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Multiscale homogenization of elastic properties in hypereutectoid steel

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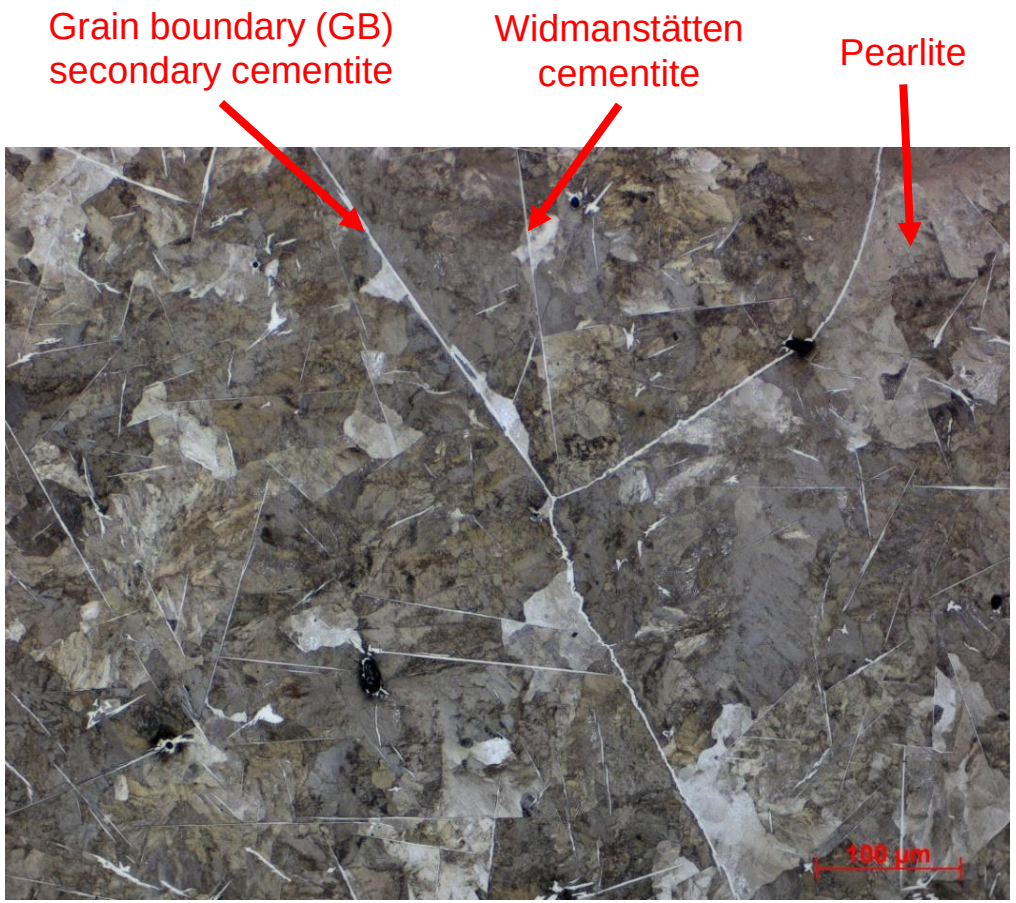
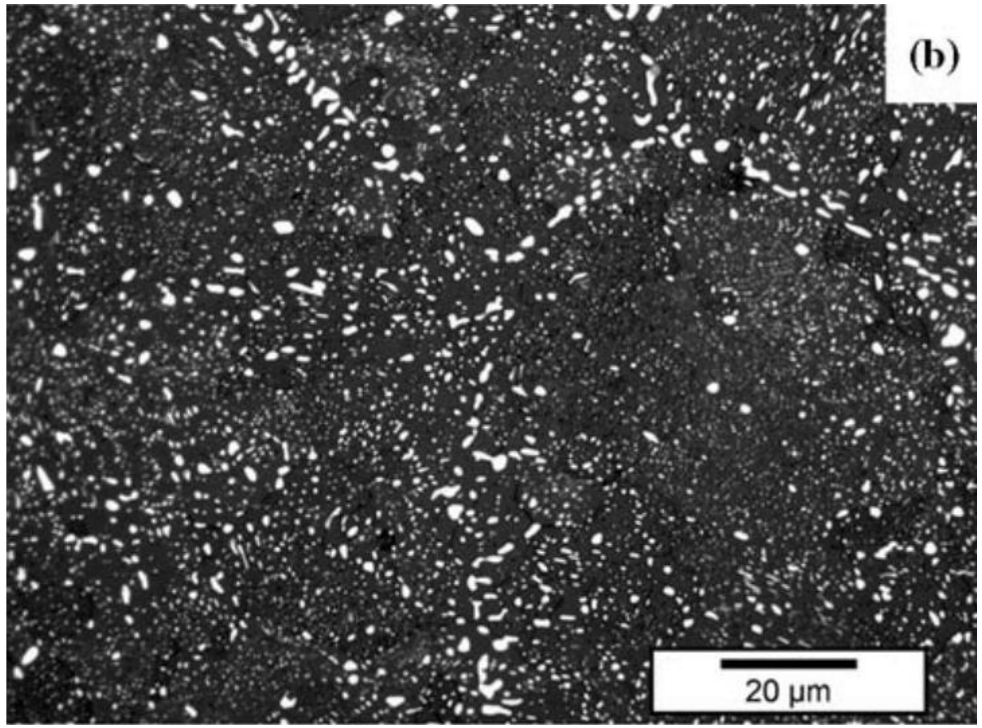
The microstructure of hypereutectoid steels



Bright field light microscopy micrograph of an as-cast hypereutectoid steel (1.2wt%C – 1wt%Mn – 1wt%Cu)



Micrograph of spheroidized microstructure with GB cementite network (1.04wt%C – 0.25wt%Si – 0.3wt%Mn – 0.53wt%Cr) [1]

Relevant parameters for hypereutectoid steel microstructure:

- Grain size
- Interlamellar spacing
- GB cementite thickness & continuity

[1] Luzginova et al., Metall. Mat. Trans. A, 39A, 2008, 513-521

Multiscale homogenization – Objectives

Investigated material properties: elastic stiffness tensor → Young's modulus, bulk modulus, shear modulus…

Statistically relevant RVE

Elastic properties of individual material phases

+

Phase morphological parameters

↓

Homogenized mean-field elastic properties

→ **Multiscale homogenization approach of the RVE**

<u>Caution:</u> rule of separation of scales!

Can we derive the macroscopic elastic properties of steel out of the elastic properties of cementite & pearlite, and of the microstructure's morphology?

Multiscale homogenization – Theoretical background

$$\boldsymbol{\Sigma} = \boldsymbol{C}^{hom} : \boldsymbol{E}$$

$$\boldsymbol{\Sigma} = \langle \boldsymbol{\sigma} \rangle \longleftrightarrow \boldsymbol{E} = \langle \boldsymbol{\varepsilon} \rangle$$

localization $\boldsymbol{\sigma}_p = \boldsymbol{B}_p : \boldsymbol{\Sigma}$

homogenization $\boldsymbol{\Sigma} = \sum_p f_p \boldsymbol{\sigma}_p$

localization $\boldsymbol{\varepsilon}_p = \boldsymbol{A}_p : \boldsymbol{E}$

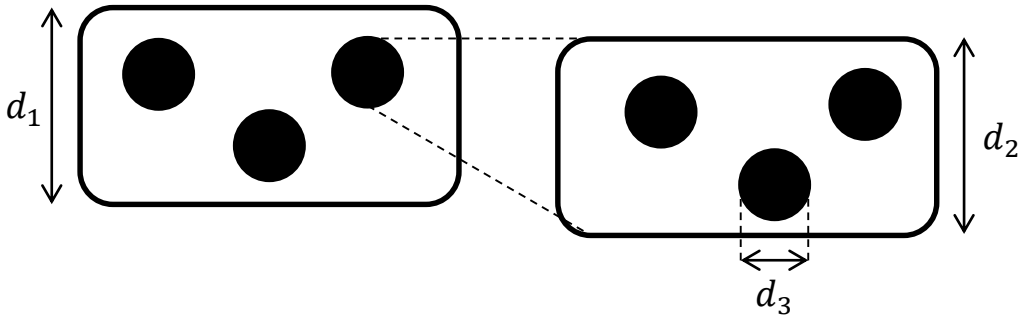
homogenization $\boldsymbol{E} = \sum_p f_p \boldsymbol{\varepsilon}_p$

$$\boldsymbol{\sigma}_p \longleftrightarrow \boldsymbol{\varepsilon}_p$$

$$\boldsymbol{\sigma}_p = \boldsymbol{C}_p : \boldsymbol{\varepsilon}_p$$

Separation of scales:

$$\boldsymbol{d_1} \gg \boldsymbol{d_2} \gg \boldsymbol{d_3}$$



How to derive $\boldsymbol{C}^{hom}$ from $\boldsymbol{C}_p$?

$$\boxed{\boldsymbol{C}^{hom} = \sum_p f_p \boldsymbol{C}_p : \boldsymbol{A}_p}$$

Multiscale homogenization – Model parametrization

Using matrix-inclusion calculations [1]:

$$\boldsymbol{C}^{\mathrm{hom}} = \sum_p f_p \boldsymbol{C}_p : \left[\boldsymbol{I} + \boldsymbol{P}_p^{\boldsymbol{0}} : \left(\boldsymbol{C}_p - \boldsymbol{C}^0\right)\right]^{-\boldsymbol{1}} : \left\{\sum_q f_q \left[\boldsymbol{I} + \boldsymbol{P}_{\boldsymbol{q}}^{\boldsymbol{0}} : \left(\boldsymbol{C}_q - \boldsymbol{C}^0\right)\right]^{-1}\right\}^{-1}$$

$\boldsymbol{C}^0$: accounts for interactions between phases

- Mori-Tanaka [2]
  → $\boldsymbol{C}^0 = \boldsymbol{C}_{\mathrm{matrix}}$
  → matrix-inclusion composites
- Classical self-consistent scheme (CSCS) [3]
  → $\boldsymbol{C}^0 = \boldsymbol{C}^{\mathrm{hom}}$
  → polycrystals & aggregates
- Generalized self-consistent scheme (GSCS) [4]
  → set of equations → $\boldsymbol{C}^0$
  → polycrystals with layer

For lamellar pearlite:

Generalized pearlitic aspect ratio:

$$\omega = \frac{\lambda}{l_{\mathrm{lam}}}$$

λ: Interlamellar spacing
l_{lam}: length of pearlite lamellae

$\boldsymbol{P}_p^{\boldsymbol{0}}$: 4th order Hill tensor, accounts for shape of inclusion p inside matrix $(\boldsymbol{C}^0)$

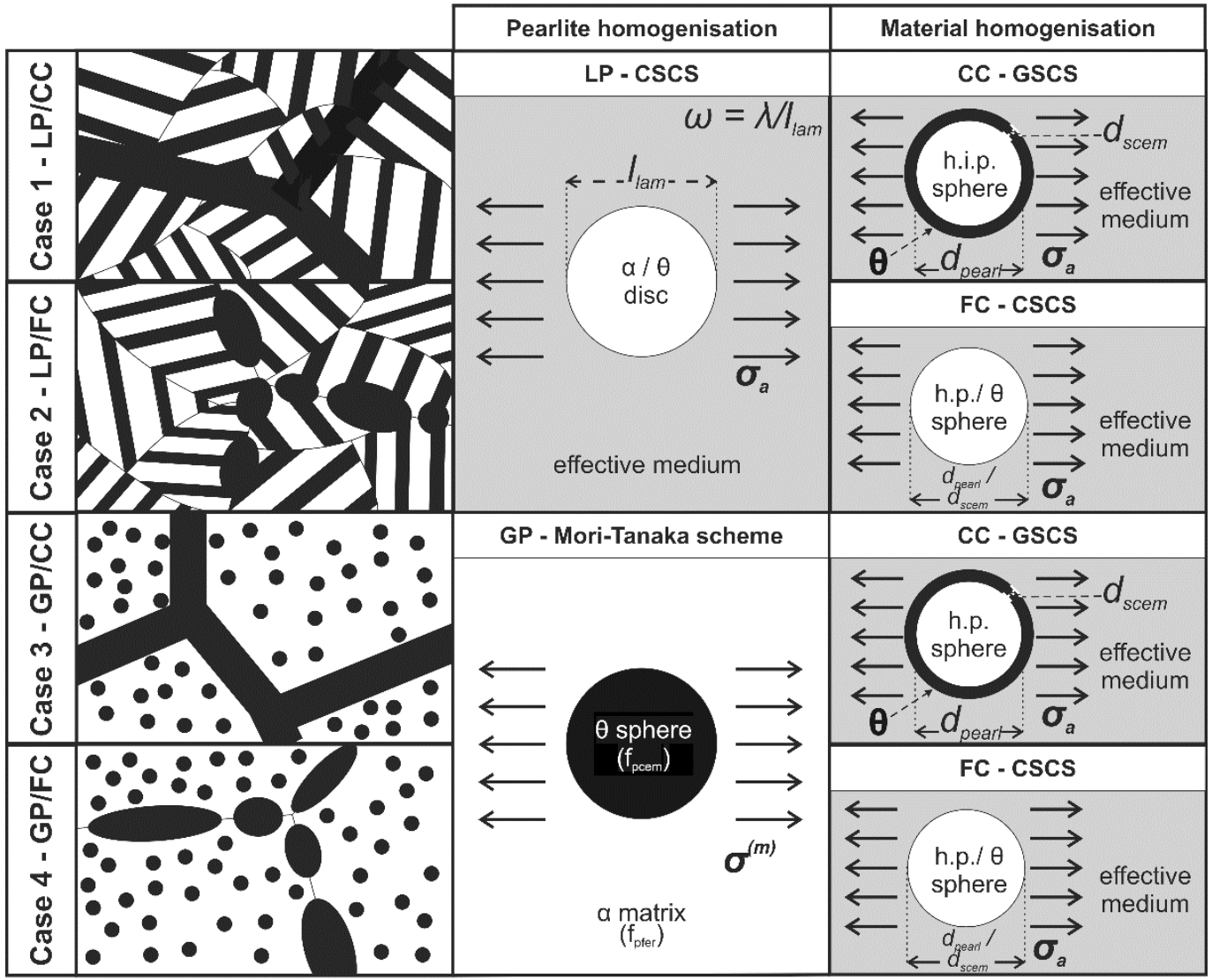
[1] Eshelby, Proc. R. Soc. London A, 241, 1957, 376-396

[2] Benveniste, Mech. Mater., 6, 1987, 147-157

[3] Hill, J. Mech. Phys. Solids, 13, 1965, 213-222

[4] Benveniste, J. Mech. Phys. Solids, 56, 2008, 2984-3002

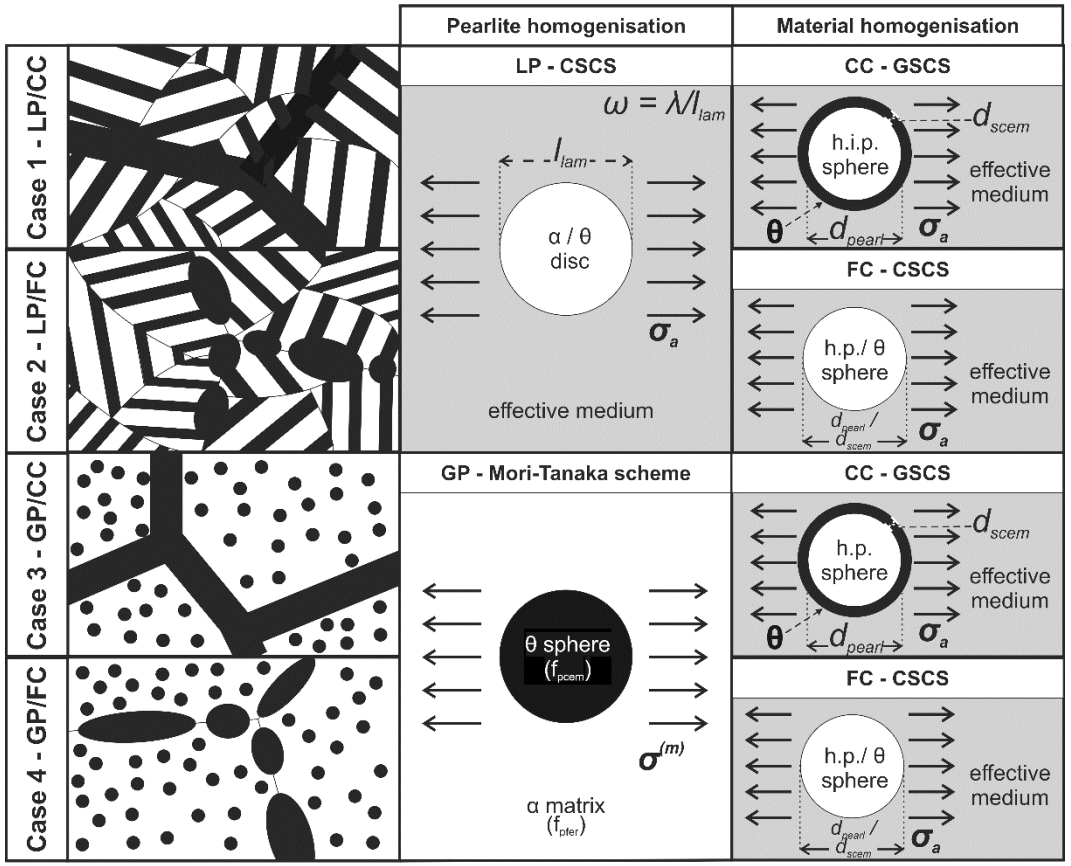
Model setup



Schematic representation of the microstructure types and the different steps of the multiscale modeling approach [1]

[1] Vogric, Povoden-Karadeniz, IJMR, 112, 2021, 348-358

Model setup



Schematic representation of the microstructure types and the different steps of the multiscale modeling approach [1]

- Minimal value of the generalized aspect ratio:

$$\omega \geq \frac{4.5\,\lambda}{d_{\mathrm{pearl}}}$$

d_{pearl}: size of a pearlite colony

- Diversity factor Δ for pearlite isotropy

- Material input data:

Ferrite [2]		Cementite [3]	
Bulk modulus (GPa)	Shear modulus (GPa)	Bulk modulus (GPa)	Shear modulus (GPa)
167	82	168	90

Microstructural parameters to investigate:

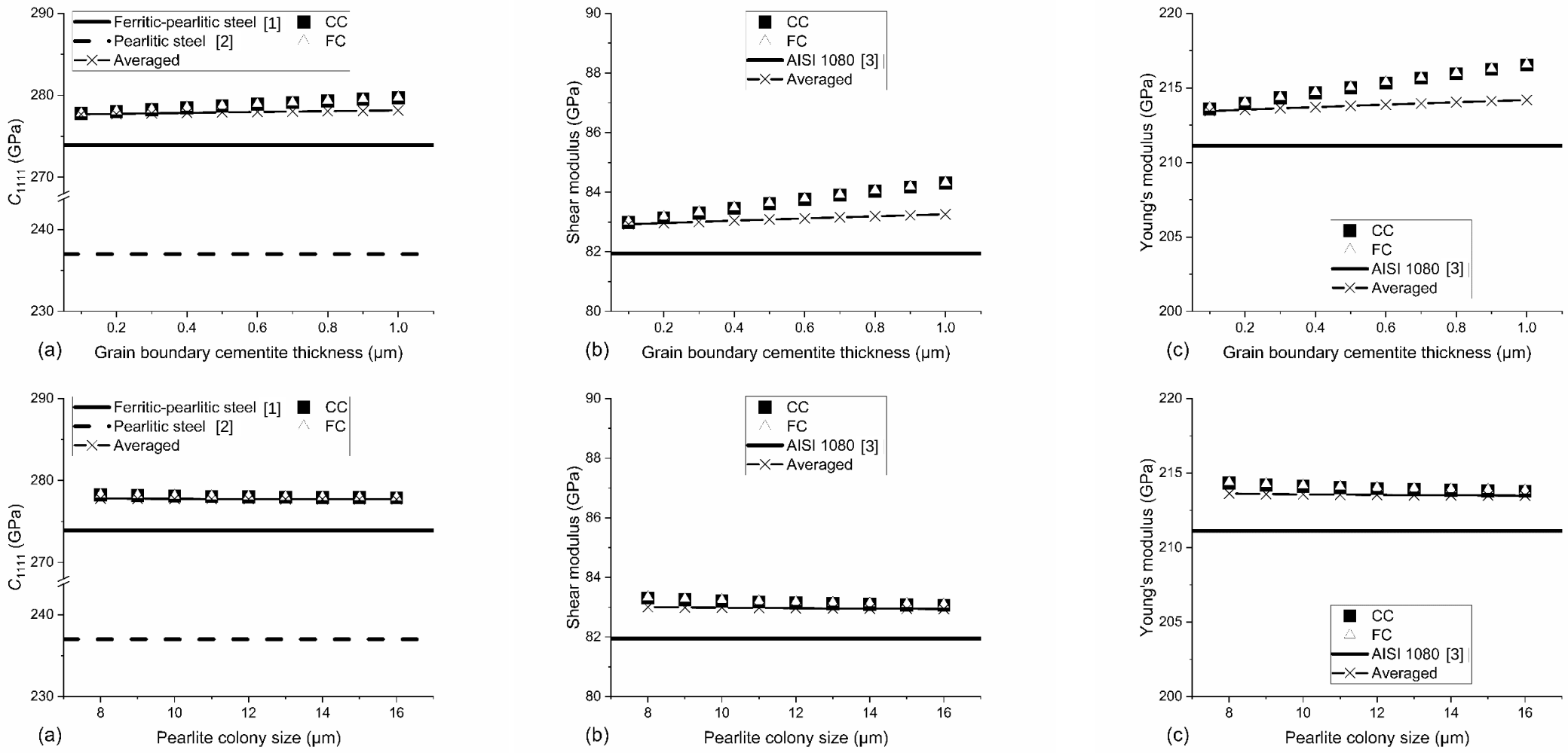
- GB cementite thickness d_{scem} (0.1 µm .. 1 µm)
- Pearlite colony size d_{pearl} (8 µm .. 16 µm)

[1] Vogric, Povoden-Karadeniz, IJMR, 112, 2021, 348-358

[2] Kim, Johnson, Mater. Sci. Eng. A, 452-453, 2007, 633-639

[3] Ledbetter, Mater. Sci. Eng. A, 527, 2010, 2657-2661

Results – Function of d_{scem} and d_{pearl}



[1] Kim, Johnson, Mater. Sci. Eng. A, 452-453, 2007, 633-639

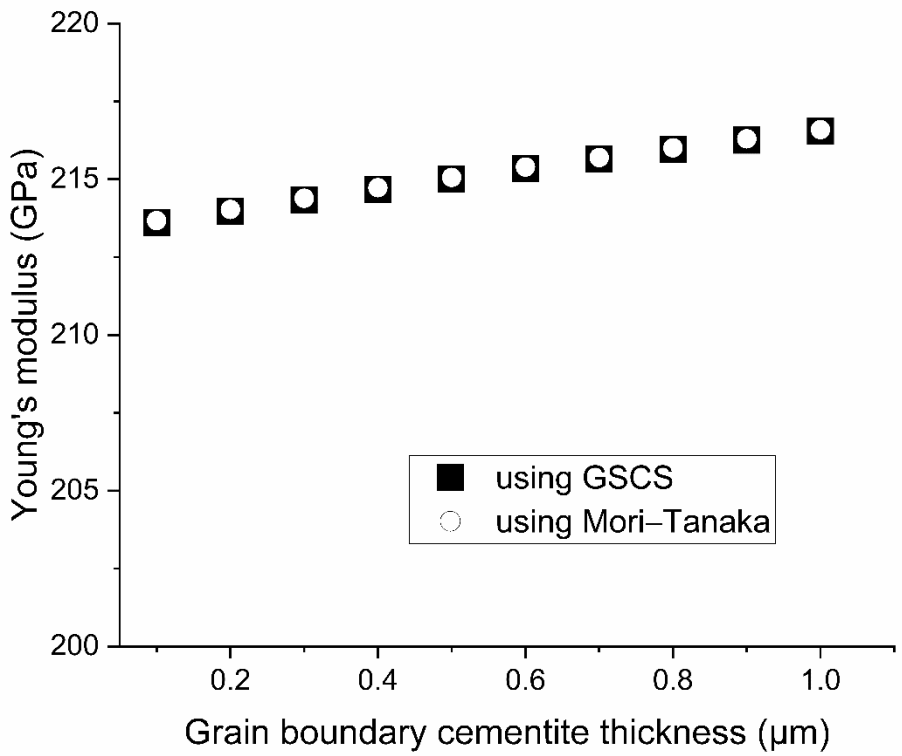
[2] Durgaprasad et al., Acta Mater., 129, 2017, 278-289

[3] Freitas et al., Mater. Sci. Eng. A, 527, 2010, 4431-4437

Results – Breaking the rule of separation of scales

Impact of variations of λ or ω is erased by the diversity factor Δ

→ Need to avoid the constraint of isotropic pearlite
→ Mori-Tanaka method for the LP/CC case BUT breaks the rule of separation of scale



Conclusion & Outlook

Proof of concept for *multiscale* modeling of elastic properties of hypereutectoid steels:

- 4 types of microstructures ⇒ 4 calculation schemes
- Maximum 4 different microstructure parameters

Calculated elastic properties are very close to the experimentally determined values of lamellar pearlitic steels

Next steps:

- Consideration of anisotropy of elastic properties
- Consideration of plasticity

} ⇒ Indentation of pearlite colonies with various orientations

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