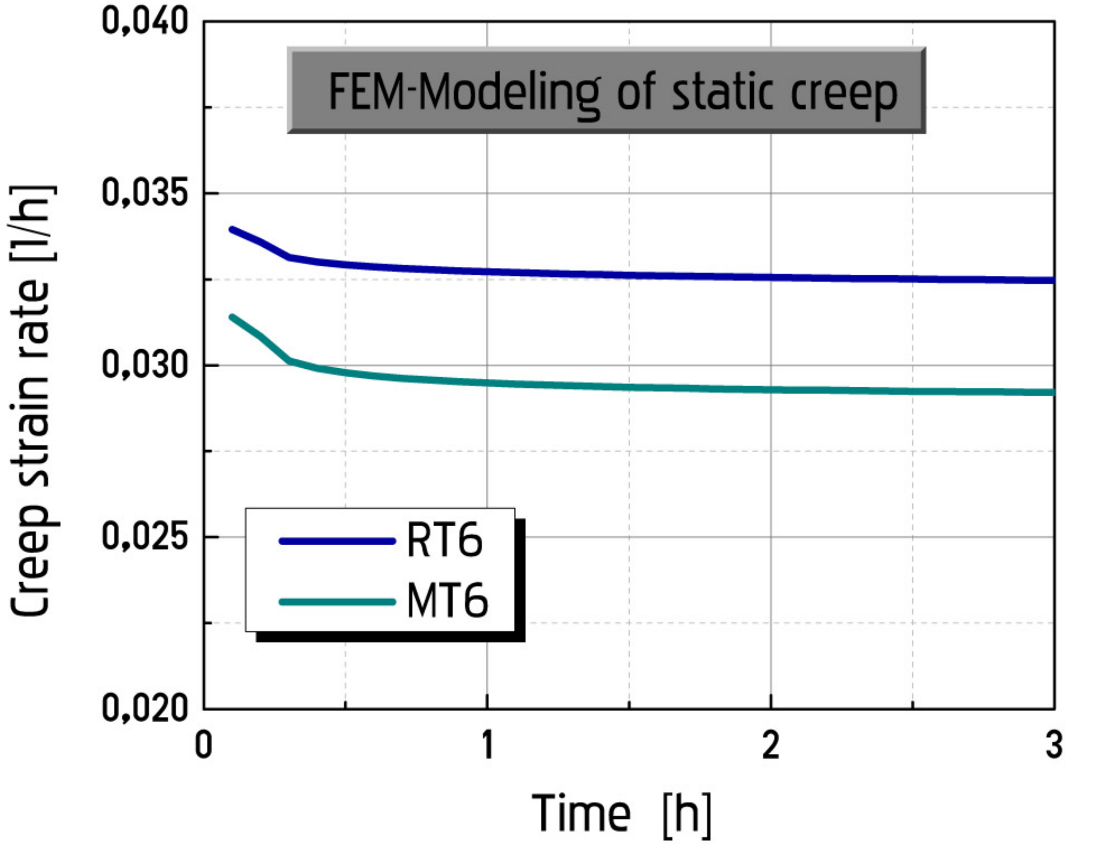
Material RT6



Material MT6

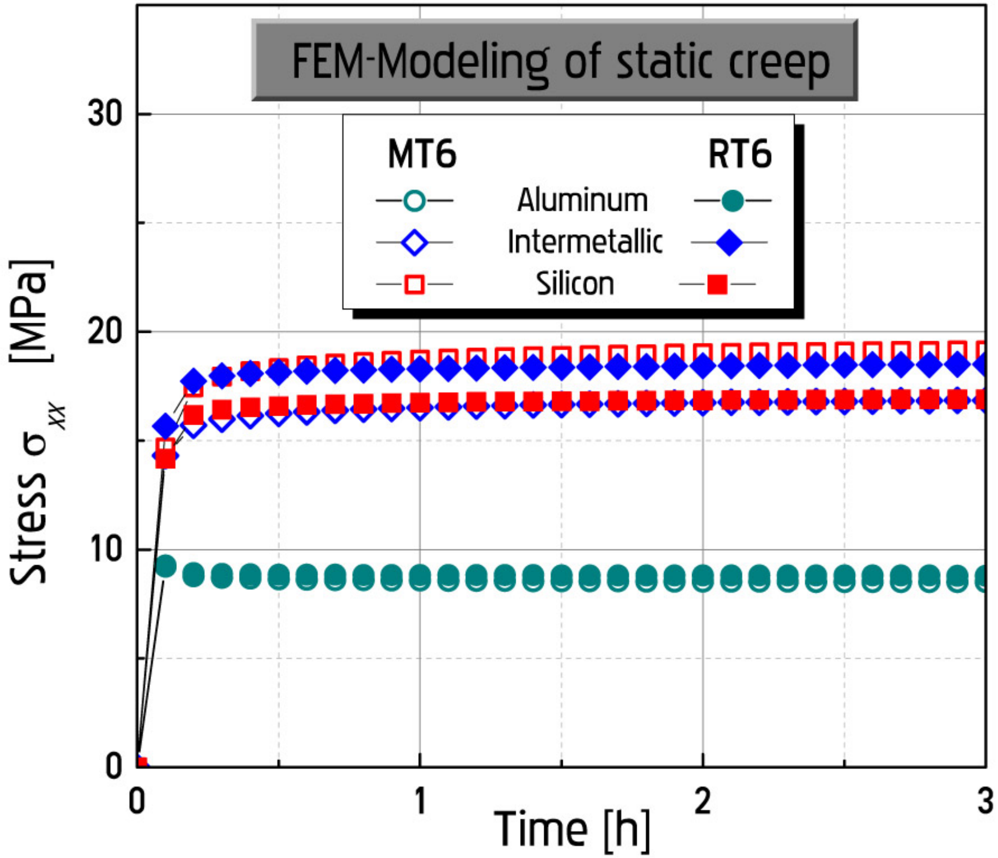
Results of the FE-Modeling. Monotonic creep

Creep Strain ε_{xx}^{in} for Aluminium



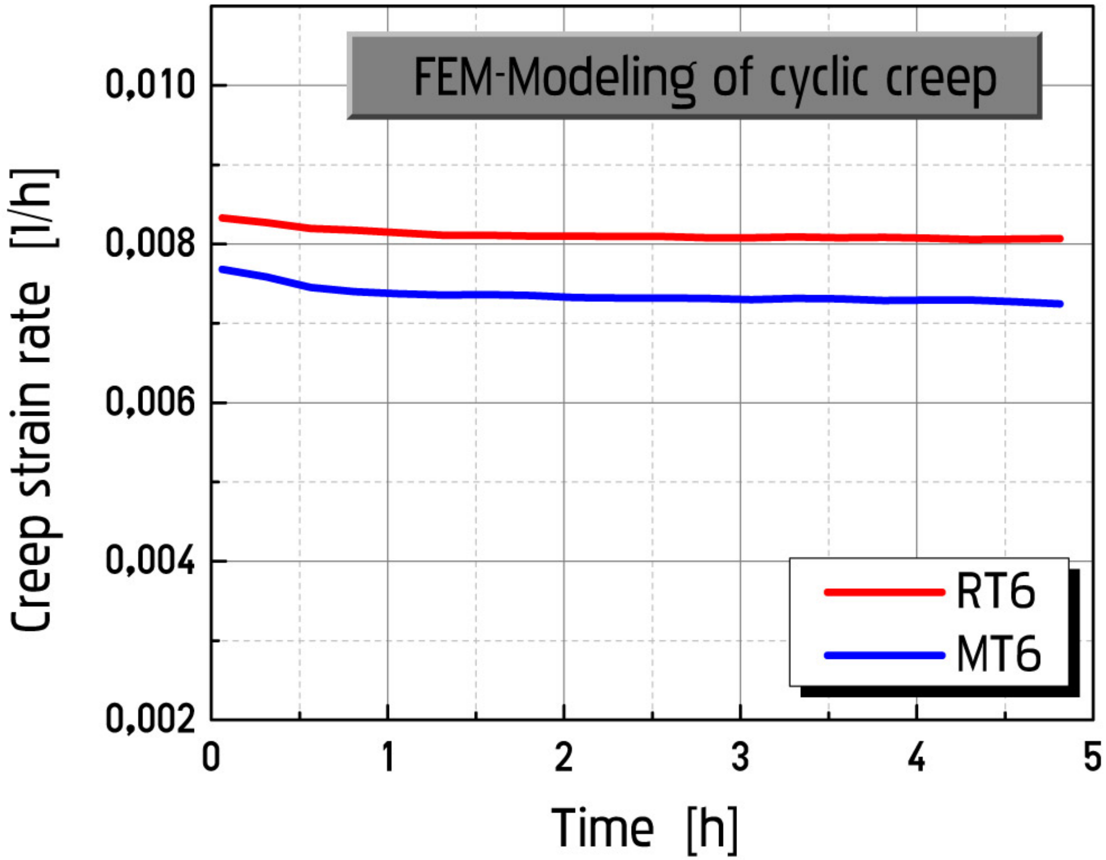
Results of the FE-Modeling. Monotonic creep

Averaged Stress Values σ_{xx} in the Constituents



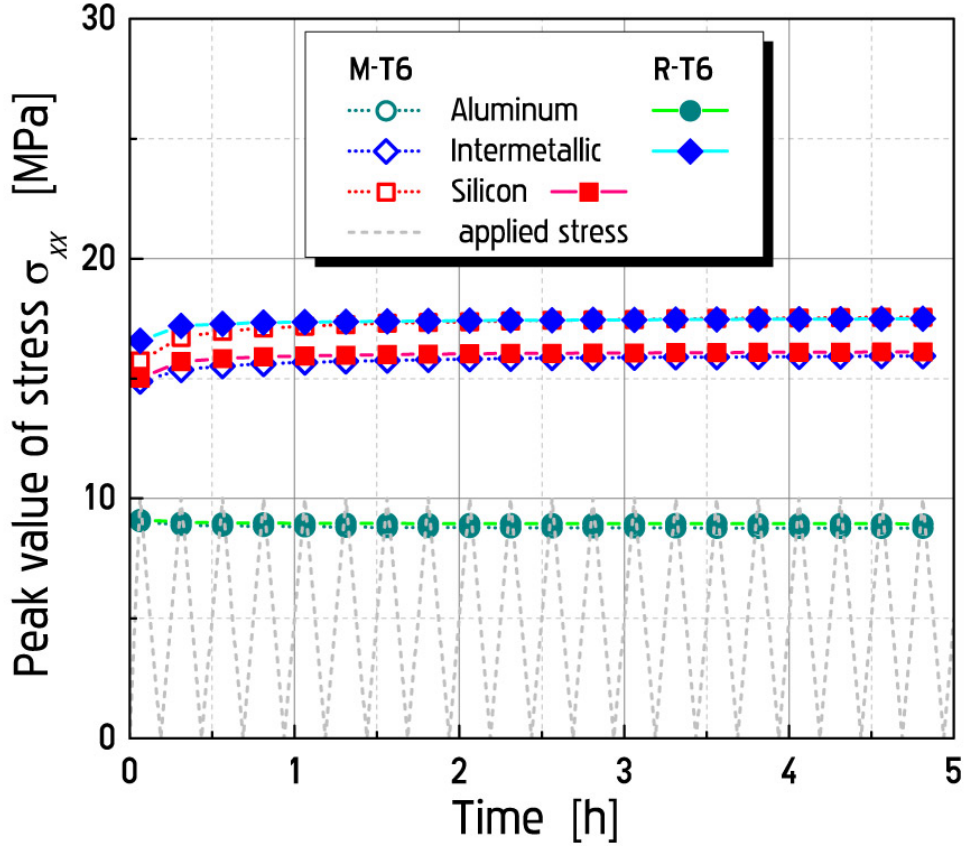
Results of the FE-Modeling. Cyclic creep

Maximum Creep Strain Rate $\varepsilon_{xx}^{\mathrm{in}}$ of Aluminium



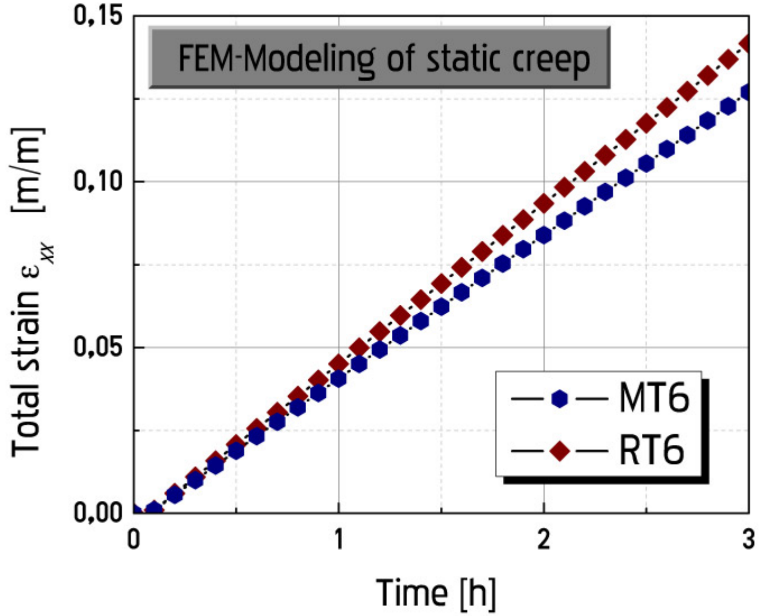
Results of the FE-Modeling. Cyclic creep

Averaged Stress Values σ_{xx} in the Constituents

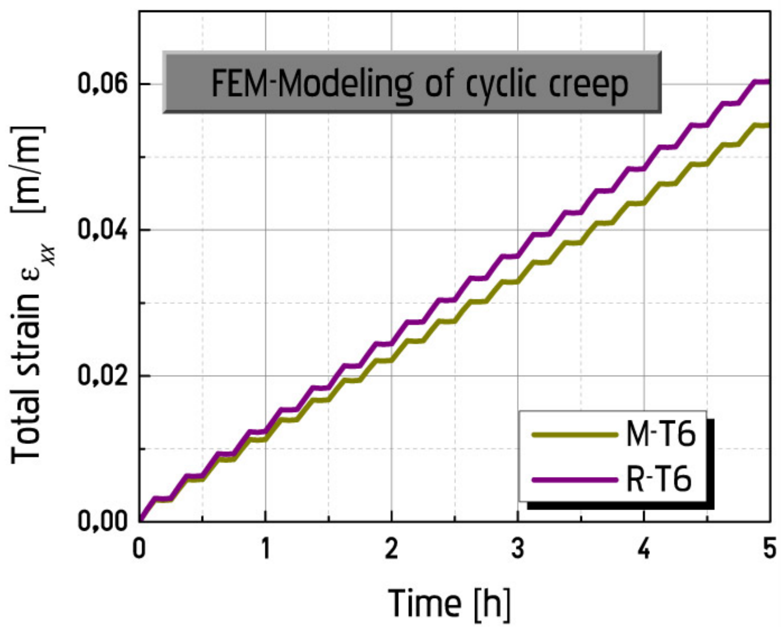


Results of the FE-Modeling. Static & Cyclic Creep

Averaged Values ε_{xx}

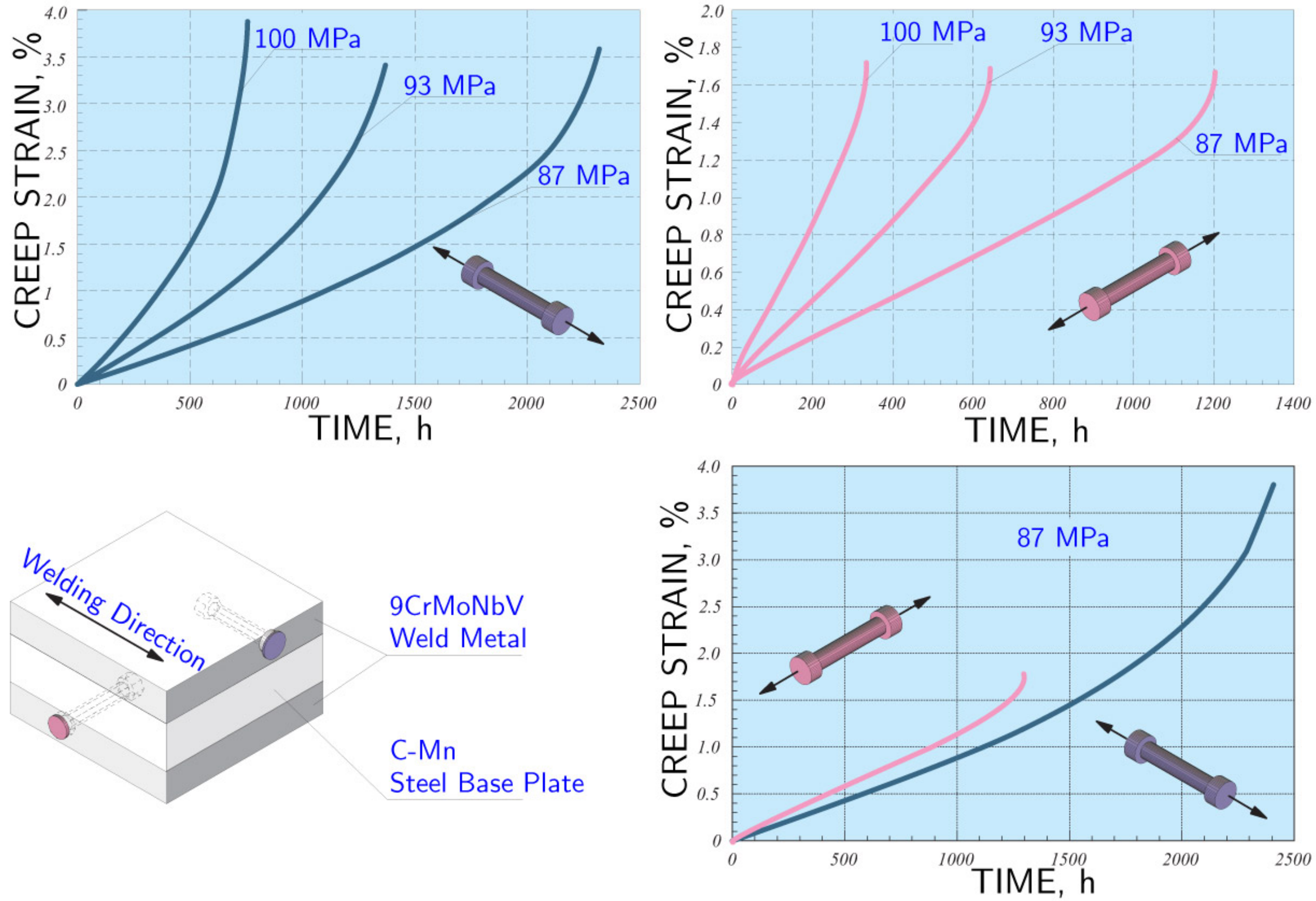


Averaged Values ε_{xx}



Creep Behavior of a Weld Metal

9CrMoNbV (P91) at 650° C (after Hyde et al., 2003)

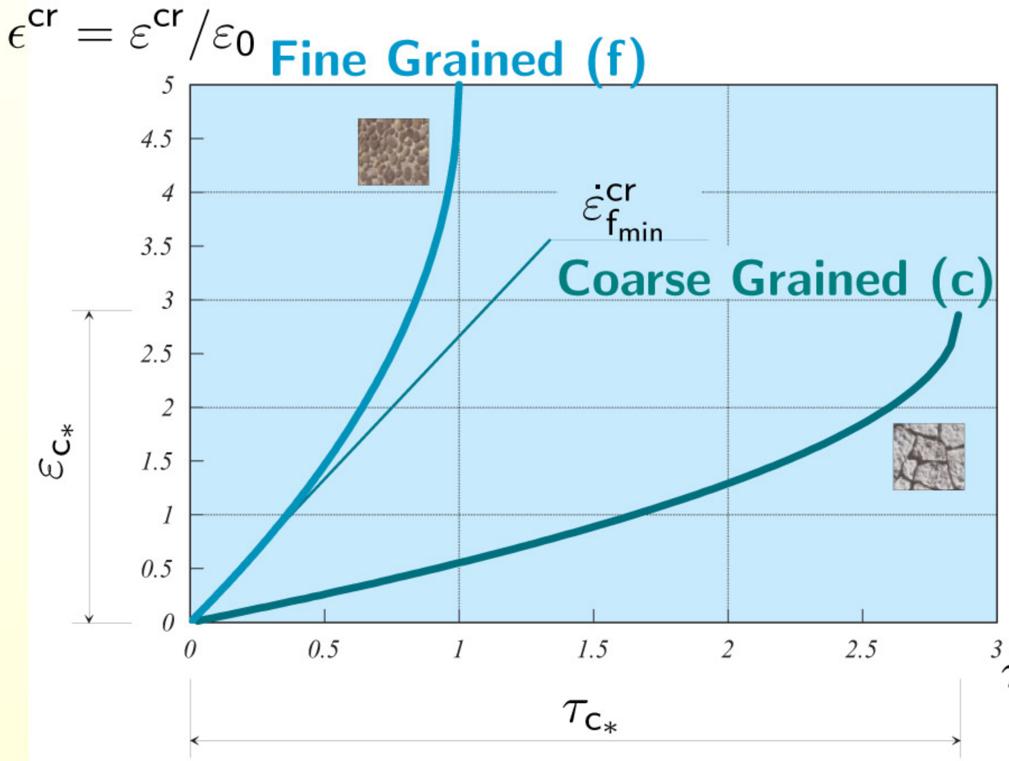


Creep Behavior of Constituents (I)

Experimental data (grain size influence)

Kowalewski (1992), Wohlfahrt & Brinkmann (2001), Matsui et al. (2001), Wu et al. (2004)

$$
\left\{
\begin{aligned}
\dot{\varepsilon}^{\mathrm{cr}} &= \frac{a\sigma^{n}}{(1-\omega)^{n}} \\
\dot{\omega} &= \frac{b\sigma^{k}}{(1-\omega)^{l}}
\end{aligned}
\right.
$$



$$\ln \dot{\varepsilon}^{\mathrm{cr}}_{\mathrm{min}} = \ln a + n \ln \sigma$$

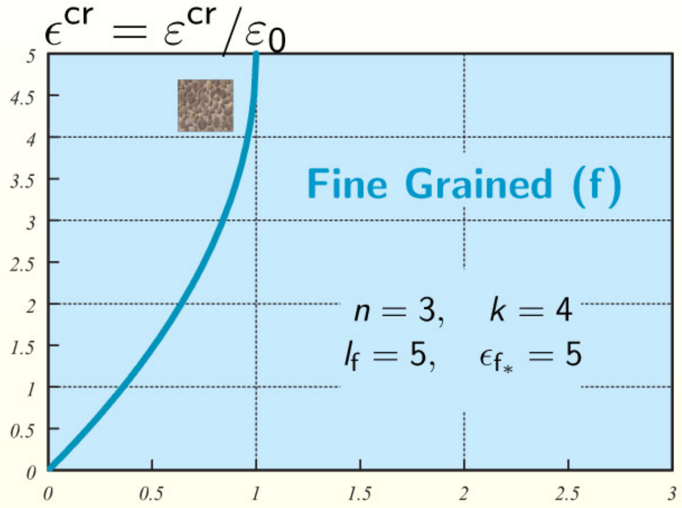
$$t_* = \frac{1}{(l+1)b\sigma^{k}}$$

$$\varepsilon^{\mathrm{cr}}_{*} = \frac{a\sigma^{n-k}}{b(l+1-n)}$$

Leckie & Hayhurst, (1977)

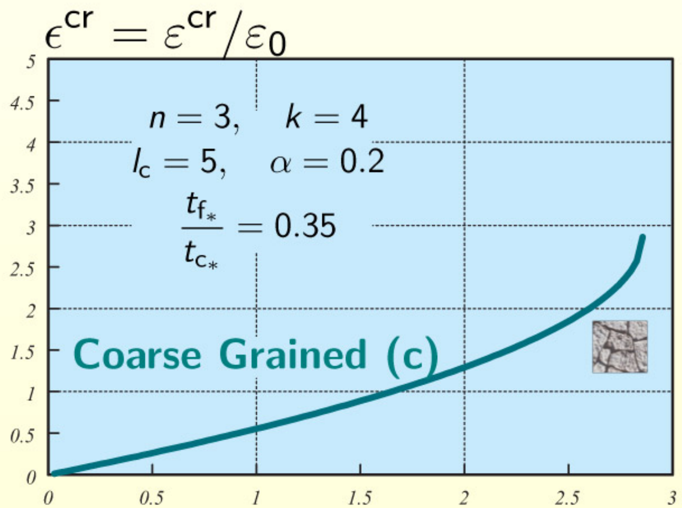
$\tau = t/t_{\mathrm{f}_*}$

Creep Behavior of Constituents (II)



$$\begin{cases} \dfrac{d}{d\tau}\epsilon_f^{cr} = \epsilon_{f_*}\left(1 - \dfrac{n}{l_f + 1}\right)\left(\dfrac{\tilde{\sigma}}{1 - \omega_f}\right)^n \\ \dfrac{d}{d\tau}\omega_f = \dfrac{1}{l_f + 1}\dfrac{\tilde{\sigma}^k}{(1 - \omega_f)^{l_f}} \end{cases}$$

$$\tilde{\sigma} = \frac{\sigma}{\sigma_0}, \qquad \varepsilon_0 = \frac{\sigma_0}{E}$$



$$\begin{cases} \dfrac{d}{d\tau}\epsilon_c^{cr} = \alpha\epsilon_{f_*}\left(1 - \dfrac{n}{l_f + 1}\right)\left(\dfrac{\tilde{\sigma}}{1 - \omega_c}\right)^n \\ \dfrac{d}{d\tau}\omega_c = \beta\dfrac{1}{l_f + 1}\dfrac{\tilde{\sigma}^k}{(1 - \omega_c)^{l_c}} \end{cases}$$

$$\alpha = \frac{\dot{\varepsilon}^{cr}_{c_{min}}}{\dot{\varepsilon}^{cr}_{f_{min}}}, \qquad \beta = \frac{t_{f_*}}{t_{c_*}}\frac{l_f + 1}{l_c + 1}$$

Binary Structure (I)

- Assumptions:

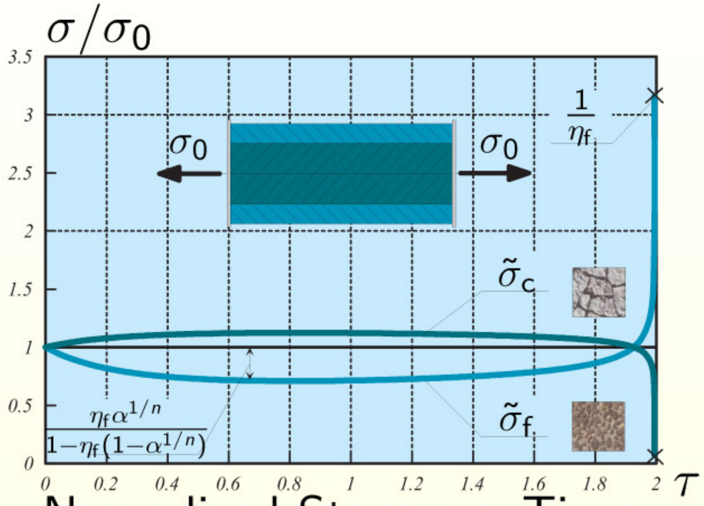
$$\varepsilon_{\mathsf{f}} = \varepsilon_{\mathsf{c}} \quad \Rightarrow \quad \dot{\varepsilon}_{\mathsf{f}} = \dot{\varepsilon}_{\mathsf{c}},$$

$$\sigma_0 = \eta_{\mathsf{f}}\sigma_{\mathsf{f}} + (1-\eta_{\mathsf{f}})\sigma_{\mathsf{c}} = \text{const},$$

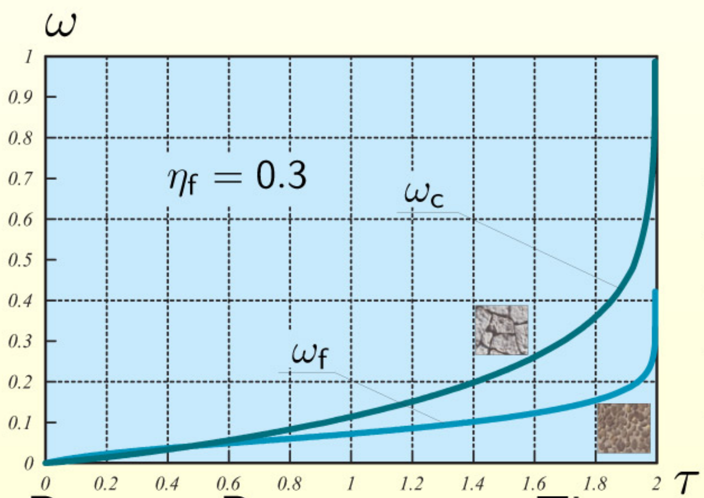
$$\sigma_{\mathsf{f}} = E(1-\omega_{\mathsf{f}})(\varepsilon - \varepsilon_{\mathsf{f}}^{\mathsf{cr}}),$$

$$\sigma_{\mathsf{c}} = E(1-\omega_{\mathsf{c}})(\varepsilon - \varepsilon_{\mathsf{c}}^{\mathsf{cr}}),$$

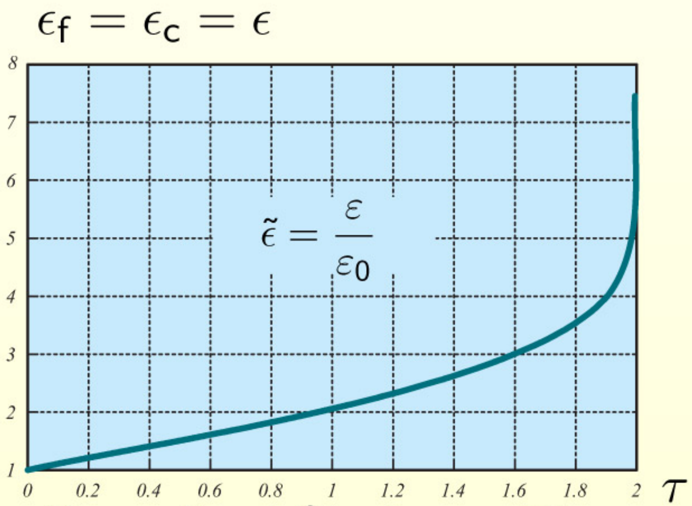
$$\begin{cases} \dot{\sigma_{\mathsf{f}}} = g_1(\sigma_{\mathsf{f}}, \omega_{\mathsf{f}}, \omega_{\mathsf{c}}) \\ \dot{\omega_{\mathsf{f}}} = g_2(\sigma_{\mathsf{f}}, \omega_{\mathsf{f}}, \omega_{\mathsf{c}}) \\ \dot{\omega_{\mathsf{c}}} = g_3(\sigma_{\mathsf{f}}, \omega_{\mathsf{f}}, \omega_{\mathsf{c}}) \end{cases}$$



Normalized Stress vs. Time

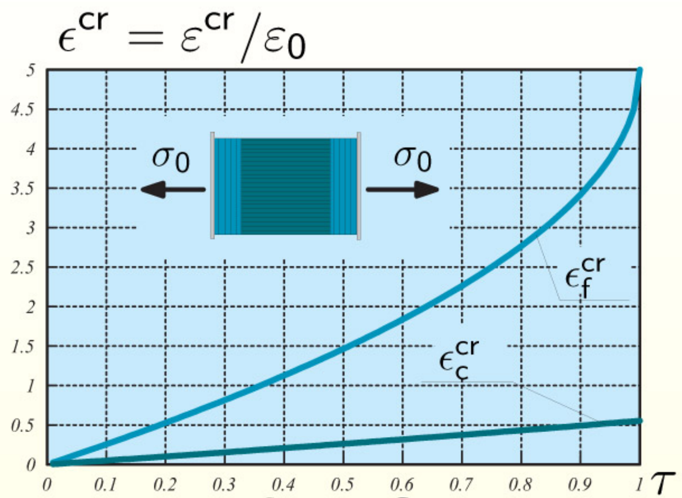


Damage Parameter vs. Time



Normalized Strain vs. Time

Binary Structure (II)

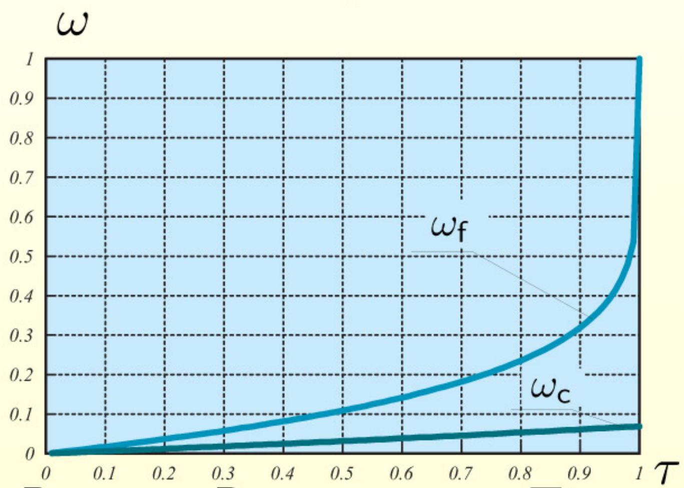


Normalized Creep Strain vs. Time

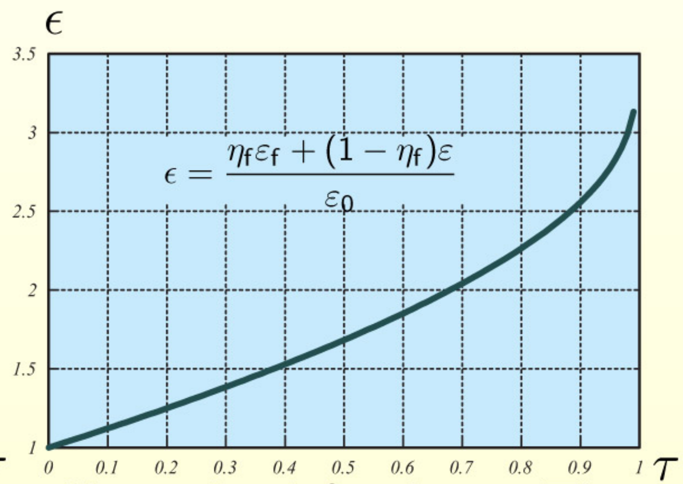
- Assumptions:

$$\sigma_0 = \sigma_f = \sigma_c = \text{const},$$

$$\varepsilon = \eta_f \varepsilon_f + (1 - \eta_f)\varepsilon_c$$

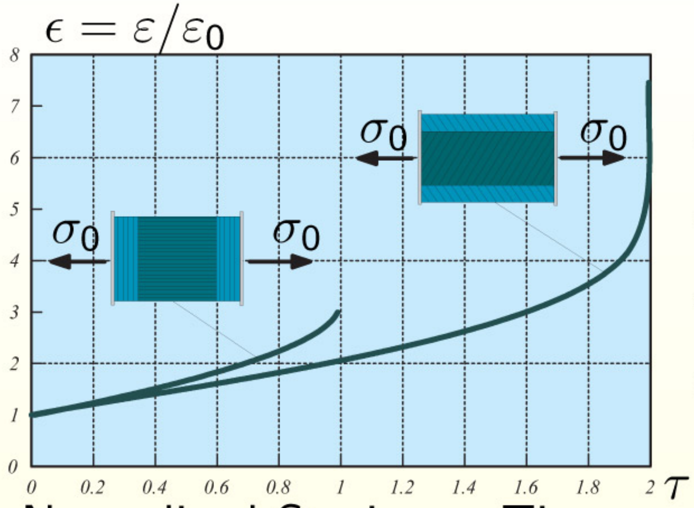


Damage Parameter vs. Time

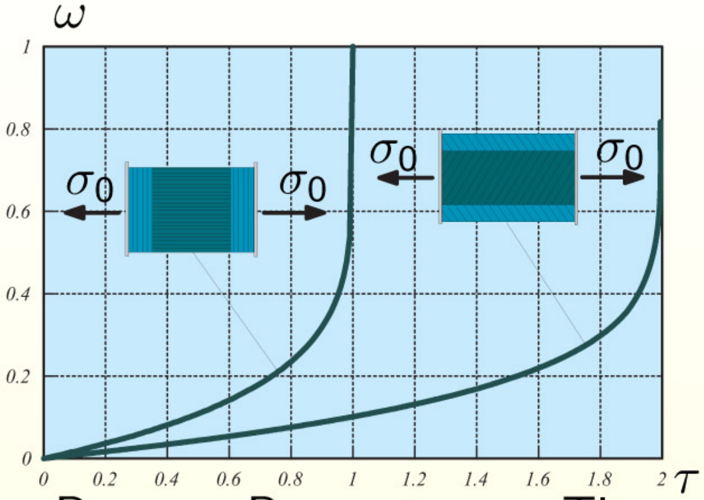


Normalized Strain vs. Time

Binary Structure (III)



Normalized Strain vs. Time



Damage Parameter vs. Time

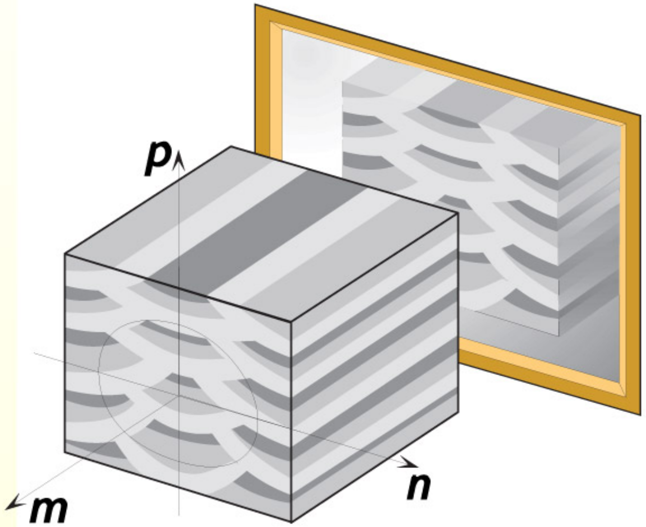
Microstructural observations of damage, Hyde et al. (2003)

- **Longitudinal specimen:** extensive voids and cracks along entire length of specimen, damage is confined to creep strong columnar regions
- **Transverse specimen:** voids and cracks are localized and are much less extensive away the fracture surface, the failure propagated through the fine-grained region

Symmetry Assumptions

Two Types of Symmetries

- Material Symmetries



- Reflection $\boldsymbol{Q}_1 = \boldsymbol{E} - 2\boldsymbol{m} \otimes \boldsymbol{m}$
- Rotation $\boldsymbol{Q}_2(\pi\boldsymbol{p}) = 2\boldsymbol{p} \otimes \boldsymbol{p} - \boldsymbol{E}$

$$\Downarrow$$

- Reflection $\boldsymbol{Q}_3 = \boldsymbol{Q}_1 \cdot \boldsymbol{Q}_2 = \boldsymbol{E} - 2\boldsymbol{n} \otimes \boldsymbol{n}$

- Physical Symmetries
  - Assumptions:
    a) Transverse Isotropy: $\boldsymbol{Q}(\varphi\boldsymbol{m}), \pm\boldsymbol{Q}(\pi\boldsymbol{p}), \quad -\pi < \varphi < \pi$
    b) Orthotropic Symmetry: $\pm\boldsymbol{Q}(\pi\boldsymbol{n}), \pm\boldsymbol{Q}(\pi\boldsymbol{p})$
  - Anisotropic Creep Models: Betten (2002)

Transversely-isotropic Creep

Restrictions

$$W(\boldsymbol{Q}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{Q}^{\mathsf{T}}) = W(\boldsymbol{\sigma})$$

$$\boldsymbol{Q} = \boldsymbol{m}\otimes\boldsymbol{m} + \cos\varphi(\boldsymbol{E} - \boldsymbol{m}\otimes\boldsymbol{m}) + \sin\varphi\boldsymbol{m}\times\boldsymbol{E}$$

$$-\pi < \varphi < \pi, \quad \boldsymbol{m} = \text{const}, \quad \boldsymbol{m}\cdot\boldsymbol{m} = 1$$

Invariants

$$W(\boldsymbol{Q}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{Q}^{\mathsf{T}}) = W(\boldsymbol{\sigma}) \quad \Rightarrow \quad (\boldsymbol{m}\times\boldsymbol{\sigma} - \boldsymbol{\sigma}\times\boldsymbol{m})\cdot\cdot\frac{\partial W}{\partial\boldsymbol{\sigma}} = 0$$

Characteristic system: $\dfrac{d\boldsymbol{\sigma}}{ds} = (\boldsymbol{m}\times\boldsymbol{\sigma} - \boldsymbol{\sigma}\times\boldsymbol{m})$

Solutions: $\boldsymbol{\sigma}^k(s) = \boldsymbol{Q}(s\boldsymbol{m})\cdot\boldsymbol{\sigma}_0^k\cdot\boldsymbol{Q}^{\mathsf{T}}(s\boldsymbol{m}), \quad k = 1,2,3$

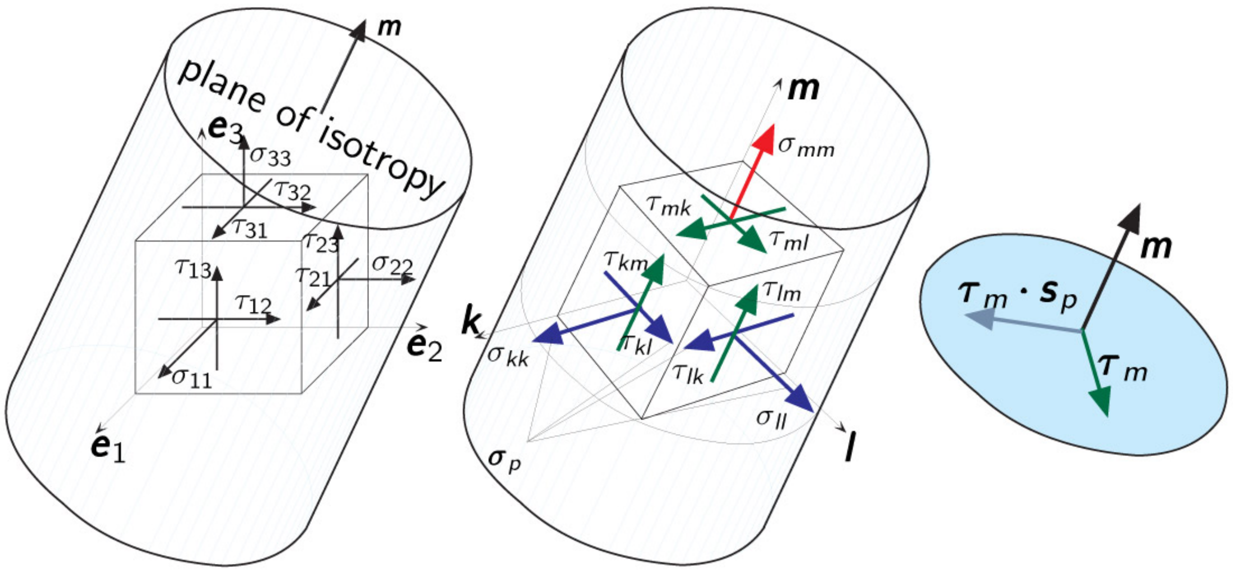
Integrals: $\mathrm{tr}\boldsymbol{\sigma}, \quad \mathrm{tr}\boldsymbol{\sigma}^2, \quad \mathrm{tr}\boldsymbol{\sigma}^3,$

$\boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m}, \quad \boldsymbol{m}\cdot\boldsymbol{\sigma}^2\cdot\boldsymbol{m}, \quad \boldsymbol{m}\cdot\boldsymbol{\sigma}^2\cdot(\boldsymbol{m}\times\boldsymbol{\sigma}\cdot\boldsymbol{m})$

Sets of transversely-isotropic invariants: Bruhns et al. (1999)

Transversely-isotropic Invariants

New Split of the Stress Tensor



$$\boldsymbol{\sigma} = \boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m}\,\boldsymbol{m}\otimes\boldsymbol{m} + \boldsymbol{\sigma}_p + \boldsymbol{\tau}_m\otimes\boldsymbol{m} + \boldsymbol{m}\otimes\boldsymbol{\tau}_m,$$

$$\boldsymbol{\sigma}_p = \boldsymbol{s}_p + \frac{1}{2}\mathrm{tr}\boldsymbol{\sigma}_p(\boldsymbol{E} - \boldsymbol{m}\otimes\boldsymbol{m}), \quad \mathrm{tr}\boldsymbol{s}_p = 0,$$

$$I_{1m} = \boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m}, \quad I_{2m} = \frac{1}{2}\mathrm{tr}\boldsymbol{\sigma}_p, \quad I_{3m} = \mathrm{tr}\boldsymbol{s}_p^2, \quad I_{4m} = \boldsymbol{\tau}_{\boldsymbol{m}}\cdot\boldsymbol{\tau}_{\boldsymbol{m}}$$

$$I_{5m} = \boldsymbol{\tau}_{\boldsymbol{m}}\cdot\boldsymbol{s}_p\cdot\boldsymbol{\tau}_{\boldsymbol{m}}, \quad I_{6m} = \boldsymbol{m}\cdot(\boldsymbol{\tau}_{\boldsymbol{m}}\cdot\boldsymbol{s}_p\times\boldsymbol{\tau}_{\boldsymbol{m}})$$

$$\boxed{I_{6m}^2 = I_{3m}I_{4m} - I_{5m}^2}$$

von Mises Type Creep Equation

- Equivalent Stress

$$\sigma_{\text{eq}}^2 = J_0^2 + 3\alpha_1 J_1 + 3\alpha_2 J_2, \quad \alpha_1 > 0, \quad \alpha_2 > 0$$

$$\begin{aligned} J_0 &= \boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m} - \frac{1}{2}\text{tr}\boldsymbol{\sigma}_p = \frac{1}{2}(3\boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m} - \text{tr}\boldsymbol{\sigma}) \\ \text{tr}\boldsymbol{\sigma}_p &= \text{tr}\boldsymbol{\sigma} - \boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m} \\ 2J_1 &= \text{tr}\boldsymbol{s}_p^2 = \text{tr}\boldsymbol{\sigma}^2 - 2\boldsymbol{m}\cdot\boldsymbol{\sigma}^2\cdot\boldsymbol{m} + (\boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m})^2 - \frac{1}{2}(\text{tr}\boldsymbol{\sigma}_p)^2 \\ J_2 &= \boldsymbol{\tau}_m\cdot\boldsymbol{\tau}_m = \boldsymbol{m}\cdot\boldsymbol{\sigma}^2\cdot\boldsymbol{m} - (\boldsymbol{m}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{m})^2 \end{aligned}$$

- Norton-Bailey-Odqvist Potential

$$W = \frac{a}{n+1}\sigma_{\text{eq}}^{n+1} \qquad \text{(power law creep)}$$

- Creep Equation

$$\boldsymbol{D}^{\text{cr}} = \frac{3}{2}a\sigma_{\text{eq}}^{n-1}\left[J_0(\boldsymbol{m}\otimes\boldsymbol{m} - \frac{1}{3}\boldsymbol{E}) + \alpha_1\boldsymbol{s}_p + \alpha_2(\boldsymbol{\tau}_m\otimes\boldsymbol{m} + \boldsymbol{m}\otimes\boldsymbol{\tau}_m)\right]$$

- Classical Case: $\alpha_1 = \alpha_2 = 1$

Material Constants I

- Creep Equation

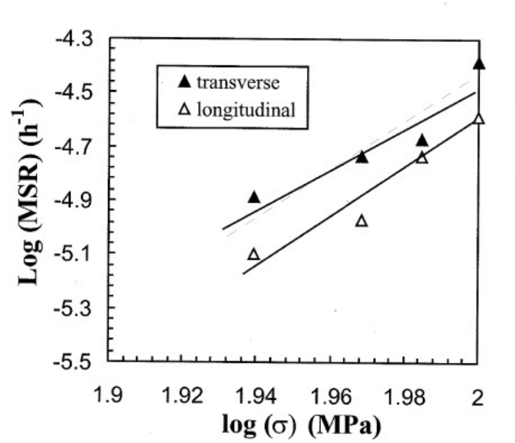
$$\boldsymbol{D}^{\text{cr}} = \frac{3}{2} a \sigma_{\text{eq}}^{n-1} \left[J_0 \left(\boldsymbol{m} \otimes \boldsymbol{m} - \frac{1}{3} \boldsymbol{E} \right) + \alpha_1 \boldsymbol{s}_p + \alpha_2 (\boldsymbol{\tau}_m \otimes \boldsymbol{m} + \boldsymbol{m} \otimes \boldsymbol{\tau}_m) \right]$$

- Creep tests in longitudinal (welding) direction

$$\boldsymbol{\sigma} = \sigma_0 \boldsymbol{m} \otimes \boldsymbol{m} : \quad \dot{\varepsilon}^{\text{cr}} = \boldsymbol{m} \cdot \boldsymbol{D}^{\text{cr}} \cdot \boldsymbol{m} = a \sigma_0^n, \quad \sigma_0 [87 - 100] \text{MPa}$$

- Creep tests in transverse direction

$$\sigma = \sigma_0 \boldsymbol{p} \otimes \boldsymbol{p}, \quad \boldsymbol{p} \cdot \boldsymbol{m} = 0, \quad \dot{\varepsilon}^{\text{cr}} = \boldsymbol{p} \cdot \boldsymbol{D}^{\text{cr}} \cdot \boldsymbol{p} = a \gamma^{n+1} \sigma_0^n,$$
$$\alpha_1 = \frac{1}{3}(4\gamma^2 - 1), \quad \sigma_0 [87 - 100] \text{MPa}$$



$$a = 1.15 \cdot 10^{-22} \text{MPa}^{-n}/\text{h}, \quad n = 8.64$$

$$\alpha_1 = 1.23$$

Minimum Creep Rate vs. Stress, Hyde et al. (2003)

Material Constants I

- Creep Equation

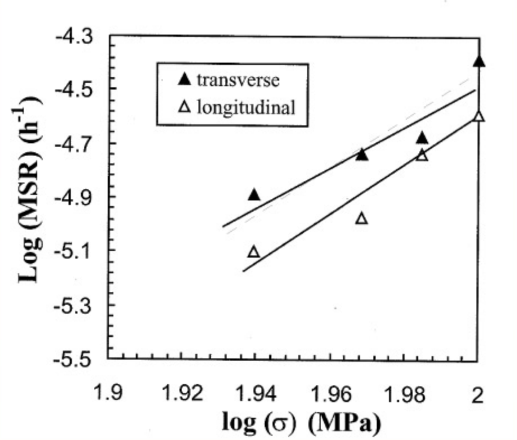
$$\mathbf{D}^{\mathrm{cr}}=\frac{3}{2}a\sigma_{\mathrm{eq}}^{n-1}\left[J_0\left(\mathbf{m}\otimes\mathbf{m}-\frac{1}{3}\mathbf{E}\right)+\alpha_1\mathbf{s}_p+\alpha_2(\boldsymbol{\tau}_m\otimes\mathbf{m}+\mathbf{m}\otimes\boldsymbol{\tau}_m)\right]$$

- Creep tests in longitudinal (welding) direction

$$\boldsymbol{\sigma}=\sigma_0\mathbf{m}\otimes\mathbf{m}:\quad \dot{\varepsilon}^{\mathrm{cr}}=\mathbf{m}\cdot\mathbf{D}^{\mathrm{cr}}\cdot\mathbf{m}=a\sigma_0^n,\quad \sigma_0[87-100]\mathrm{MPa}$$

- Creep tests in transverse direction

$$\sigma=\sigma_0\mathbf{p}\otimes\mathbf{p},\quad \mathbf{p}\cdot\mathbf{m}=0,\quad \dot{\varepsilon}^{\mathrm{cr}}=\mathbf{p}\cdot\mathbf{D}^{\mathrm{cr}}\cdot\mathbf{p}=a\gamma^{n+1}\sigma_0^n,$$
$$\alpha_1=\frac{1}{3}(4\gamma^2-1),\quad \sigma_0[87-100]\mathrm{MPa}$$



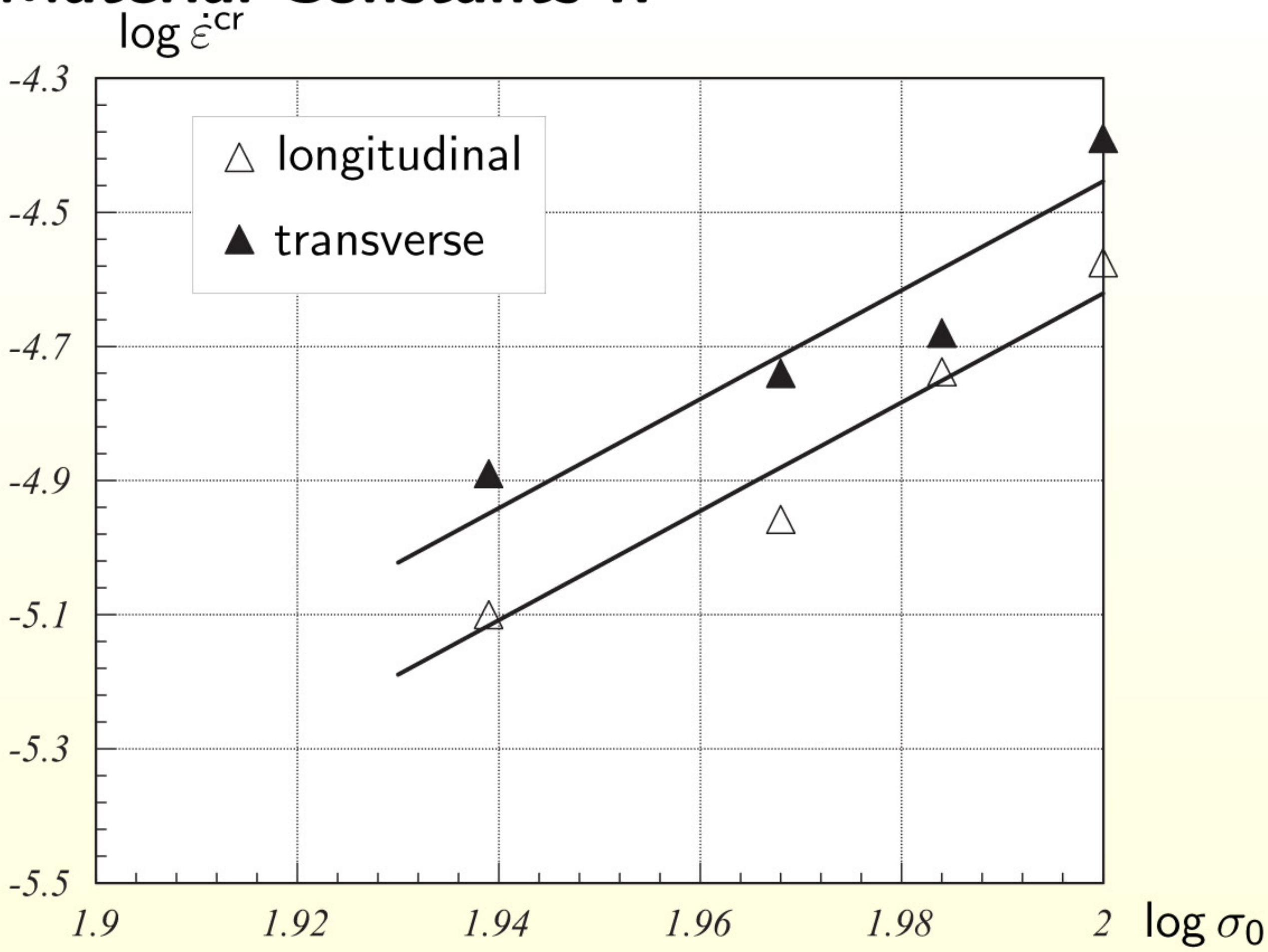
$$a=1.15\cdot10^{-22}\mathrm{MPa}^{-n}/\mathrm{h},\quad n=8.64$$

$$\alpha_1=1.23$$

$$\alpha_2=??$$

Minimum Creep Rate vs. Stress,
Hyde et al. (2003)

Material Constants II



$a = 1.38 \cdot 10^{-21} \mathrm{MPa}^{-n}/\mathrm{h}, \quad n = 8.12, \quad \alpha_1 = 1.17$

$\alpha_2 = ??$

Balance of Momentum and Moment of Momentum

Deformable plane surface

Integral Form

$$\boldsymbol{\mathcal{F}}_s^* \equiv \int\limits_{\mathcal{M}_*} \boldsymbol{q}\,\mathrm{d}A + \int\limits_{\mathcal{C}_*} \boldsymbol{t}_s\,ds = \boldsymbol{0},$$

$$\boldsymbol{\mathcal{M}}_s^* \equiv \int\limits_{\mathcal{M}_*} (\boldsymbol{x} \times \boldsymbol{q} + \boldsymbol{c})\,\mathrm{d}A + \int\limits_{\mathcal{C}_*} (\boldsymbol{x} \times \boldsymbol{t}_s + \boldsymbol{m}_s)\,\mathrm{d}s = \boldsymbol{0}$$

Constitutive Equations

Strain Energy Density - Isotropic Case

$$
\begin{aligned}
2W &= \alpha_1 \mathrm{tr}^2 \boldsymbol{\epsilon}_{||} + \alpha_2 \mathrm{tr} \boldsymbol{\epsilon}_{||}^2 + \alpha_3 \mathrm{tr}\left(\boldsymbol{\epsilon}_{||} \cdot \boldsymbol{\epsilon}_{||}^{\mathsf{T}}\right) + \alpha_4 \boldsymbol{n} \cdot \boldsymbol{\epsilon}^{\mathsf{T}} \cdot \boldsymbol{\epsilon} \cdot \boldsymbol{n} \\
&\quad + \beta_1 \mathrm{tr}^2 \boldsymbol{\kappa}_{||} + \beta_2 \mathrm{tr} \boldsymbol{\kappa}_{||}^2 + \beta_3 \mathrm{tr}\left(\boldsymbol{\kappa}_{||} \cdot \boldsymbol{\kappa}_{||}^{\mathsf{T}}\right) + \beta_4 \boldsymbol{n} \cdot \boldsymbol{\kappa}^{\mathsf{T}} \cdot \boldsymbol{\kappa} \cdot \boldsymbol{n}
\end{aligned}
$$

Here $\boldsymbol{\epsilon}_{||} = \boldsymbol{\epsilon} \cdot \boldsymbol{A}$, $\boldsymbol{\kappa}_{||} = \boldsymbol{\kappa} \cdot \boldsymbol{A}$, and α_i, β_i are the elastic constants, $i = 1, 2, 3, 4$.

$$
\boldsymbol{T} \equiv \frac{\partial W}{\partial \boldsymbol{\epsilon}} = \alpha_1 \boldsymbol{A} \mathrm{tr} \boldsymbol{\epsilon}_{||} + \alpha_2 \boldsymbol{\epsilon}_{||}^{\mathsf{T}} + \alpha_3 \boldsymbol{\epsilon}_{||} + \alpha_4 \boldsymbol{\epsilon} \cdot \boldsymbol{n} \otimes \boldsymbol{n},
$$

$$
\boldsymbol{M} \equiv \frac{\partial W}{\partial \boldsymbol{\kappa}} = \beta_1 \boldsymbol{A} \mathrm{tr} \boldsymbol{\kappa}_{||} + \beta_2 \boldsymbol{\kappa}_{||}^{\mathsf{T}} + \beta_3 \boldsymbol{\kappa}_{||} + \beta_4 \boldsymbol{\kappa} \cdot \boldsymbol{n} \otimes \boldsymbol{n}
$$

Elastic Moduli

Constraints

$$\begin{aligned}&2\alpha_1+\alpha_2+\alpha_3>0, \quad \alpha_2+\alpha_3>0, \quad \alpha_3-\alpha_2>0, \quad \alpha_4>0,\\ &2\beta_1+\beta_2+\beta_3>0, \quad \beta_2+\beta_3>0, \quad \beta_3-\beta_2>0, \quad \beta_4>0.\end{aligned}$$

Example Chróścielewski et al. (2004)

$$\begin{aligned}&\alpha_1=C\nu, \quad \alpha_2=0, \quad \alpha_3=C(1-\nu), \quad \alpha_4=\alpha_s C(1-\nu),\\ &\beta_1=D\nu, \quad \beta_2=0, \quad \beta_3=D(1-\nu), \quad \beta_4=\alpha_t D(1-\nu),\\ &C=\frac{Eh}{1-\nu^2}, \quad D=\frac{Eh^3}{12(1-\nu^2)},\end{aligned}$$

where α_s and α_t are dimensionless coefficients.

Further Steps

- Three-dimensional Micropolar Elasticity
- Through-the-thickness integration procedure
- Micropolar Plates Constitutive Equations

Micropolar Constants for Two Materials[4]

		Foam, PU	Foam, PS
Shear modulus, MPa	$G = \frac{2\mu+\kappa}{2}$	1.1	104
Poisson's ratio,	$\nu = \frac{\lambda}{2\lambda+2\mu+\kappa}$	0.07	0.4
Characteristic length (torsion), mm	$l_t = \sqrt{\frac{\beta+\gamma}{2\mu+\kappa}}$	3.8	0.62
Characteristic length (bending), mm	$l_b = \sqrt{\frac{\gamma}{2(2\mu+\kappa)}}$	5.0	0.33
Coupling number,	$N^2 = \frac{\kappa}{2\mu+\kappa}$	0.09	0.04
Polar ratio,	$\Psi = \frac{\beta+\gamma}{\alpha+\beta+\gamma}$	1.5	1.5

- PS - low-density polystyrene closed-cell foam
- PU - high-density rigid polyurethane closed-cell foam

[4] see Lakes (1986, 1995)

Effective Stiffness for PU Foam

Elastic constants		Foam, PU	Foam, PU *
α_1, N/m 10^6	$\lambda^* h$	$0.165h$	$0.165h$
α_2, N/m 10^6	μh	$1.001h$	$1.1h$
α_3, N/m 10^6	$(\mu + \kappa)h$	$1.199h$	$1.1h$
α_4, N/m 10^6	$(\mu + \kappa)h$	$1.199h$	$1.1h$
β_1, N·m 10^6	$\alpha h - \mu \dfrac{h^3}{12}$	$-2.6 \cdot 10^{-6} h - 0.083h^3$	$-0.092h^3$
β_2, N·m 10^6	$\beta h - \lambda^* \dfrac{h^3}{12}$	$-10^{-4} h - 0.014h^3$	$-0.014h^3$
β_3, N·m 10^6	$\gamma h + (2\mu + \kappa + \lambda^*)\frac{h^3}{12}$	$1.1 \cdot 10^{-4} h + 0.197h^3$	$0.197h^3$
β_4, N·m 10^6	γh	$1.1 \cdot 10^{-4} h$	0

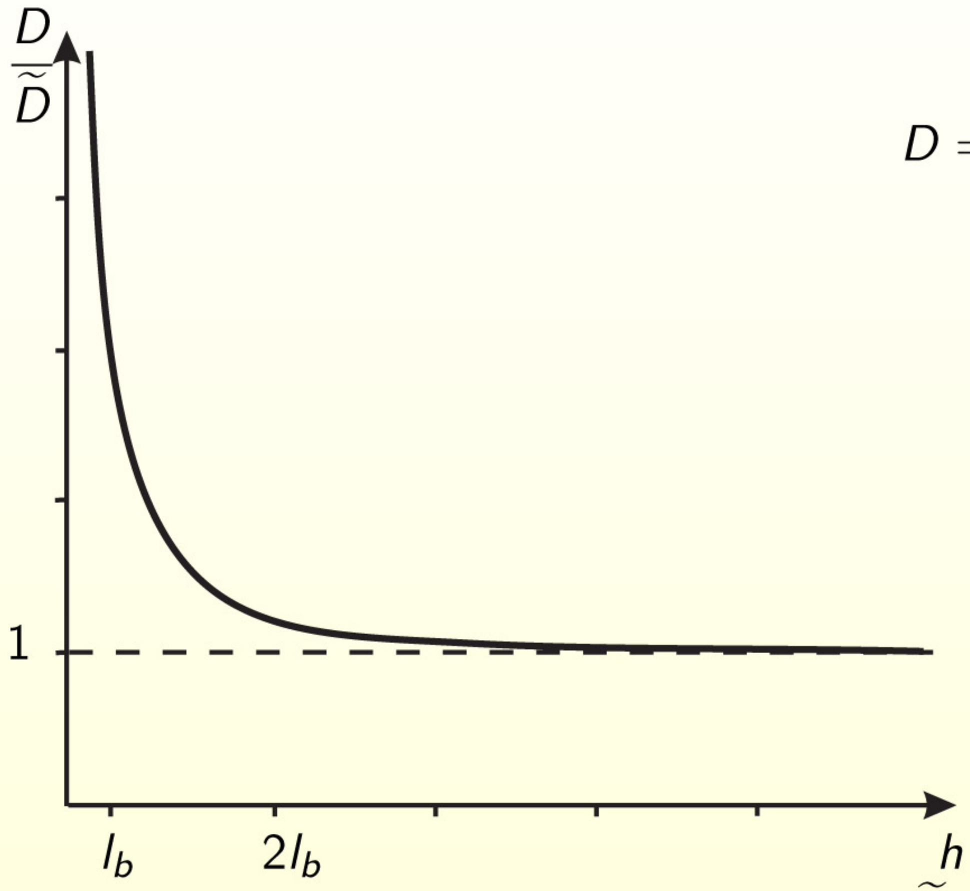
$(\ldots)^*$ - micropolar properties are neglected $(\kappa = \alpha = \beta = \gamma = 0)$

Effective Stiffness for PS Foam

Elastic constants		Foam, PS	Foam, PS *
α_1, N/m 10^6	$\lambda^* h$	$138.67h$	$138.67h$
α_2, N/m 10^6	μh	$99.84h$	$104h$
α_3, N/m 10^6	$(\mu + \kappa)h$	$108.16h$	$104h$
α_4, N/m 10^6	$(\mu + \kappa)h$	$108.16h$	$104h$
β_1, N·m 10^6	$\alpha h - \mu \dfrac{h^3}{12}$	$-6.7 \cdot 10^{-6} h - 8.3h^3$	$-8.67h^3$
β_2, N·m 10^6	$\beta h - \lambda^* \dfrac{h^3}{12}$	$-2.5 \cdot 10^{-5} h + 11.6h^3$	$-11.5h^3$
β_3, N·m 10^6	$\gamma h + (2\mu + \kappa + \lambda^*)\frac{h^3}{12}$	$4.5 \cdot 10^{-5} h + 28.9h^3$	$28.8h^3$
β_4, N·m 10^6	γh	$4.5 \cdot 10^{-5} h$	0

$(\ldots)^*$ - micropolar properties are neglected $(\kappa = \alpha = \beta = \gamma = 0)$

Dimensionless Bending Stiffness



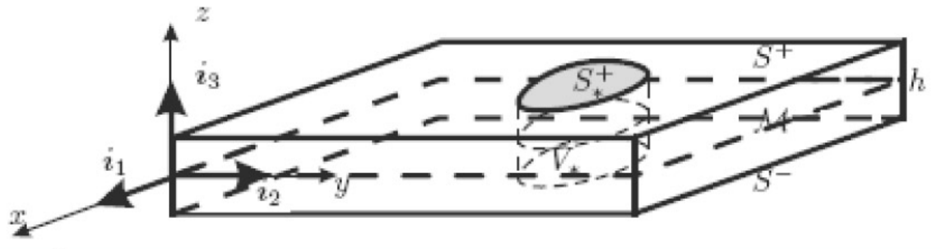
$$D = \frac{Gh^3}{12(1-\nu)}\left[1 + 2\frac{l_b^2}{h^2}\right]$$

Dimensionless bending stiffness $D/\widetilde{D}$ vs. thickness h/l_b

Theory of Capillarity

Surface Tension in the Hydrodynamics

Theory of Elasticity with Surface Stresses



Equilibrium equations

$$\nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{f} = 0, \quad \boldsymbol{n} \cdot \boldsymbol{\sigma}\big|_{z=\pm\frac{h}{2}} = \boldsymbol{t}_{\pm}.$$

Surface loads

$$\boldsymbol{t}_{\pm} = \boldsymbol{t}^0_{\pm} + \boldsymbol{t}^S_{\pm}, \quad \boldsymbol{t}^S_{\pm} = \nabla_S \cdot \boldsymbol{\tau}_{\pm},$$

Constitutive equations

$$\boldsymbol{\sigma} = 2\mu\boldsymbol{\varepsilon} + \lambda \boldsymbol{I}\,\mathrm{tr}\boldsymbol{\varepsilon}, \quad \boldsymbol{\tau}_{\pm} = 2\mu^S_{\pm}\boldsymbol{\epsilon} + \lambda^S_{\pm}\boldsymbol{A}\,\mathrm{tr}\boldsymbol{\epsilon},$$

Geometrical equations

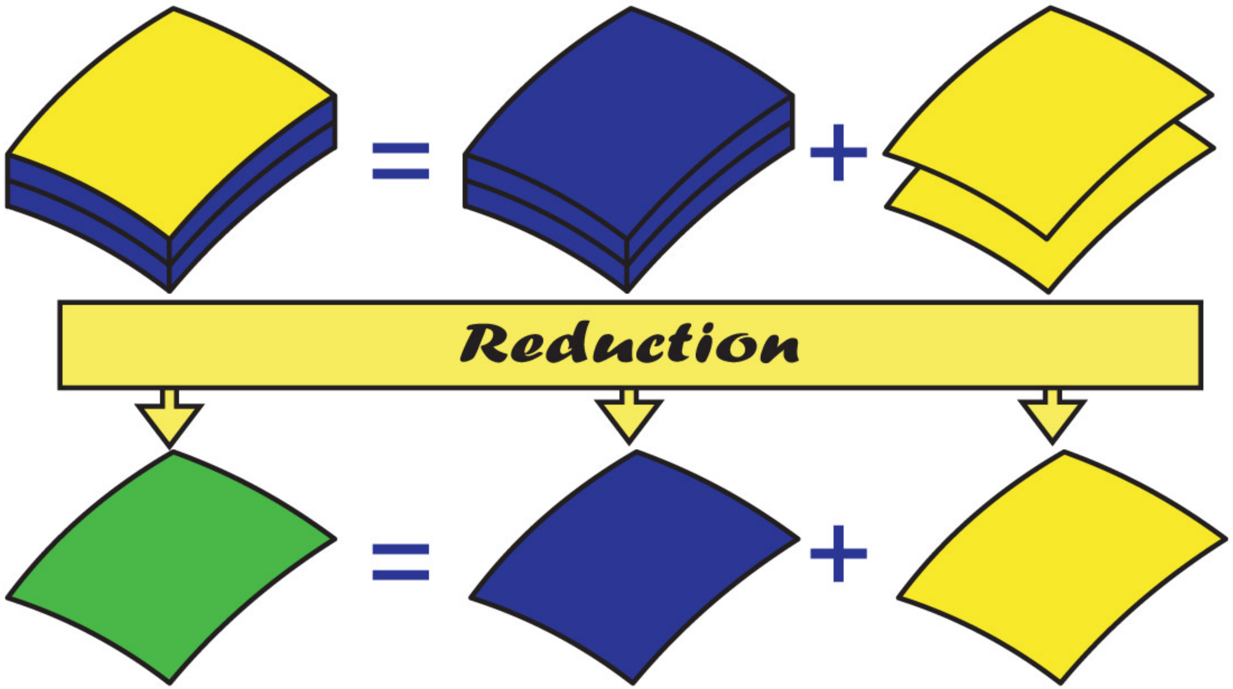
$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right), \quad \boldsymbol{\epsilon}_{\pm} = \frac{1}{2}\left(\nabla_S\boldsymbol{v}_{\pm} + (\nabla_S\boldsymbol{v}_{\pm})^T\right),$$

$\boldsymbol{I}$ - unit tensor, $\boldsymbol{A} \equiv \boldsymbol{I} - \boldsymbol{i}_3 \otimes \boldsymbol{i}_3$, $\boldsymbol{v}_{\pm} = \boldsymbol{v}_{\pm}(x, y) \equiv \boldsymbol{A} \cdot \boldsymbol{u}(x, y, \pm h/2)$

3D to 2D Reduction

Superposition of two problems

$$\mathbf{T}^* = \mathbf{T} + \mathbf{T}_S\,, \qquad \mathbf{M}^* = \mathbf{M} + \mathbf{M}_S\,,$$



$\mathbf{T}^*, \mathbf{M}^*$ $\mathbf{T}, \mathbf{M}$ $\mathbf{T}_S, \mathbf{M}_S$

Transition to 2D Equations[5]

- Averaged three-dimensional equation

$$\nabla_S \cdot \langle \boldsymbol{\sigma} \rangle + \boldsymbol{t}_+ + \boldsymbol{t}_- + \langle \rho \boldsymbol{f} \rangle = 0,$$

$$-\nabla_S \cdot \langle z\boldsymbol{\sigma} \times \boldsymbol{i}_3 \rangle - \langle \boldsymbol{i}_3 \times \boldsymbol{\sigma} \cdot \boldsymbol{i}_3 \rangle + \frac{h}{2}\boldsymbol{i}_3 \times (\boldsymbol{t}_+ - \boldsymbol{t}_-) + \langle \rho z \boldsymbol{i}_3 \times \boldsymbol{f} \rangle = 0,$$

$$\langle (\ldots) \rangle = \int_{-h/2}^{h/2} (\ldots)\, dz$$

- Resultant stresses and moment stress tensors

$$\boldsymbol{T} = \boldsymbol{A} \cdot \langle \boldsymbol{\sigma} \rangle, \quad \boldsymbol{M} = -\boldsymbol{A} \cdot \langle z\boldsymbol{\sigma} \times \boldsymbol{i}_3 \rangle,$$

$$\nabla_S \cdot \boldsymbol{T} + \nabla_S \cdot \boldsymbol{\tau}_+ + \nabla_S \cdot \boldsymbol{\tau}_- + \boldsymbol{q} = 0,$$

$$\nabla_S \cdot \boldsymbol{M} + \boldsymbol{T}_\times + \frac{h}{2}\boldsymbol{i}_3 \times (\nabla_S \cdot \boldsymbol{\tau}_+ - \nabla_S \cdot \boldsymbol{\tau}_-) + \boldsymbol{m} = 0,$$

$$\boldsymbol{q} = \boldsymbol{t}_+^0 + \boldsymbol{t}_-^0 + \langle \rho \boldsymbol{f} \rangle, \quad \boldsymbol{m} = \boldsymbol{i}_3 \times (\boldsymbol{t}_+^0 - \boldsymbol{t}_-^0)h/2 + \langle \rho z \boldsymbol{i}_3 \times \boldsymbol{f} \rangle$$

[5] Eremeyev, Altenbach & Morozov (2009)

Effective Stress and Moment Stress Tensors

- Resultant tensors

$$\boldsymbol{T}^* = \boldsymbol{T} + \boldsymbol{\tau}_+ + \boldsymbol{\tau}_-, \quad \boldsymbol{M}^* = \boldsymbol{M} - \frac{h}{2}(\boldsymbol{\tau}_+ - \boldsymbol{\tau}_-) \times \boldsymbol{i}_3.$$

- Equilibrium equations

$$\nabla_S \cdot \boldsymbol{T}^* + \boldsymbol{q} = 0, \quad \nabla_S \cdot \boldsymbol{M}^* + \boldsymbol{T}^*_\times + \boldsymbol{m} = 0.$$

Constitutive Equations (I)

- Symmetric structure, i.e. $\lambda_+^S = \lambda_-^S = \lambda^S$, $\mu_+^S = \mu_-^S = \mu^S$. Then

$$\boldsymbol{\tau}_+ + \boldsymbol{\tau}_- = 2\lambda^S \boldsymbol{A}\mathrm{tr}\boldsymbol{\epsilon} + 4\mu^S\boldsymbol{\epsilon}, \quad \boldsymbol{\tau}_+ - \boldsymbol{\tau}_- = -h\left[\lambda^S \boldsymbol{A}\mathrm{tr}\boldsymbol{\kappa} + 2\mu^S\boldsymbol{\kappa}\right]$$

- Reissner-type constitutive equations

$$\boldsymbol{T}\cdot\boldsymbol{A} = C\left[(1-\nu)\boldsymbol{\epsilon} + \nu\boldsymbol{A}\mathrm{tr}\boldsymbol{\epsilon}\right], \quad \boldsymbol{M} = D\left[(1-\nu)\boldsymbol{\kappa} + \nu\boldsymbol{A}\mathrm{tr}\boldsymbol{\kappa}\right]\times\boldsymbol{i}_3,$$

$$\boldsymbol{T}\cdot\boldsymbol{i}_3 = \Gamma\boldsymbol{\gamma}, \quad C = \frac{Eh}{1-\nu^2}, \quad D = \frac{Eh^3}{12(1-\nu^2)}, \quad \Gamma = k\mu h,$$

C and D - tangential and bending stiffness of a plate,
Γ - transverse shear stiffness,
$E = 2\mu(1+\nu)$, $\nu = \frac{\lambda}{2(\lambda+\mu)}$,
k the analogous to the shear correction factor, $\boldsymbol{\gamma} = \nabla_S w - \boldsymbol{\vartheta}$,
$w = \boldsymbol{w}\cdot\boldsymbol{i}_3$ the normal displacement

Constitutive Equations (II)

$$\boldsymbol{T}^* = C_1\boldsymbol{\epsilon} + C_2\boldsymbol{A}\mathrm{tr}\boldsymbol{\epsilon} + \varGamma\boldsymbol{\gamma} \otimes \boldsymbol{i}_3, \quad \boldsymbol{M}^* = [D_1\boldsymbol{\kappa} + D_2\boldsymbol{A}\mathrm{tr}\boldsymbol{\kappa}] \times \boldsymbol{i}_3$$

with

$$C_1 = C(1-\nu) + 4\mu^S, \quad C_2 = C\nu + 2\lambda^S,$$

$$D_1 = D(1-\nu) + h^2\mu^S, \quad D_2 = D\nu + h^2\lambda^S/2$$

Here: $\boldsymbol{T}^* \cdot \boldsymbol{i}_3 = \boldsymbol{T} \cdot \boldsymbol{i}_3$.

Conclusion:

Five independent elastic constants: C_1, C_2, D_1, D_2, $\varGamma$

Reissner's theory: four constants only C, D, ν, $\varGamma$

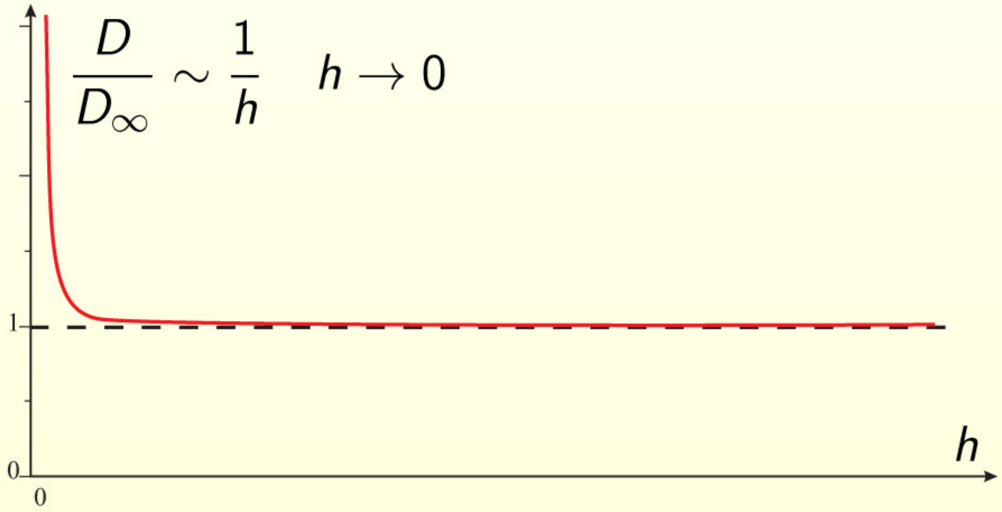
Bending Stiffness

$$D \equiv D_1 + D_2 = D_\infty + D_{surface},$$

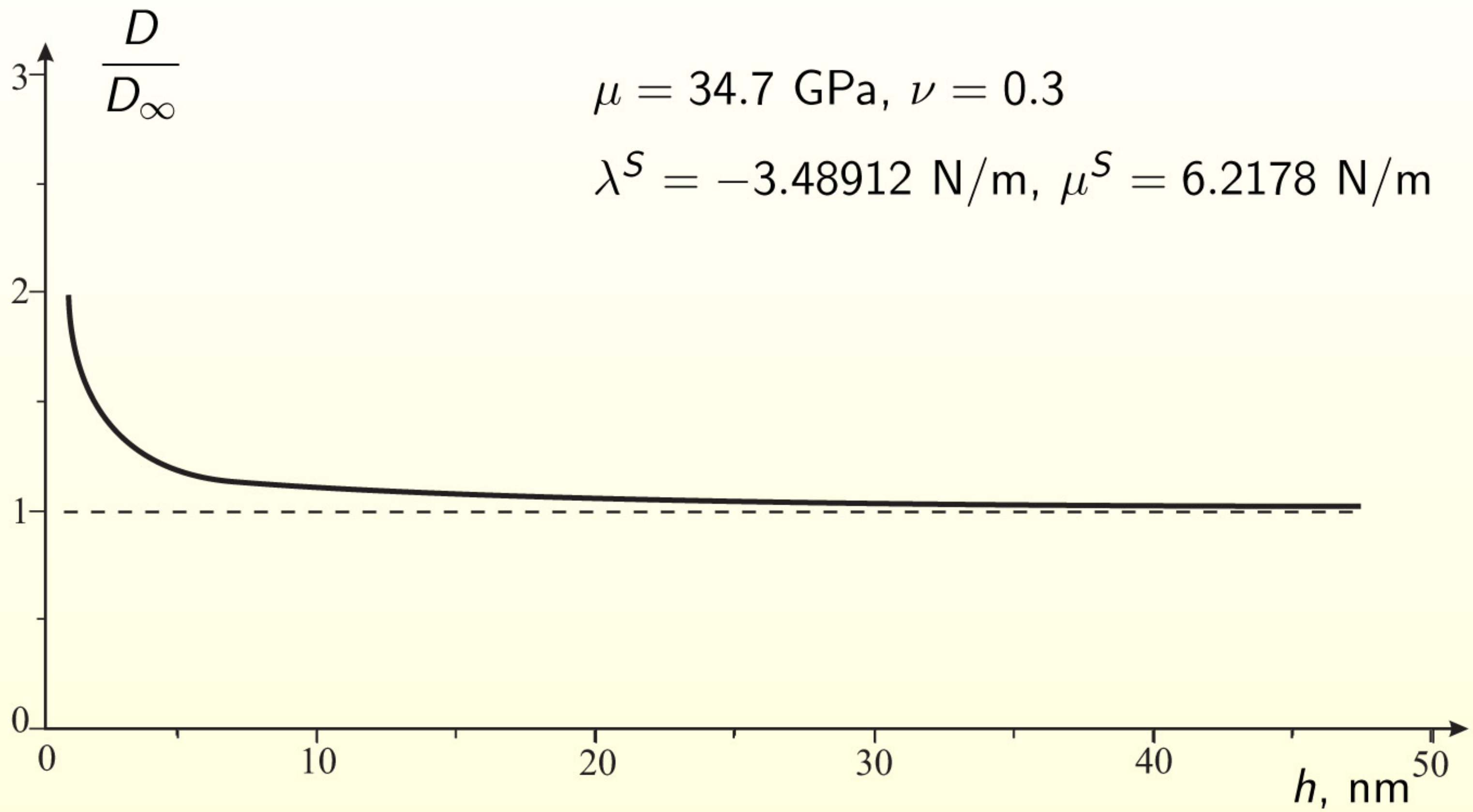
$$D_\infty = \frac{Eh^3}{12(1-\nu^2)}, \quad D_{surface} = h^2(\mu^S + \lambda^S/2)$$

From the positive definiteness of the surface energy density it follows

$$\mu_S > 0, \quad \mu_s + \lambda_S > 0 \quad \Longrightarrow \quad D_{surface} > 0$$



Bending Stiffness of a Plate made of Al[6]



$\mu = 34.7$ GPa, $\nu = 0.3$

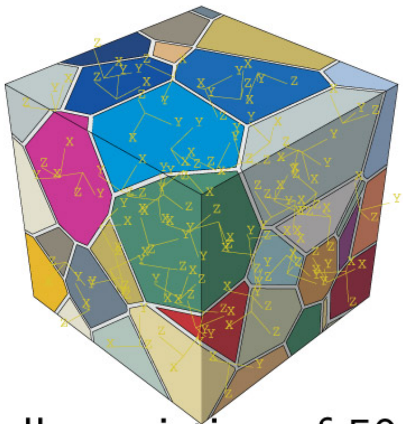
$\lambda^S = -3.48912$ N/m, $\mu^S = 6.2178$ N/m

[6] Duan et al. (2008)

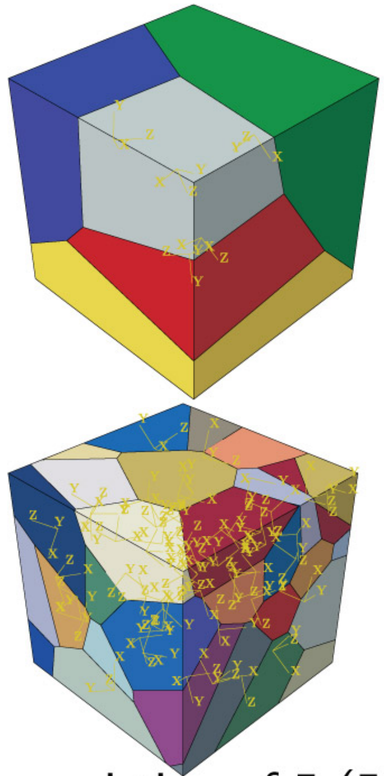
Geometrical Model of a Polycrystal

Main User Defined Parameters

- Number of grains
- Dimensions of the unit cell
- Average grain size
- Grain border thickness



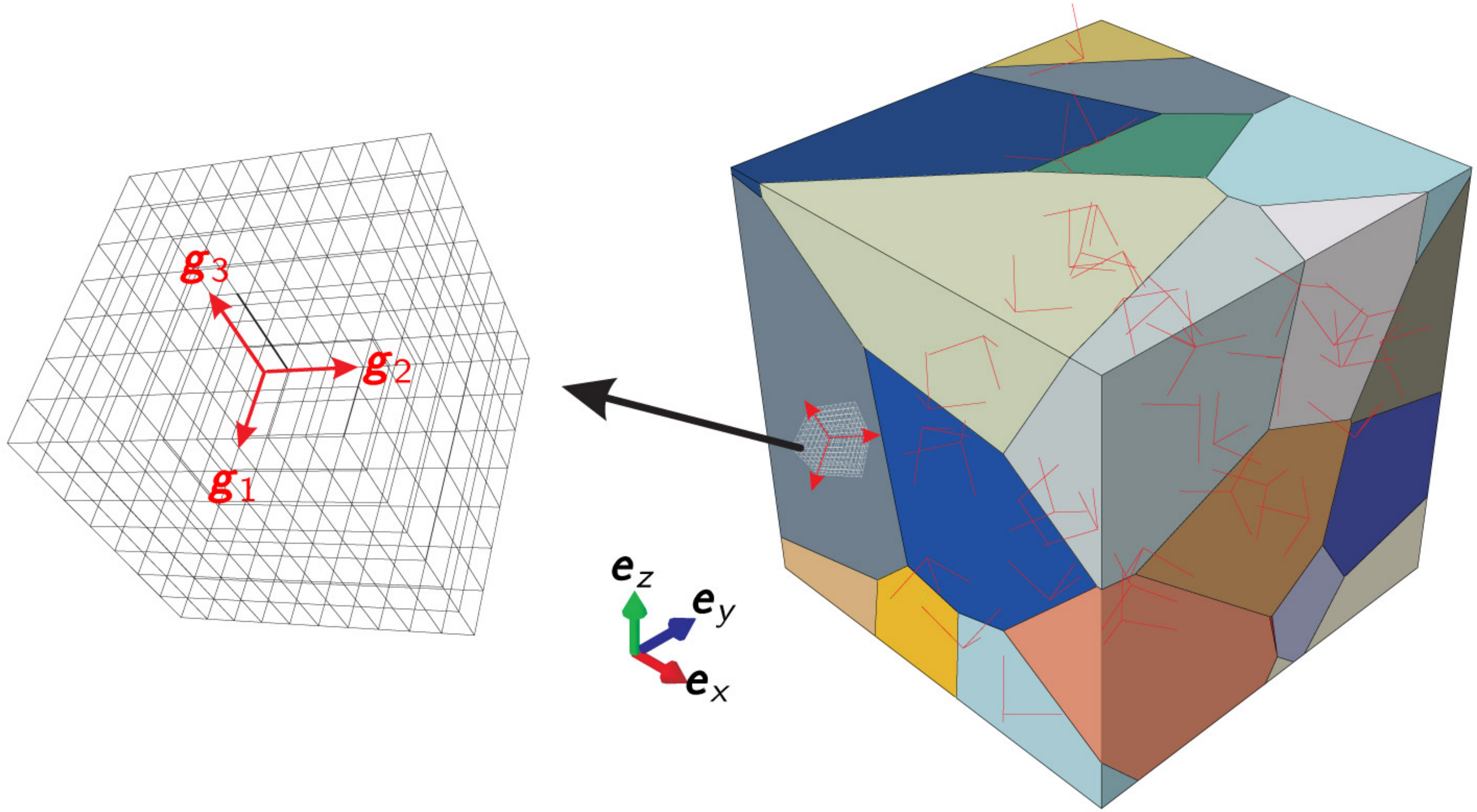
Unit cell consisting of 50 grains with non-zero grain border thickness



Unit cells consisting of 5 (50) grains with zero grain border thickness

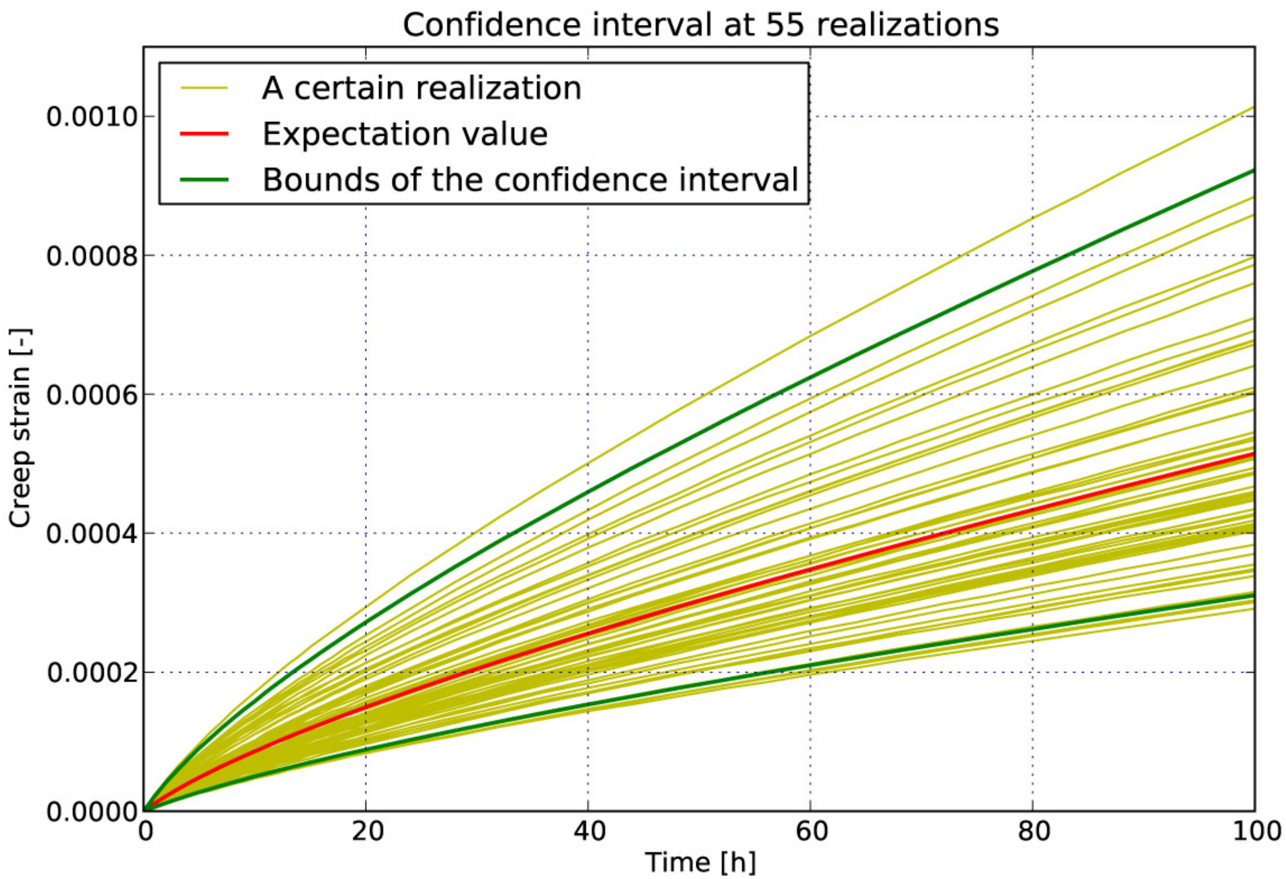
Modeling on Different Scales

Model of Polycrystal



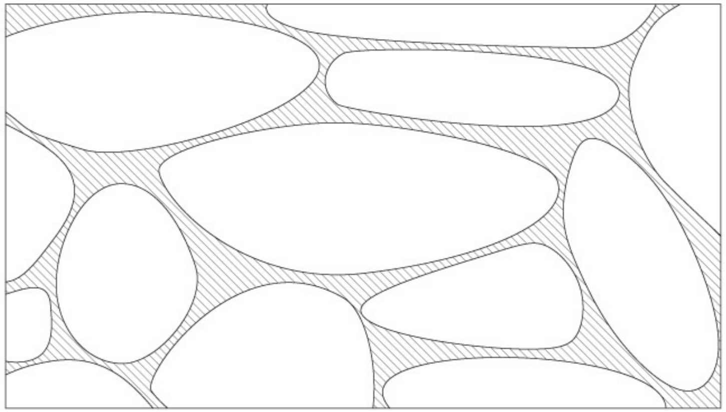
Creep Curves of 55 Realizations

Bounds of the Confidence Interval and Expectation Value

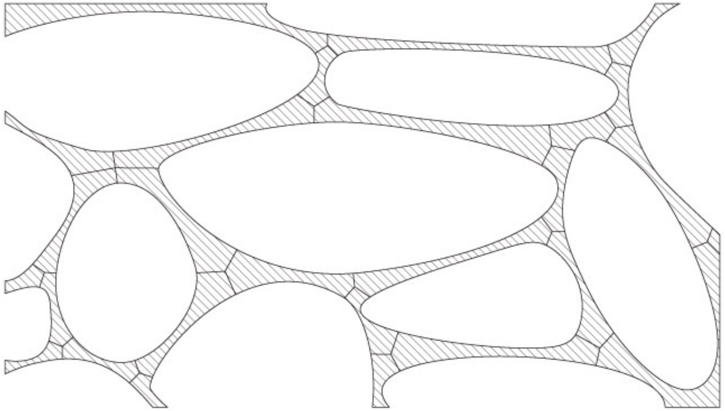


Porous Material Representation

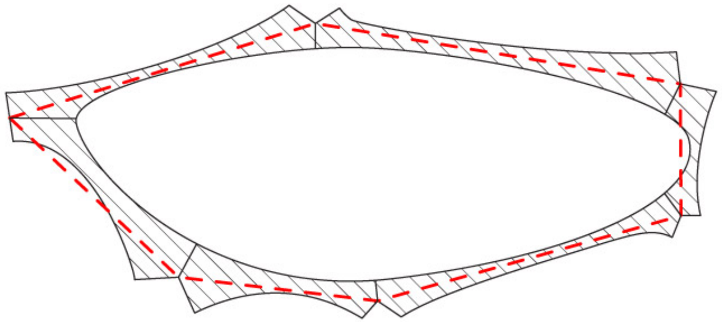
Closed Cell Foam Scheme



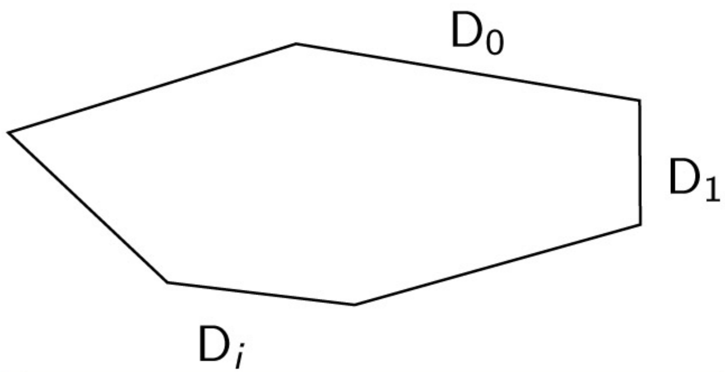
Interconnected Shells



Foam Cell



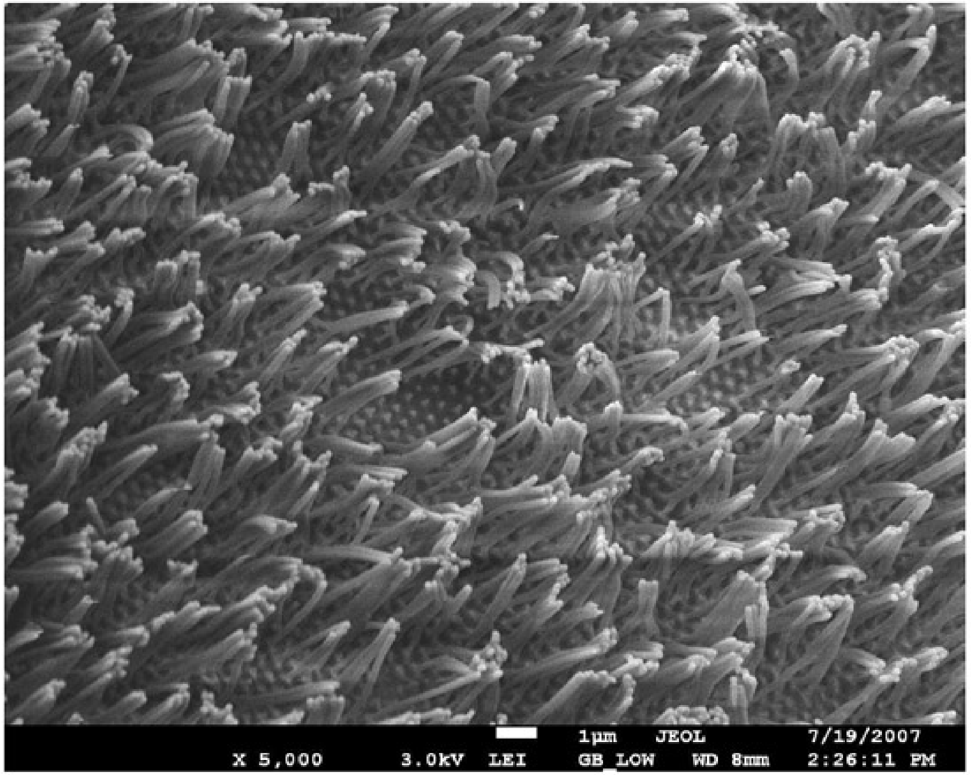
2D Voronoi Tessellation



Disordered Nanostructure

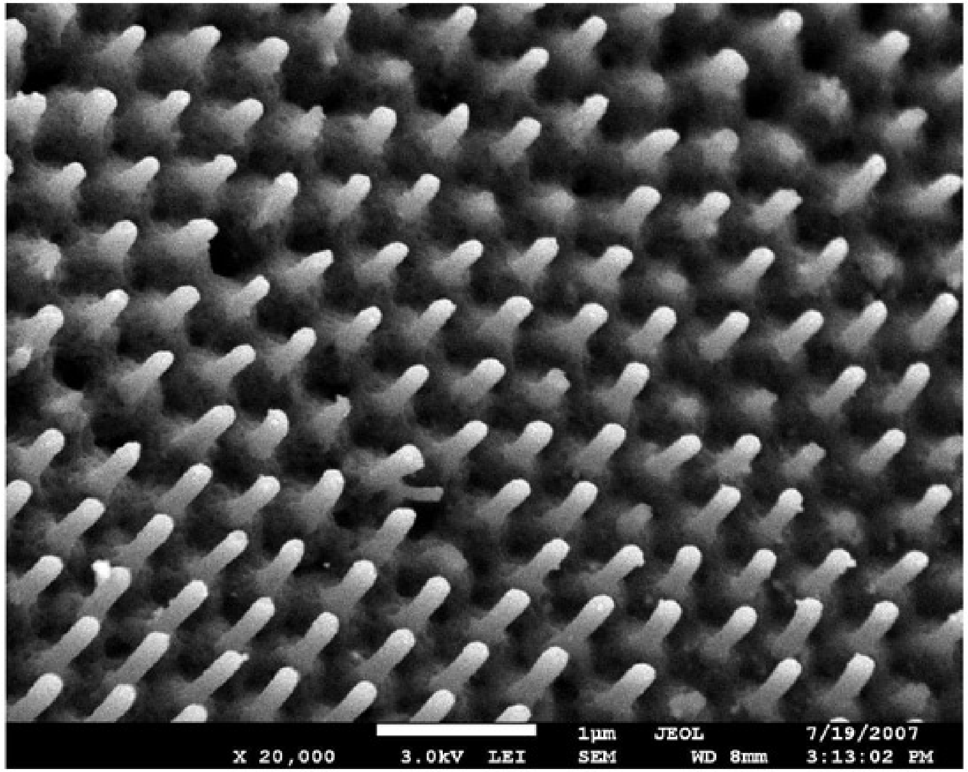
Crosslinked Polyetheracrylate: diameter: 120 nm, length: 4 μm

Disordered nanostructure as result of what:
the loss of stability (weight?) or adhesive forces



Ordered Nanostructure

Crosslinked Polyetheracrylate: diameter: 120 nm, length: 1 μm



Thank you for your attention!

Further questions:

holm.altenbach@ovgu.de