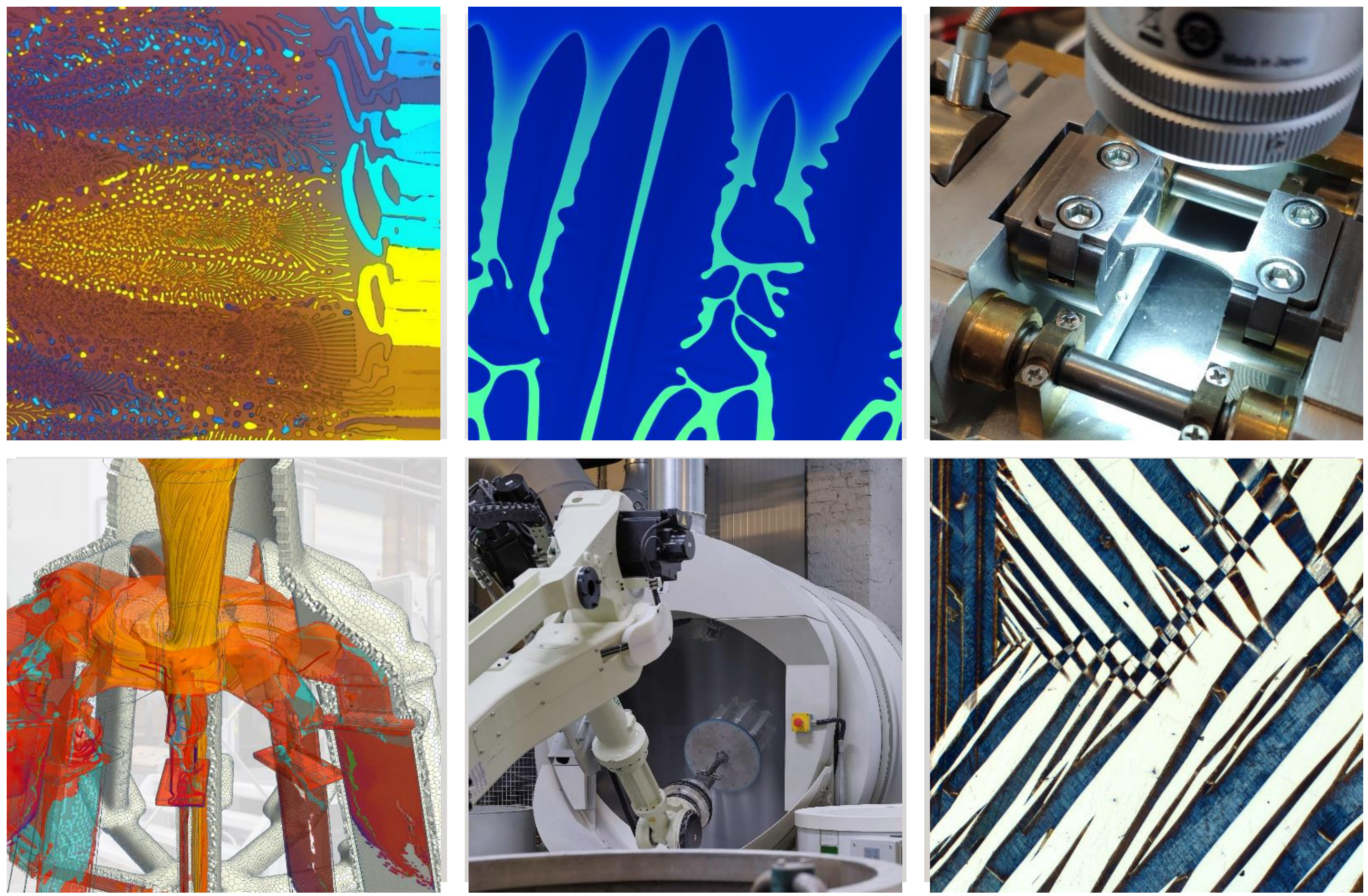
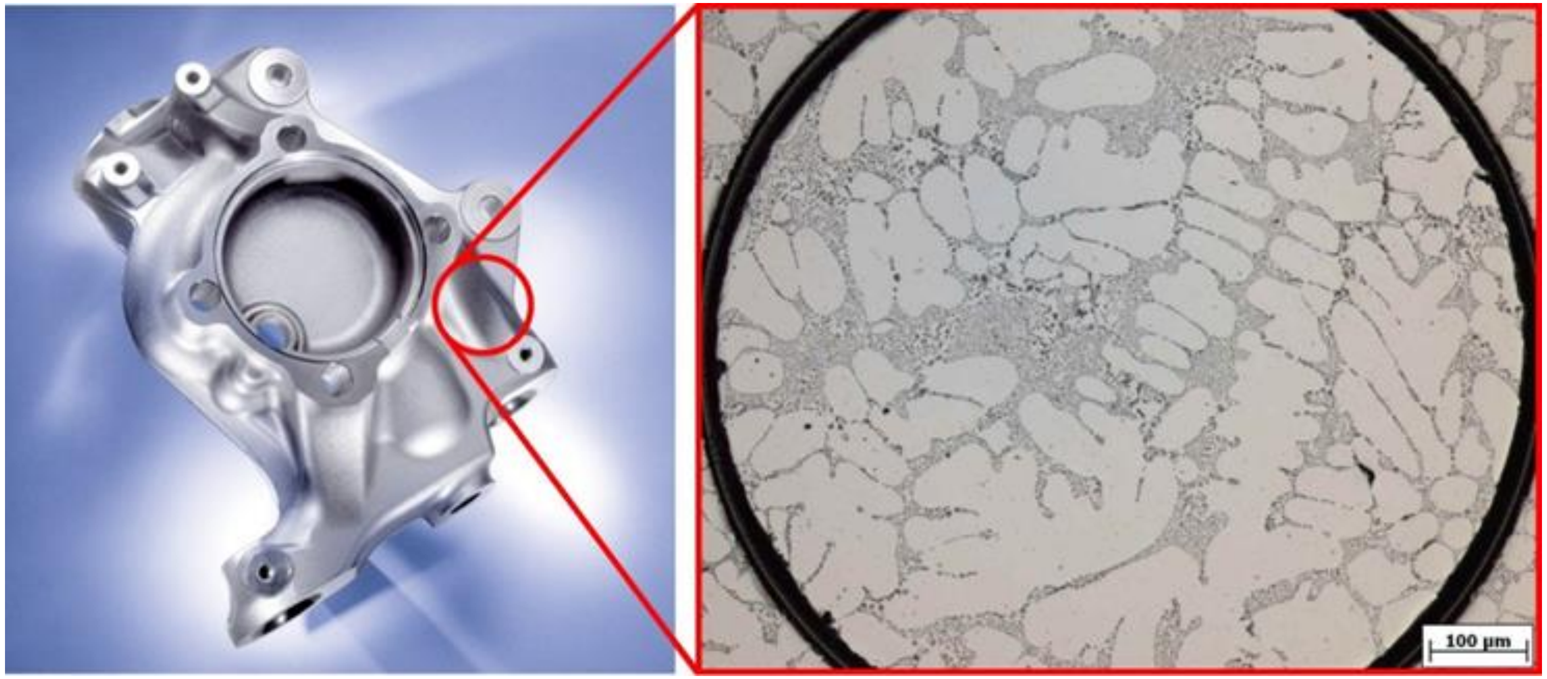


Microstructure Simulation as a Basis for Material Property and Casting Defect Predictions

M. Apel, B. Böttger, J. Eiken, B. Zhou, R. Berger, R. Altenfeld, …

Process → Microstructure → Properties → Performance

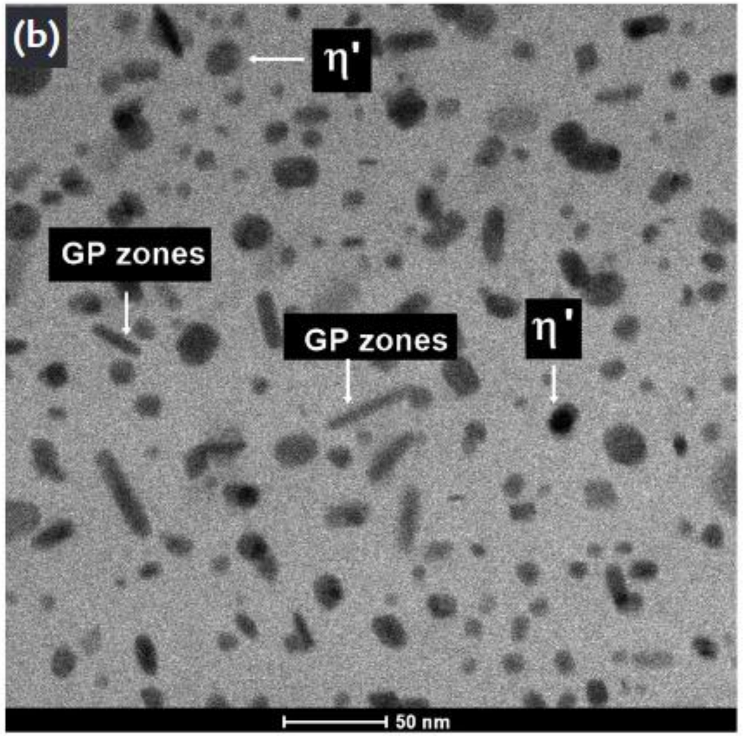


Material microstructures are the “carrier” of material properties

Microstructures are not a sole property of an alloy, but depend on processing history

➡ **Need for temporally and spatially resolved models**

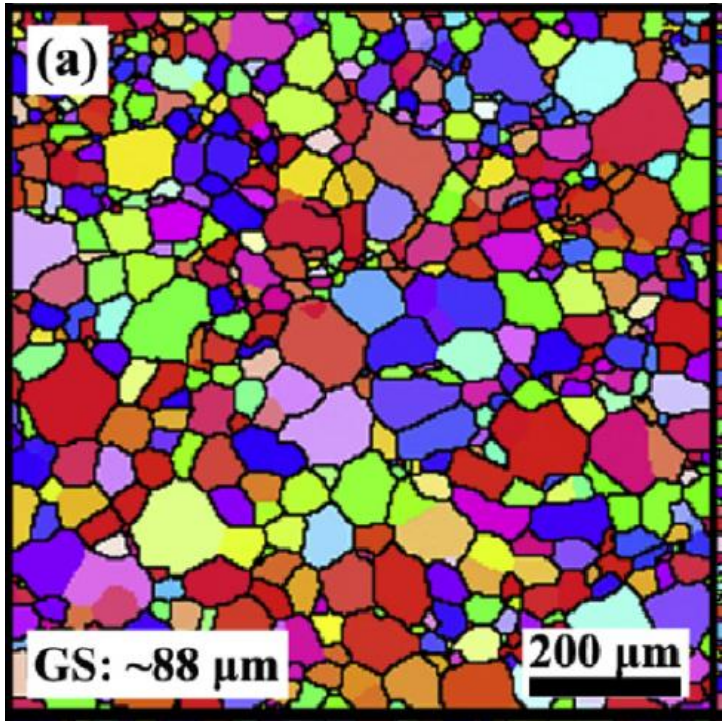
Material microstructures are naturally multiscale problems



precipitates and GP II zones in AA7050

Int. Eng. J., Ouro Preto, 69(4), 451-457 (2016)

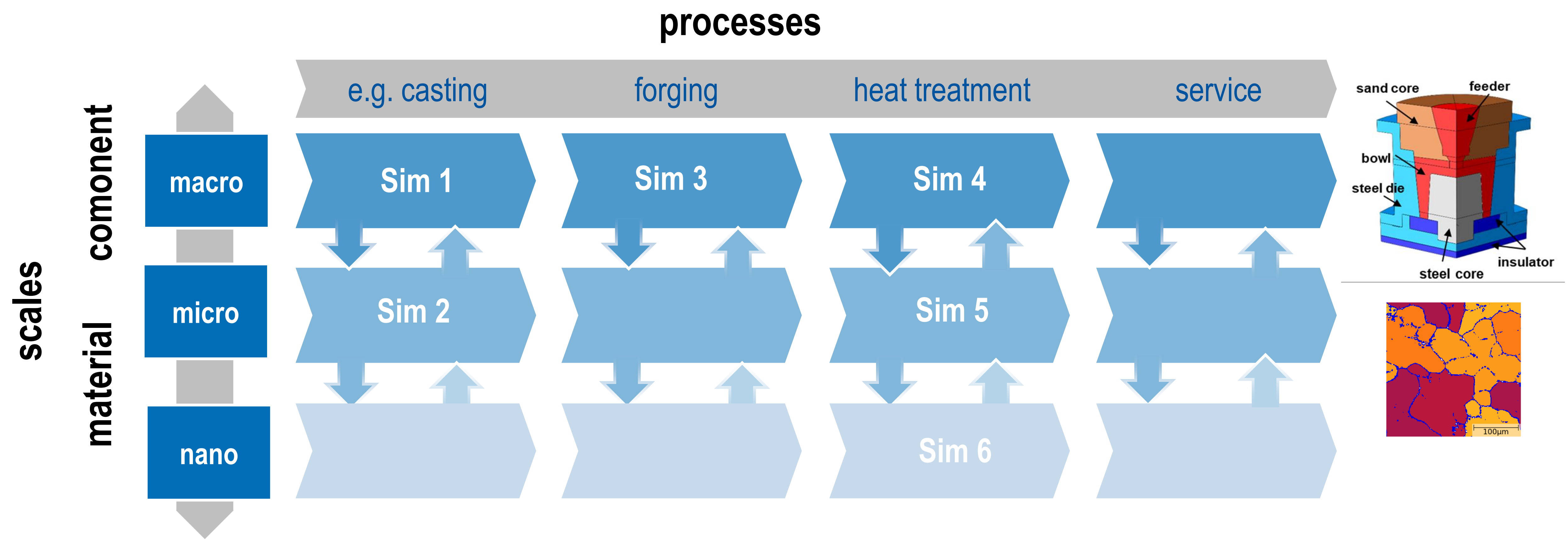
dendrites



grain structure in AA6061

Wang et al., J.Mat.Res.&Techn.,2022,pp.1566-1577

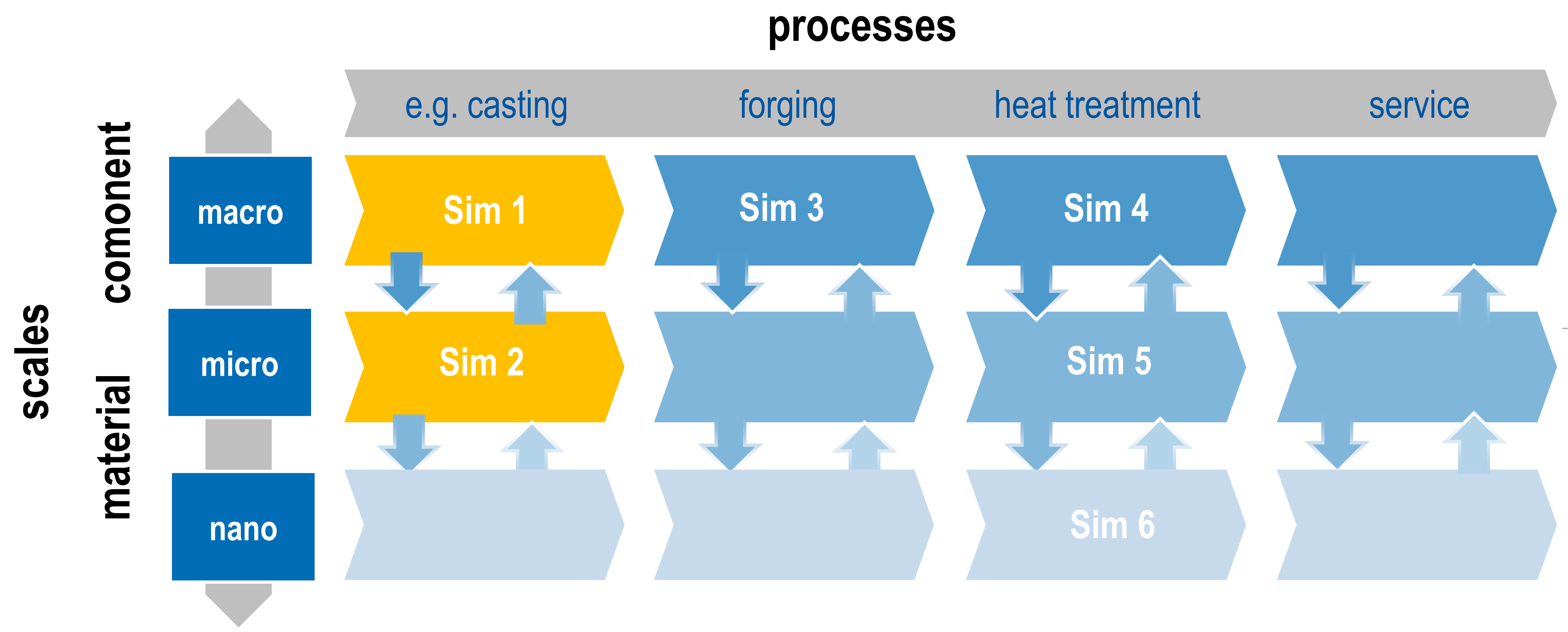
ICME: Integrated Computational Materials Engineering

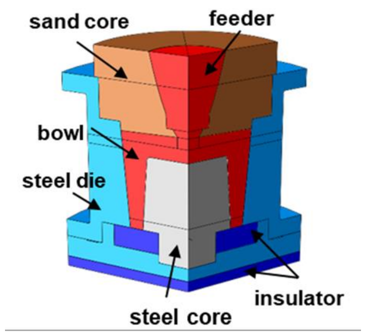


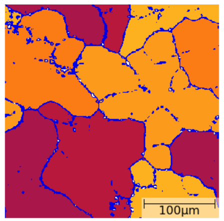
Vision:

multiscale through process modelling allows a holistic optimization of performance, costs, energy consumption, …

ICME: Integrated Computational Materials Engineering







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Outline

Solidification: microstructure informed latent heat release

→ H(T) consistent on macro- and microscale (beyond Scheil)

Microsegregation and precipitates

→ information about element distribution and nature of precipitates

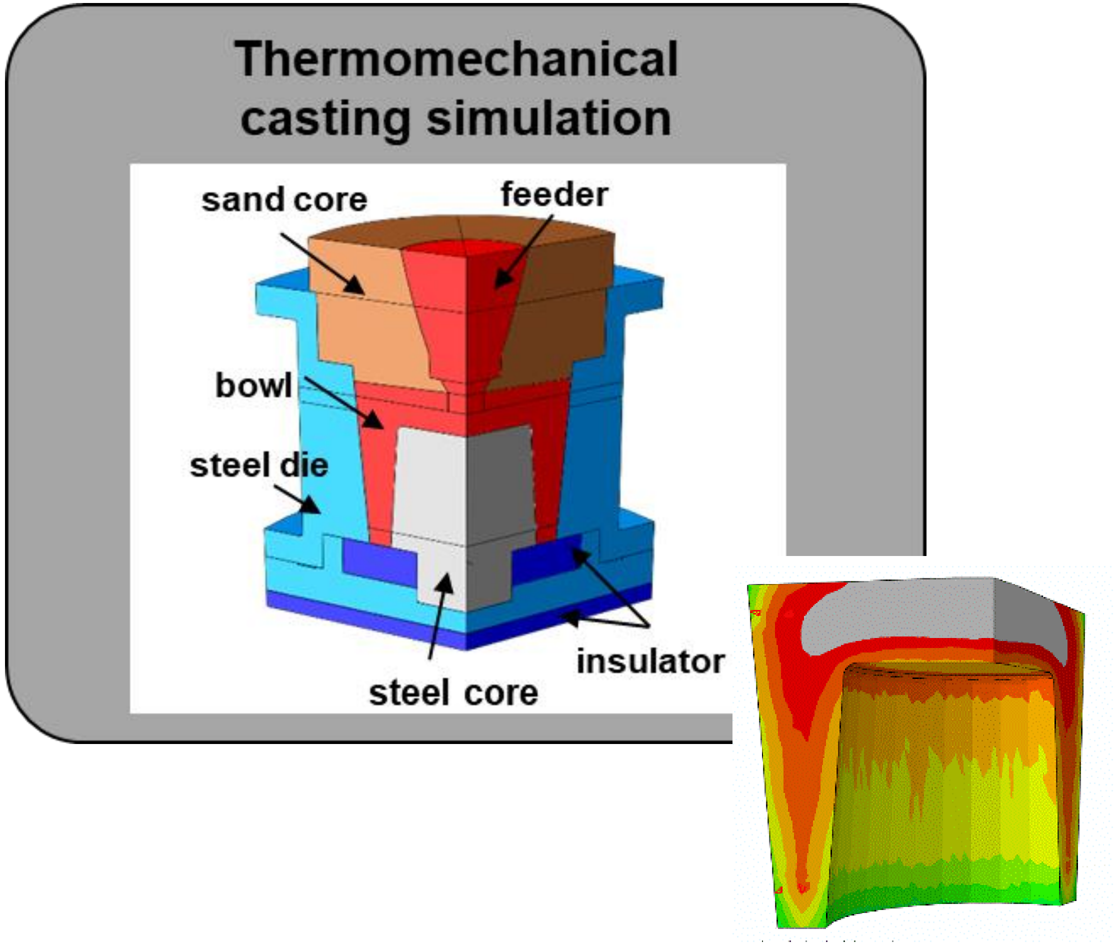
→ cheaper than EDX

→ unambitious identification of phases

Permeability of a mushy zone

→ input for hot cracking models

Microstructure informed latent heat release / enthalpy curve



Necessary input for casting simulations

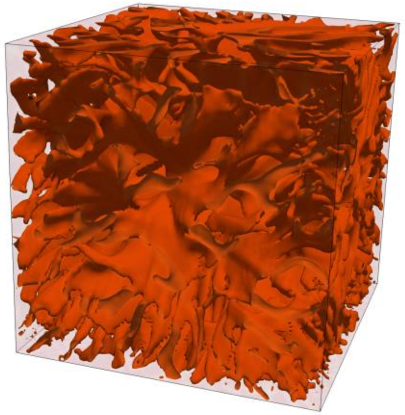
- H(T) for latent heat release, e.g. from Scheil model

Limitations of the Scheil model

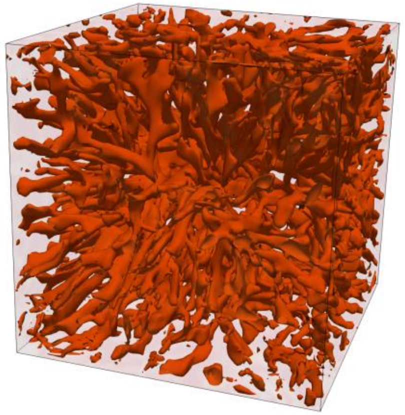
- independent of time and cooling rate
- no nucleation or growth undercooling

e.g. fails to describe the effect of Sr-modification in Al-Si

Eutectic Si morphology in A356 alloy 303µm3 RVE

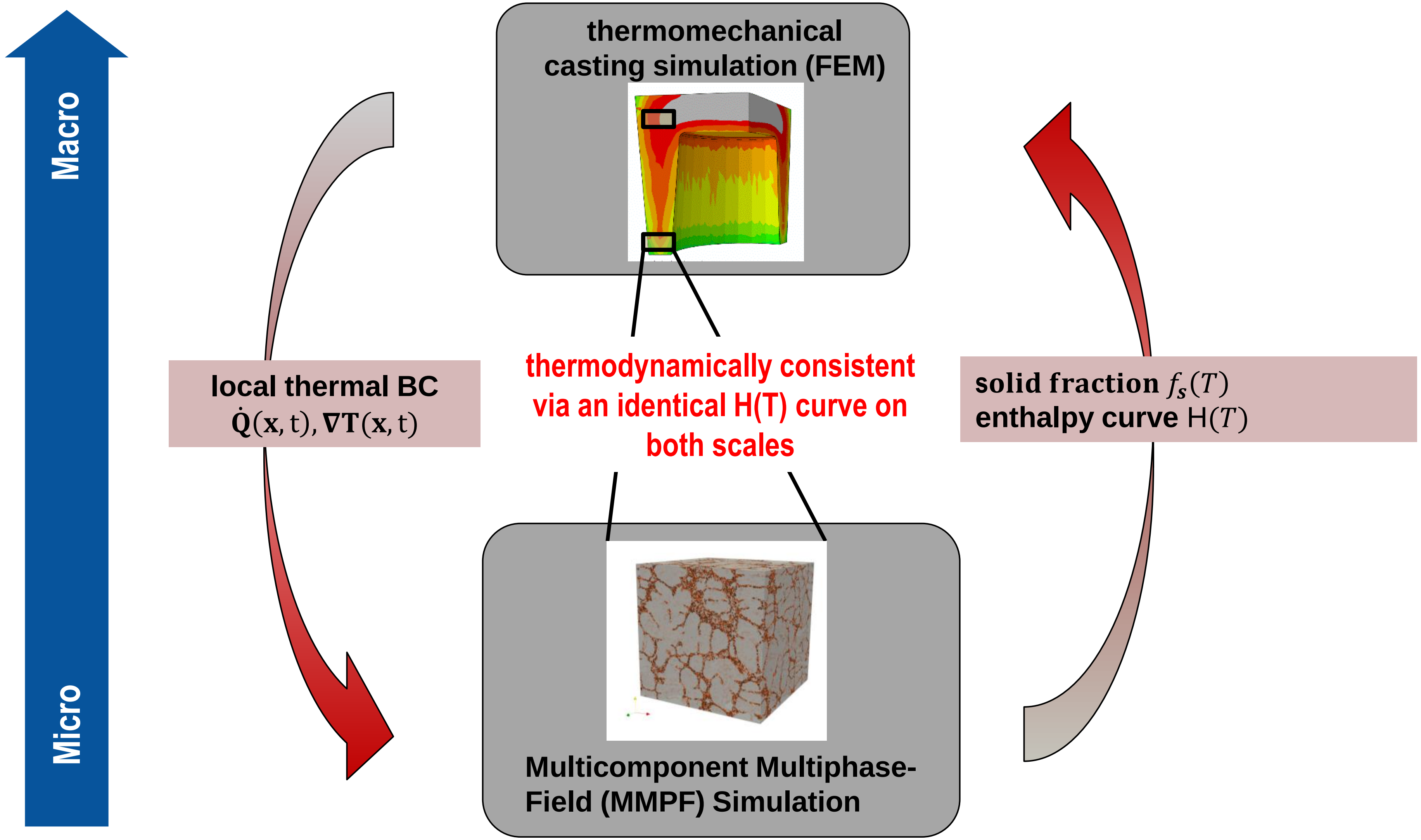


unmodified A356 alloy



Sr-modified A356 alloy

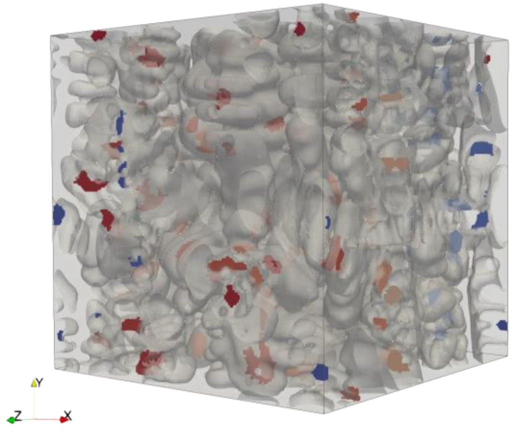
Microstructure informed latent heat release / enthalpy



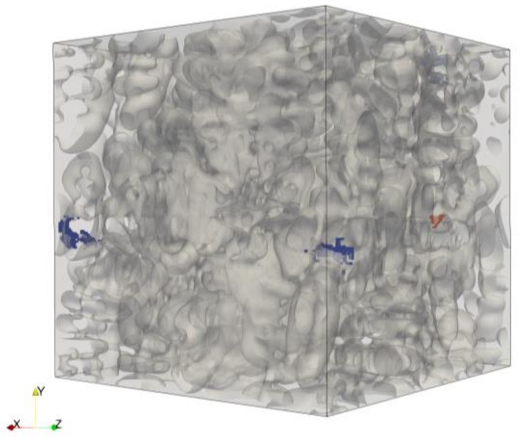
e.g. B. Zhou, G. Laschet, J. Eiken, H. Behnken, M. Apel, IOP Conf. Ser.: Mater. Sci. Eng. 861 012034 (2020)

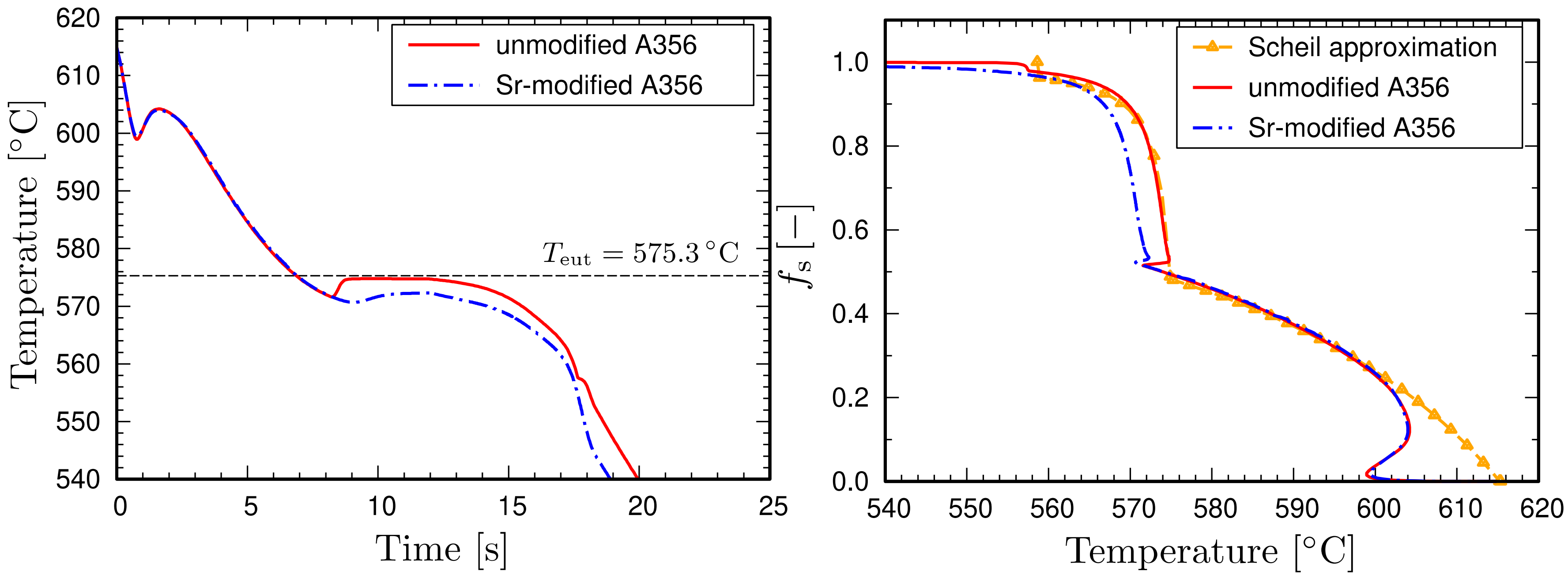
Effect of Sr-modification on solidification curve, H(T)

unmodified A356



Sr-modified A356

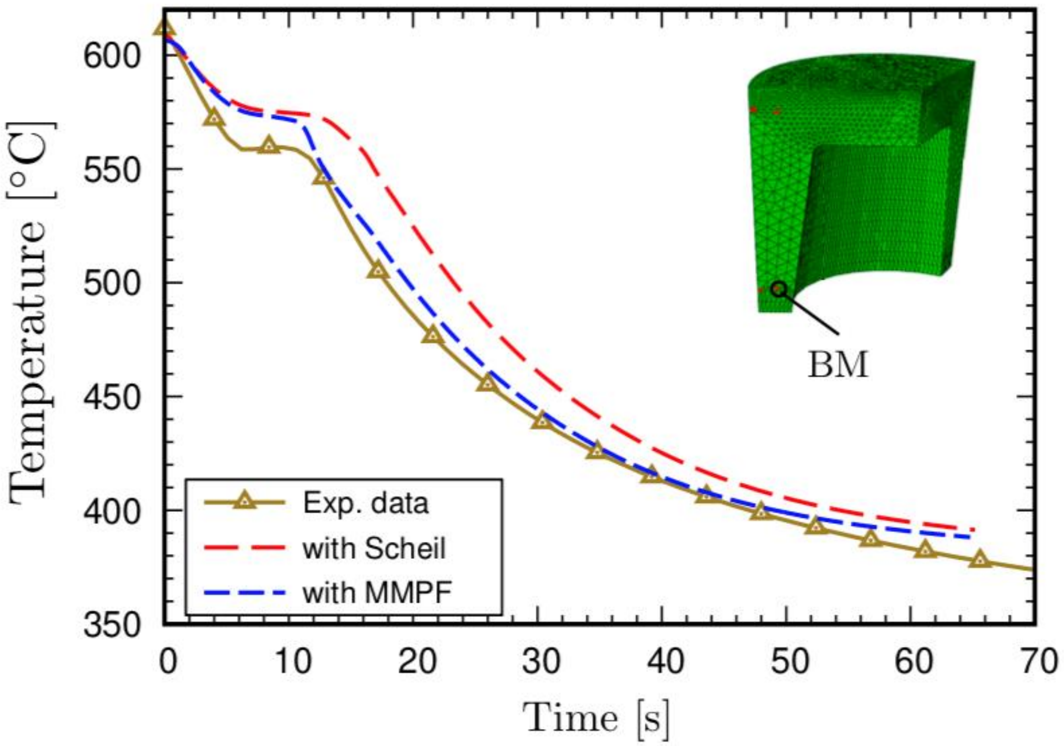


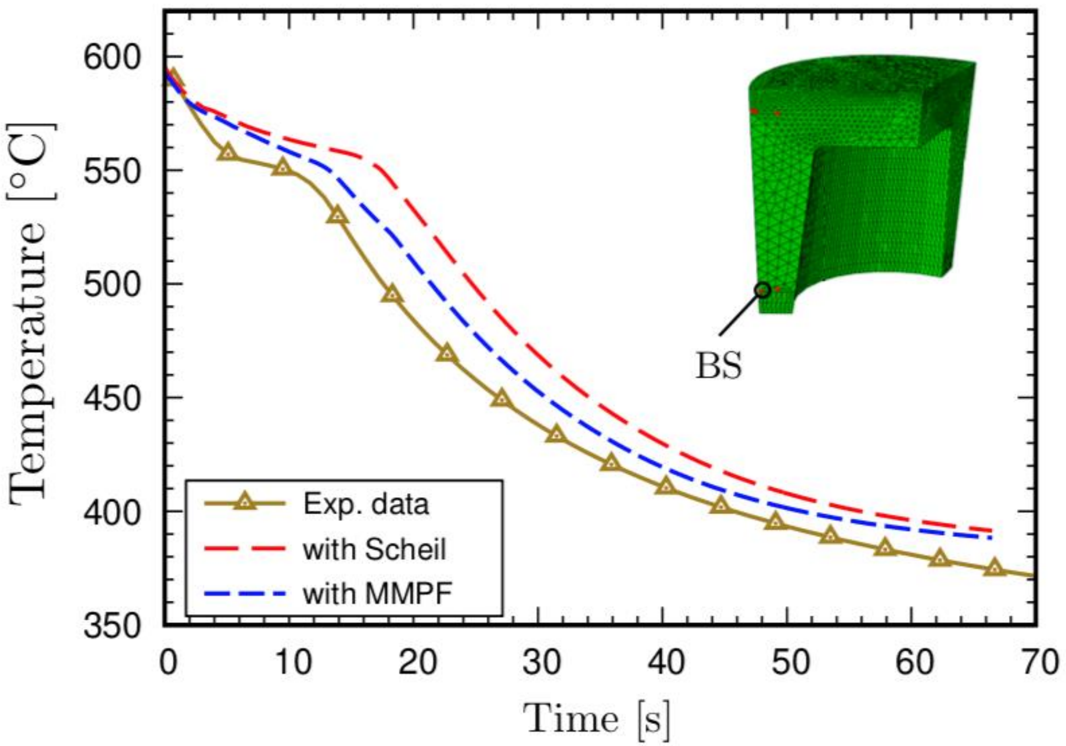


➡ higher eutectic growth undercooling due to Sr-modification

e.g. J. Eiken, M. Apel, S.-M. Liang, R. Schmid-Fetzer, Acta Materialia 98, pp. 152-163 (2015)

Effect on cooling curves from process simulation: Sr modified A356





➡ consistent and stable solution after 3-4 iterations

➡ better match to measurement, difference to Scheil solely by H(T)-curve

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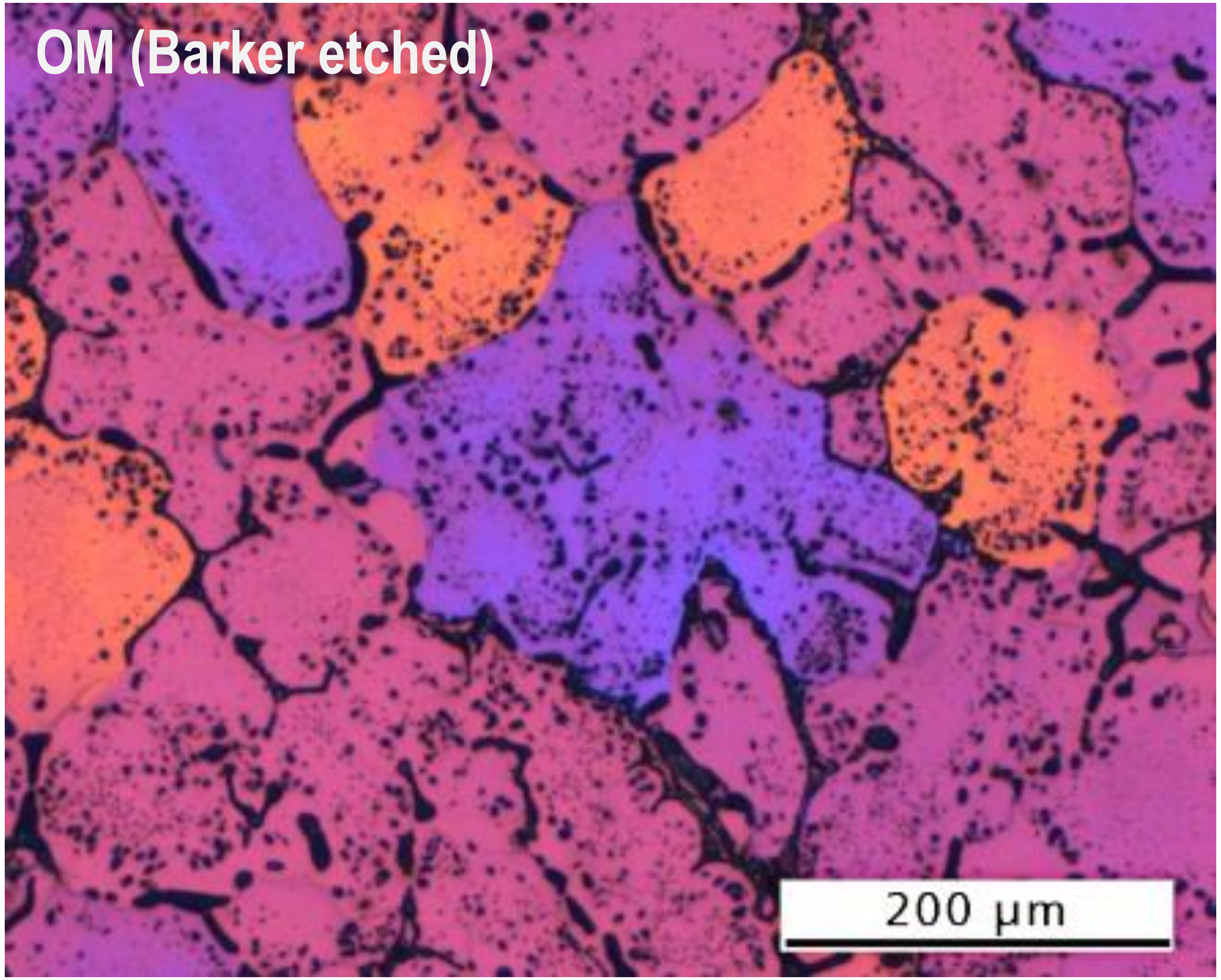
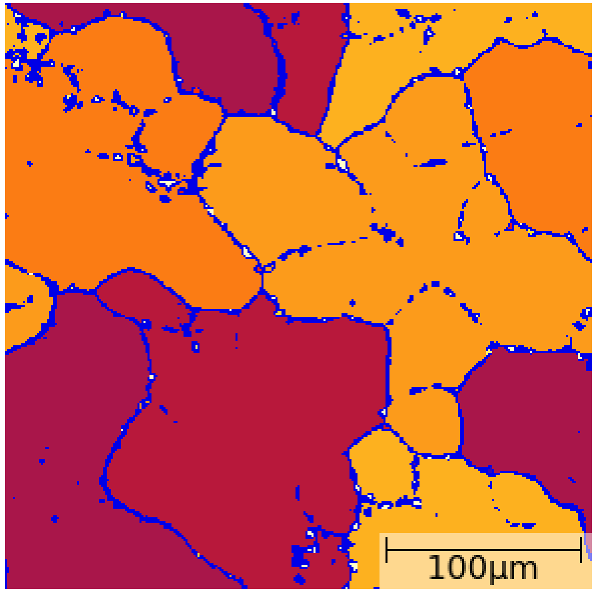
Example: AA6061

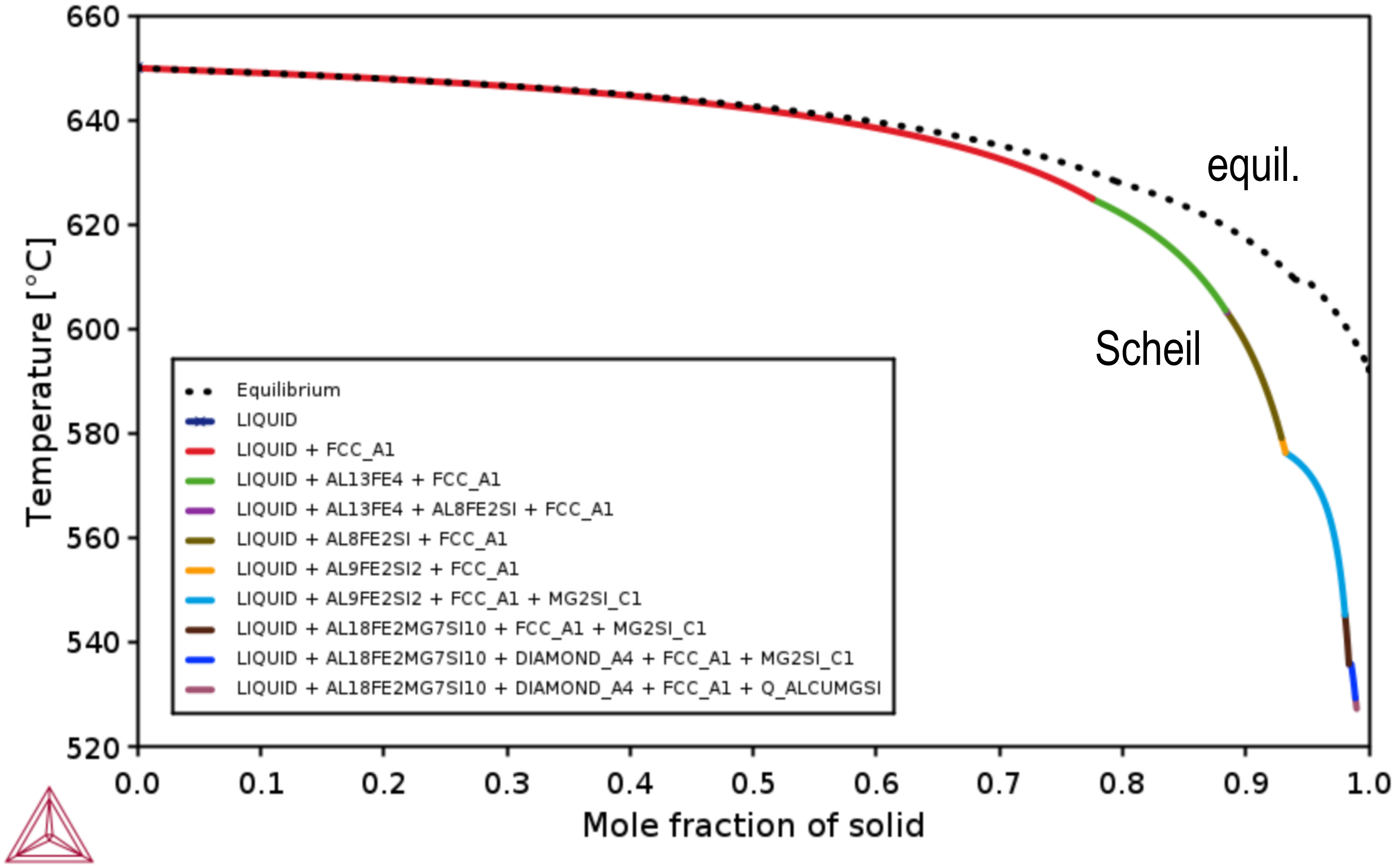


phase field simulation
(orientation)



Computational thermodynamics (CALPHAD)

AA6061	Al	bal.	Si	0.6	Mg	1.0	Cu	0.275	Fe	0.35	wt.%



equil.@ 590°C

⬇

fcc + Al8Fe2Si

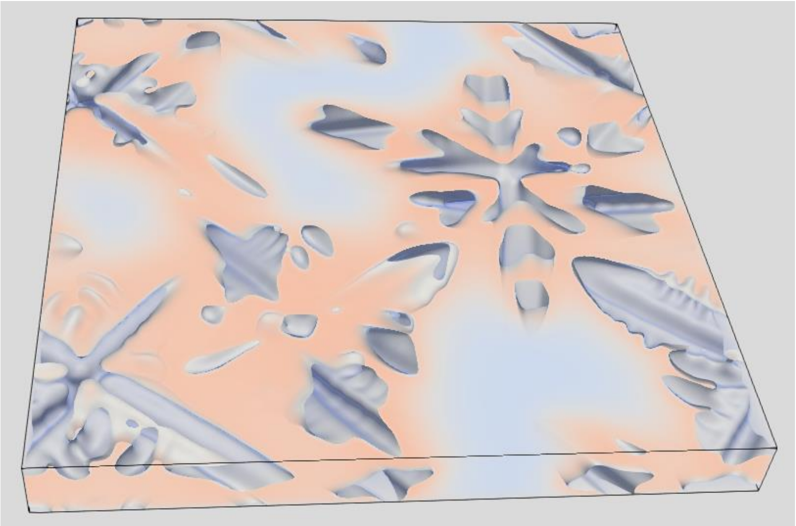
Scheil calculation

⬇

8 solid phases

➡ **Microstructures are also complex regarding "chemistry"**

domain size and resolution



250µm × 250µm × 25µm; Δx=0.75µm

thermodynamic quantities

- CALPHAD database TCAL8.2
- mobility data / diffusion

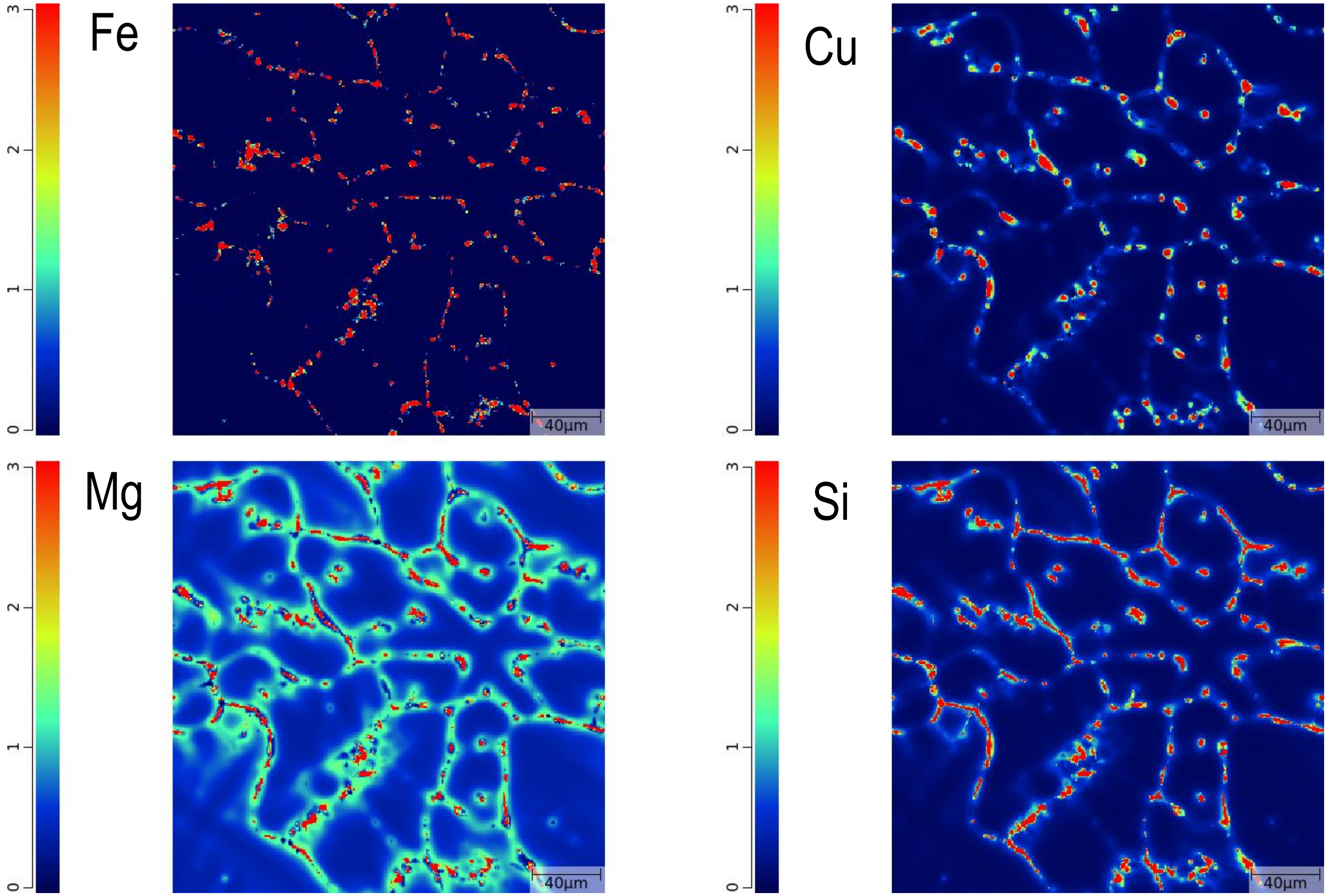
additional material properties

- interface mobilities and energies per phase pair
- anisotropies
- nucleation criteria: ΔT_{nuc}=5K

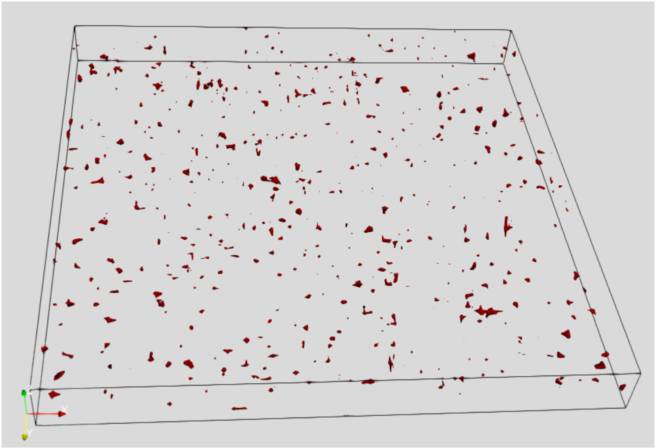
process conditions

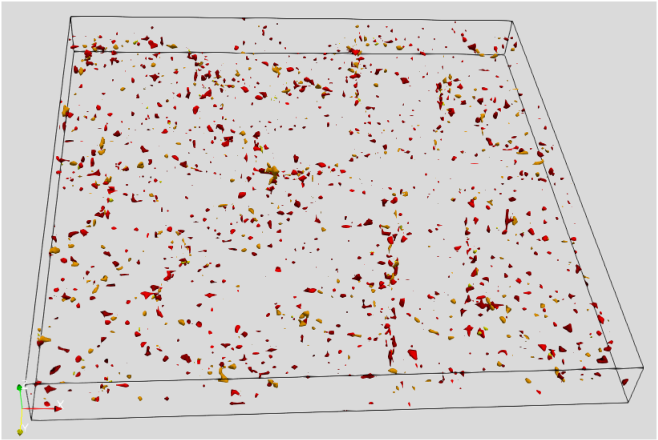
- alloy composition
- temperature or heat extraction

Microsegregation + precipitates in the as cast structure



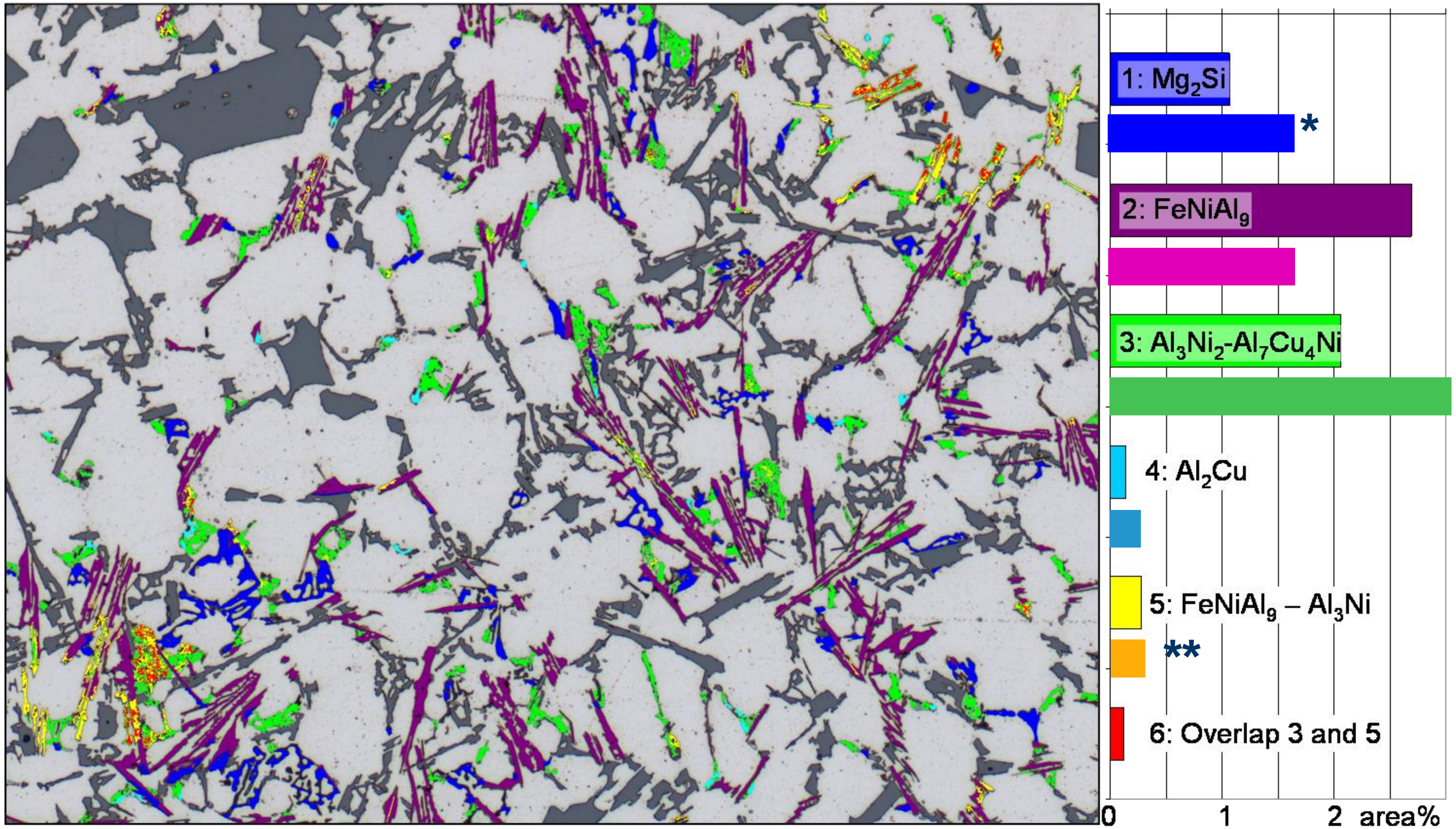
Fe13Al4: **0.317%**





all Fe-related phases: **0.842%**

Al-alloy for an automotive piston: phase analysis

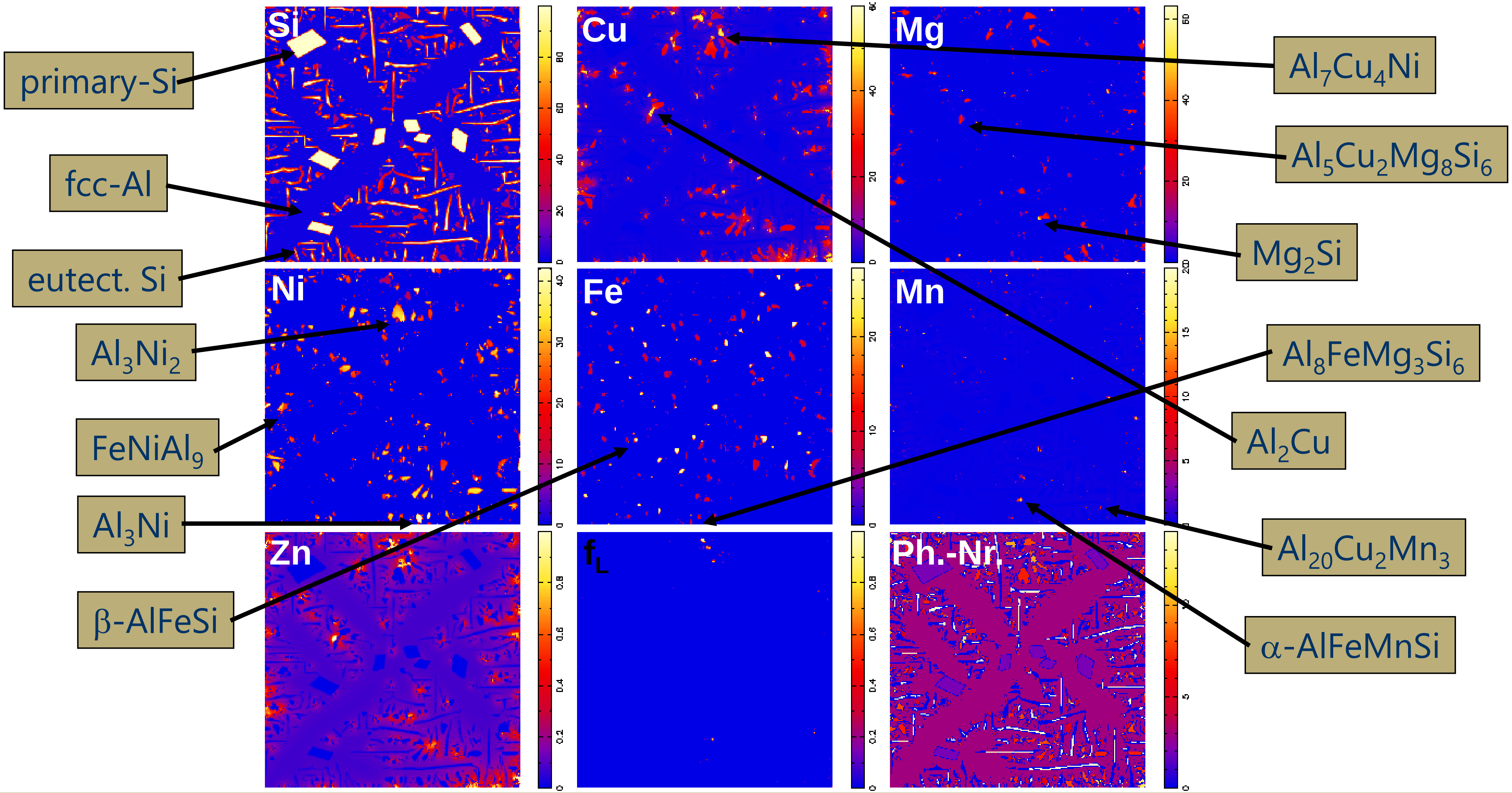


by S. Barnes, Manchester University

* *Mg_2Si + $Al_5Cu_2Mg_8Si$*

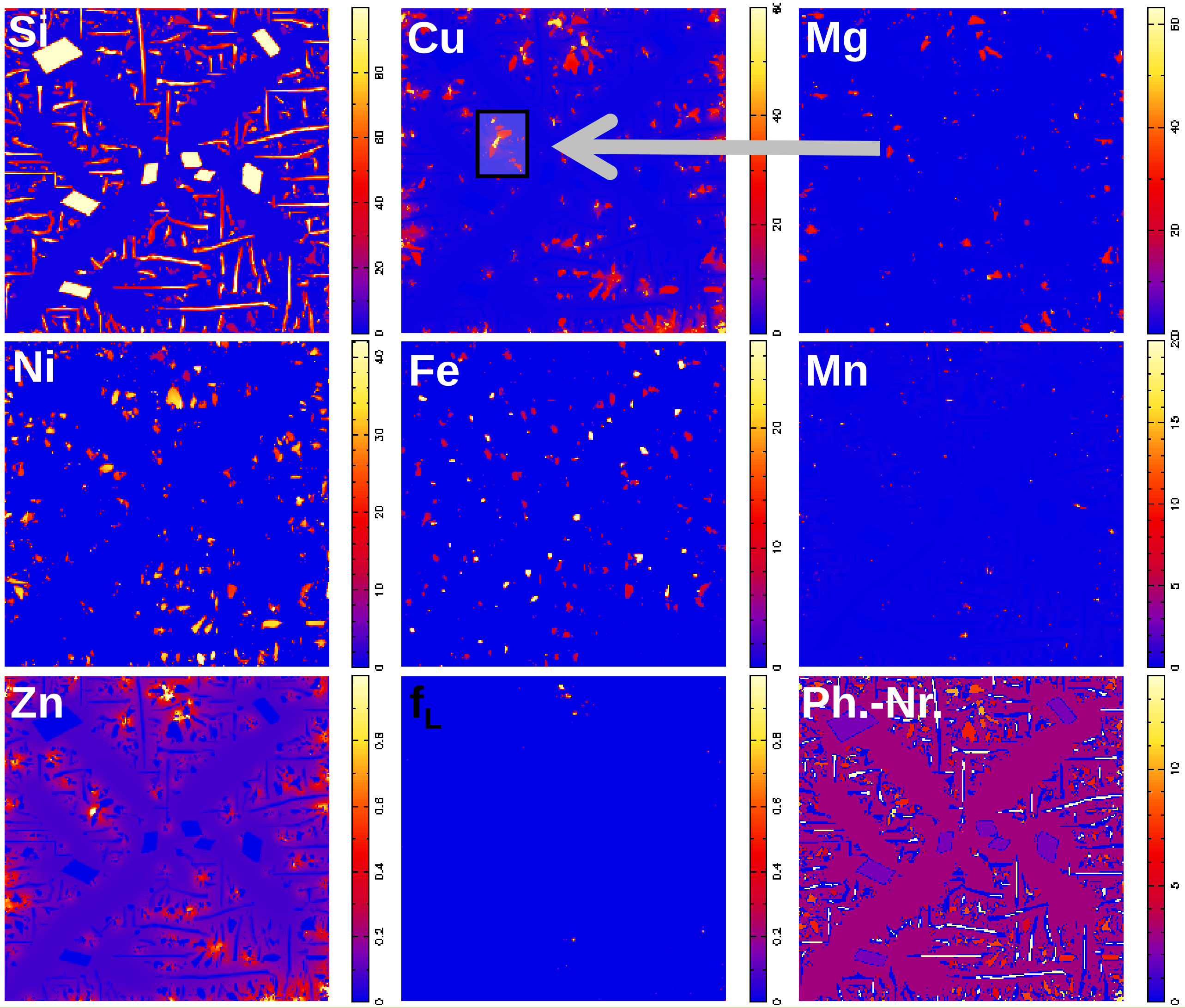
** *Al_3Ni*

Al piston alloy: 7 alloying elements, 14 phases

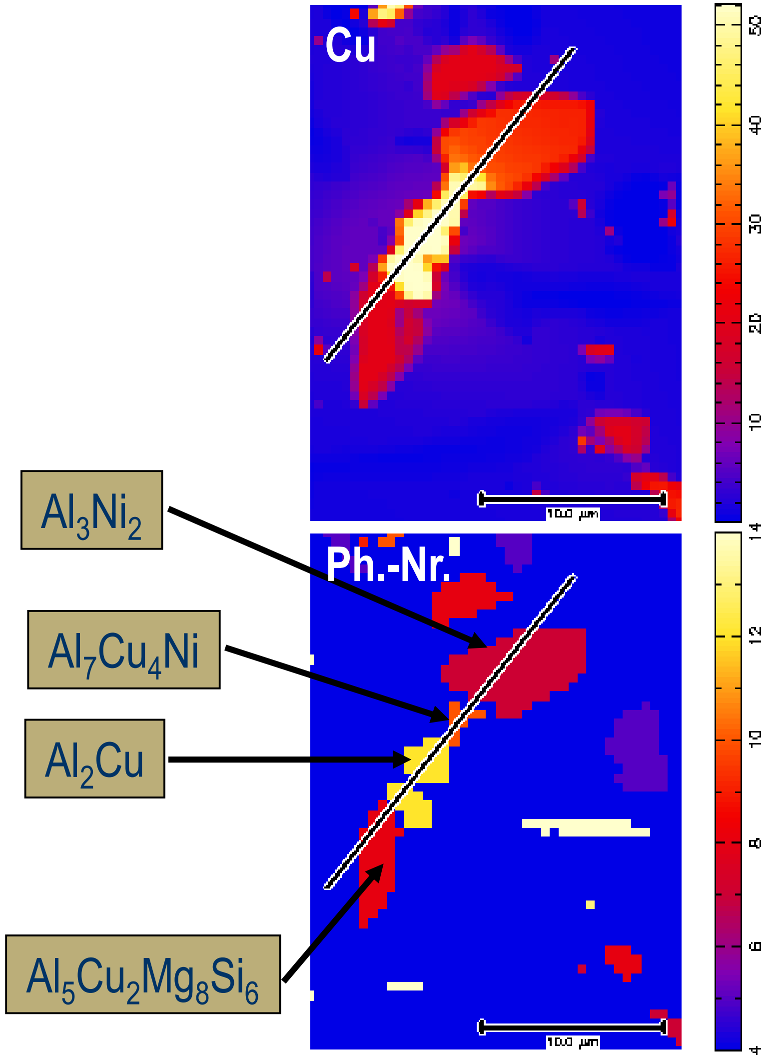


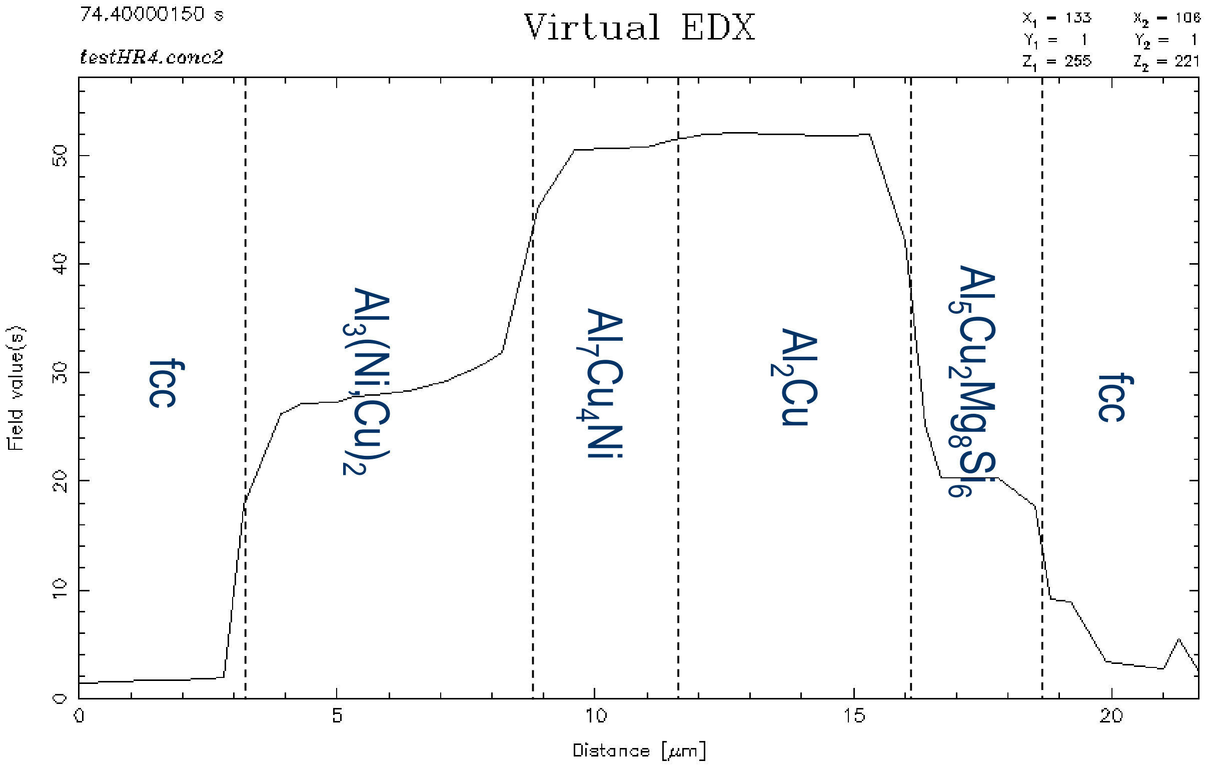
access

Spatial correlation of different phases

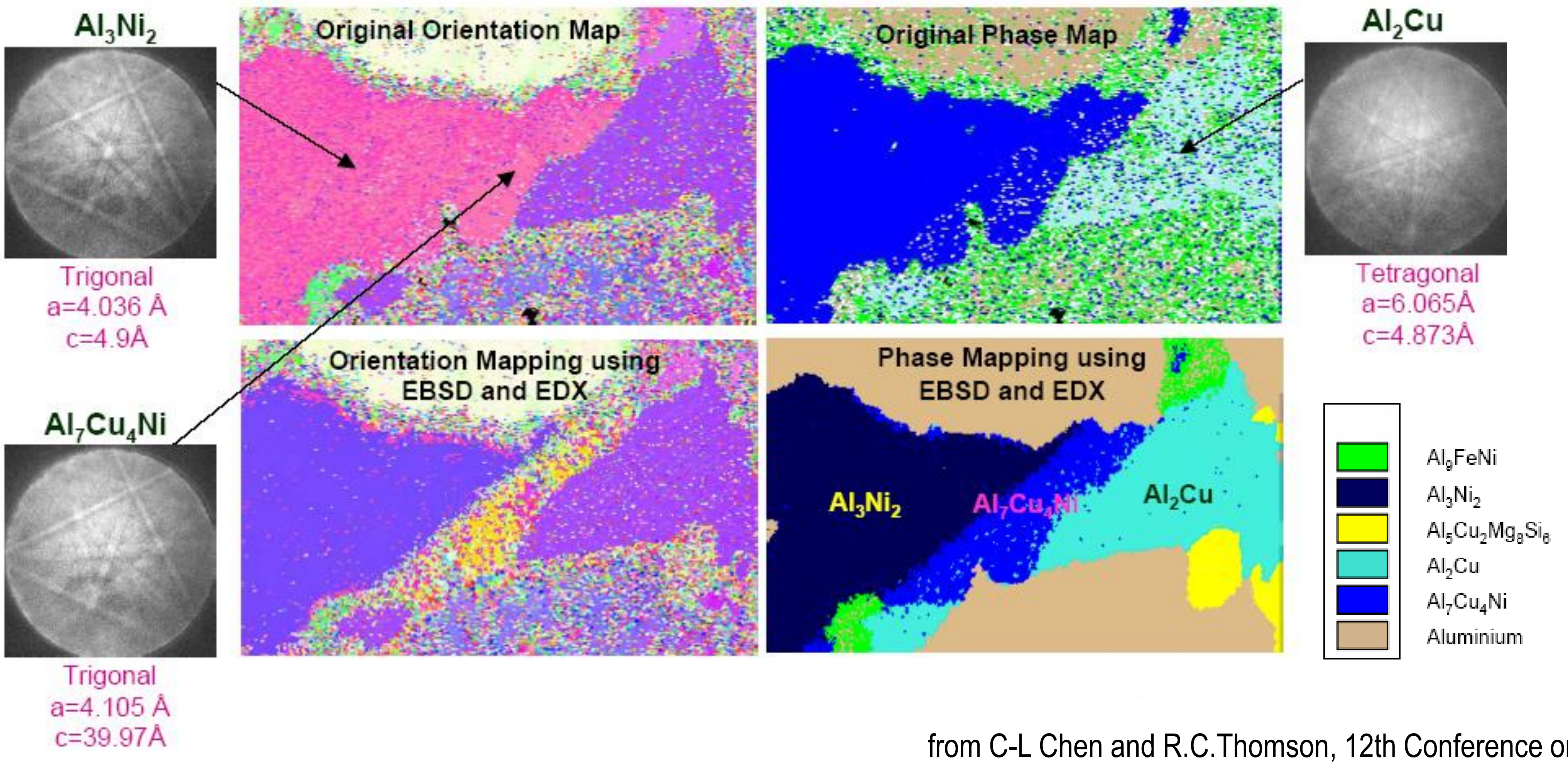


Spatial correlation of different phases





EBSD analysis: showing similar correlations



from C-L Chen and R.C.Thomson, 12th Conference on EBSD at the University of Manchester, April 2005

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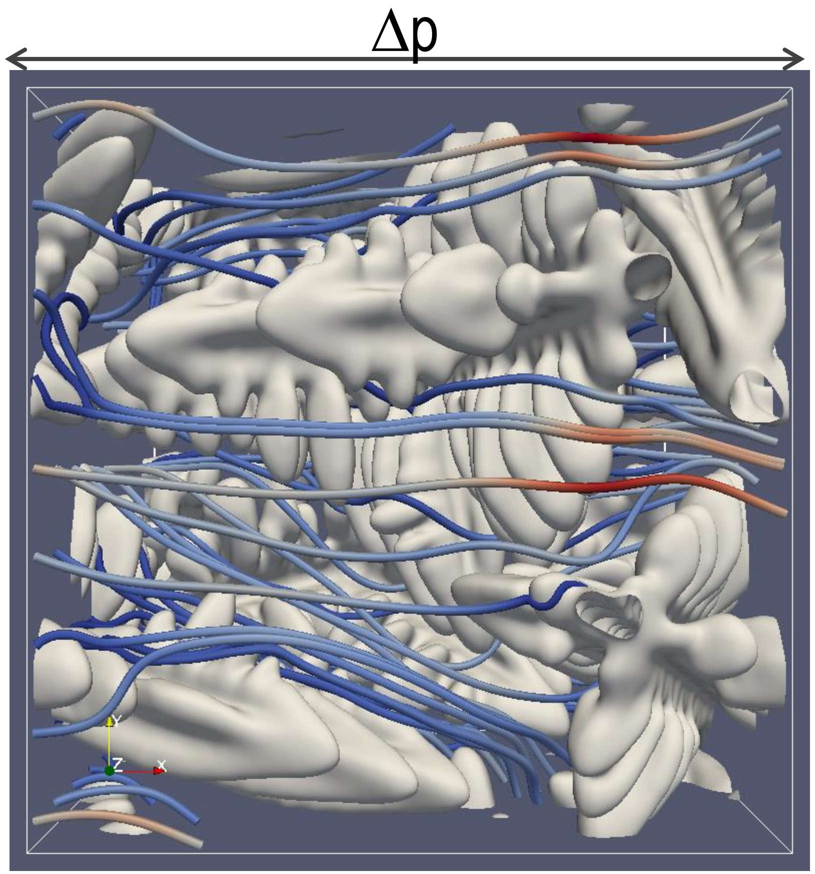
Permeability of a mushy zone

Permeability is an important input for:

- macroscopic simulation of melt flow, e.g. as boundary condition for the mushy region
- parameter for casting defect models (hot cracking, freckles, pores, …)

But: Permeability is notoriously difficult to measure, mushy zone morphology is highly time dependent

➡ **Simulate it!**

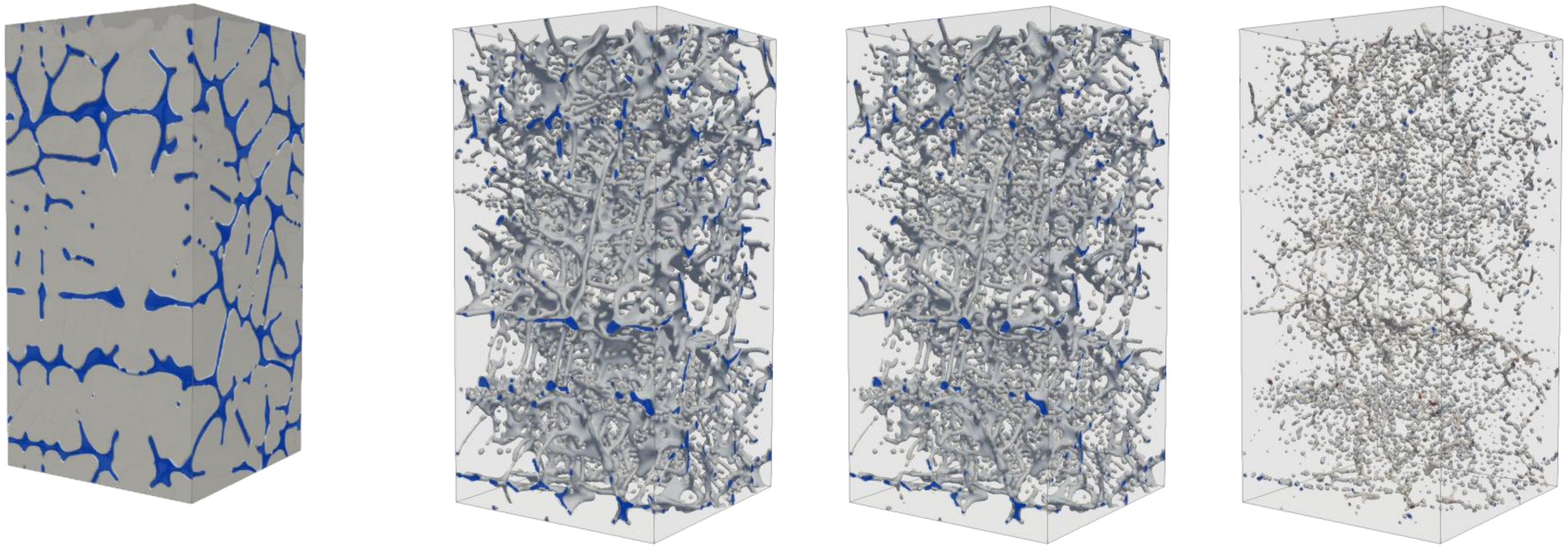


$$K = v \cdot \mu / \Delta p$$

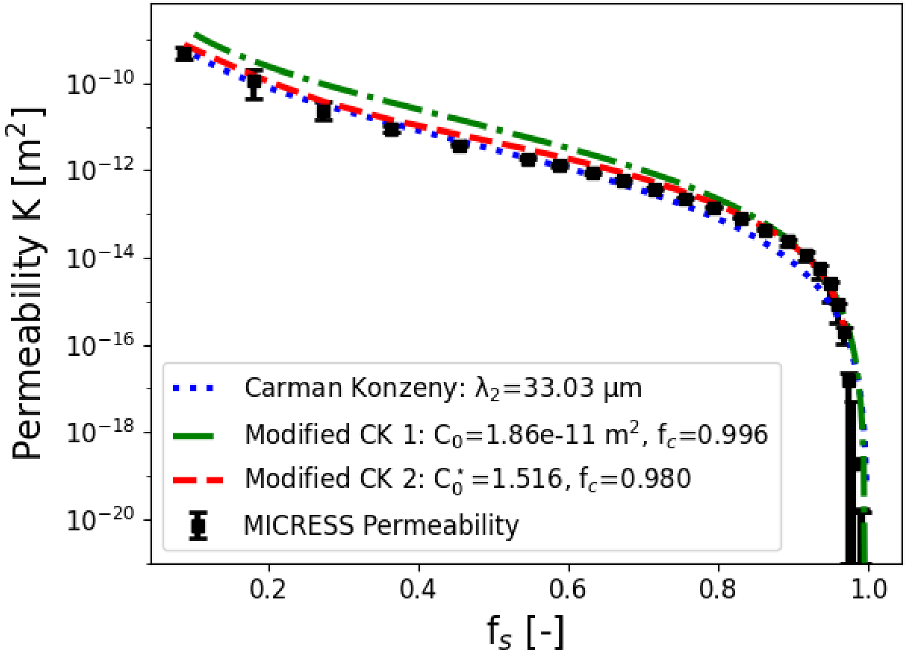
Calculation of melt flow permeability

academic example: AlCu2

$$\mathbf{k}_\mathrm{i} = c_0^* \cdot \frac{(f_c^* - f_s)^3}{\tau_i^2 \cdot S_V^2}$$



f_s=0.793 f_s=0.935 f_s=0.949 f_s=0.983



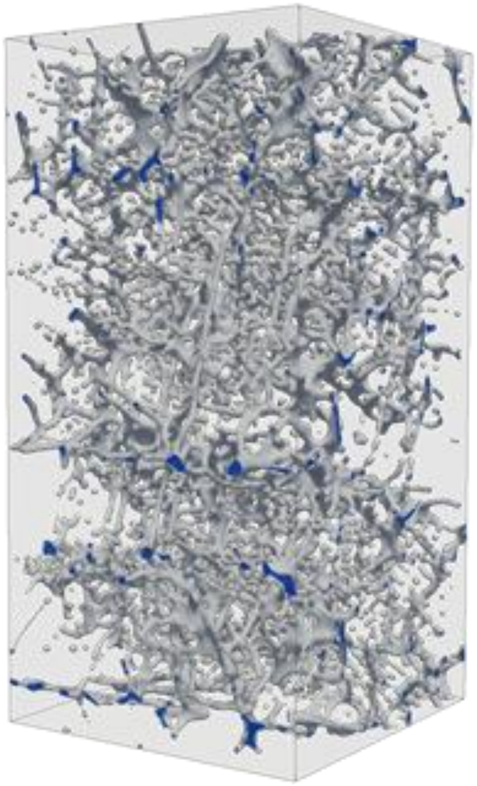
no continuous flow path above a critical solid fraction < 1

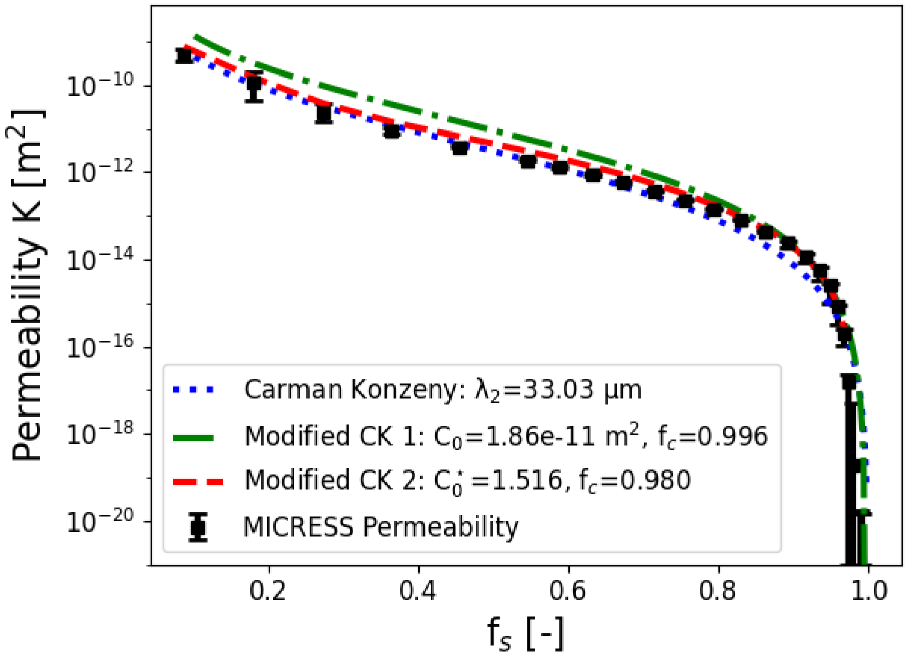
e.g. R. Berger, M. Apel, G. Laschet, Materialia, Vol.15, 2021, 100966

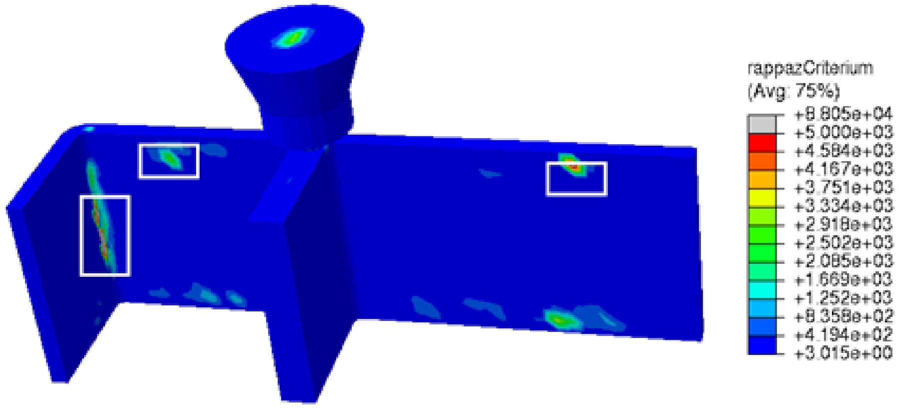
access

RDG-criteria for hot cracking

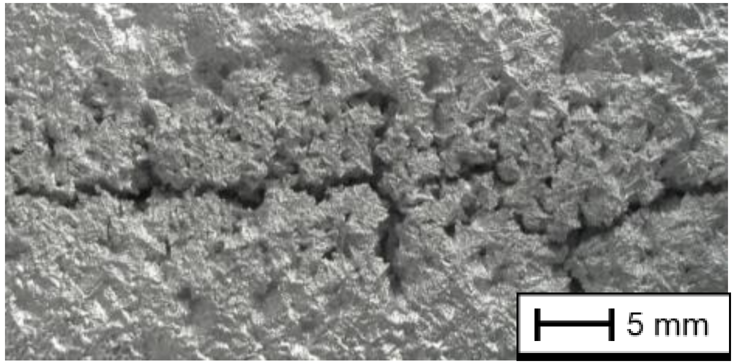
permeability and fs-curve from PF simulation → RDG-criteria implemented in FEM casting sim.





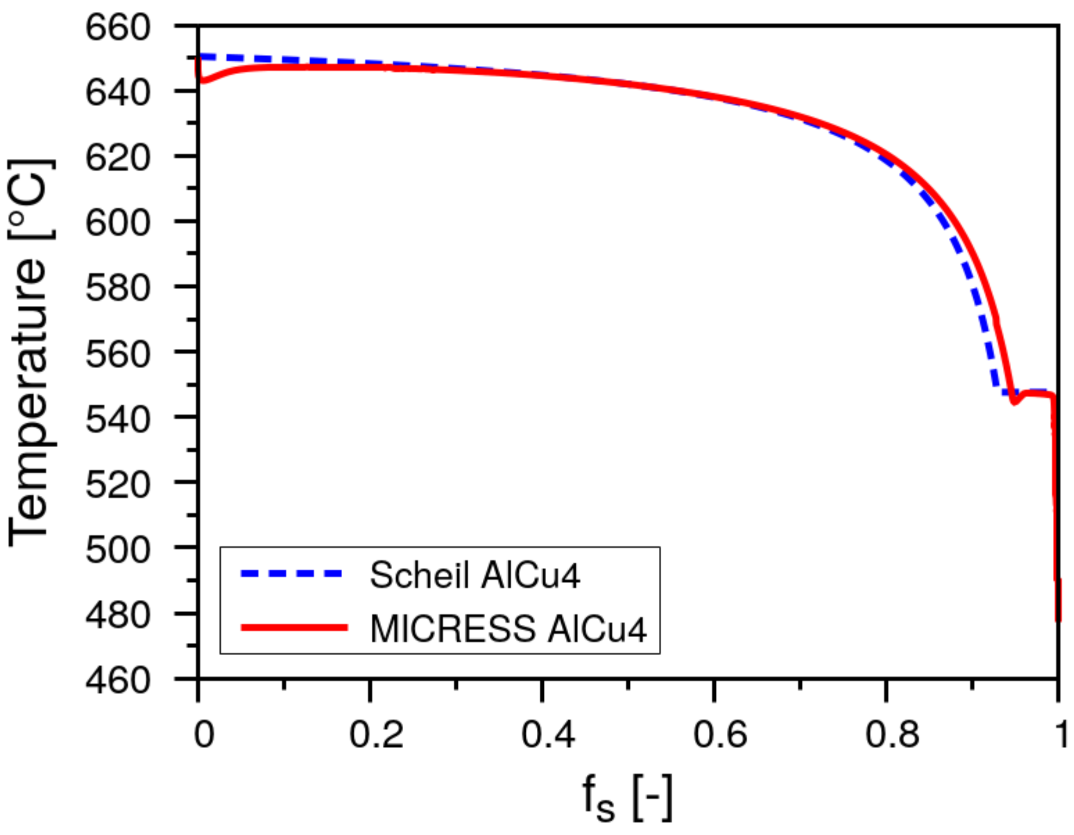


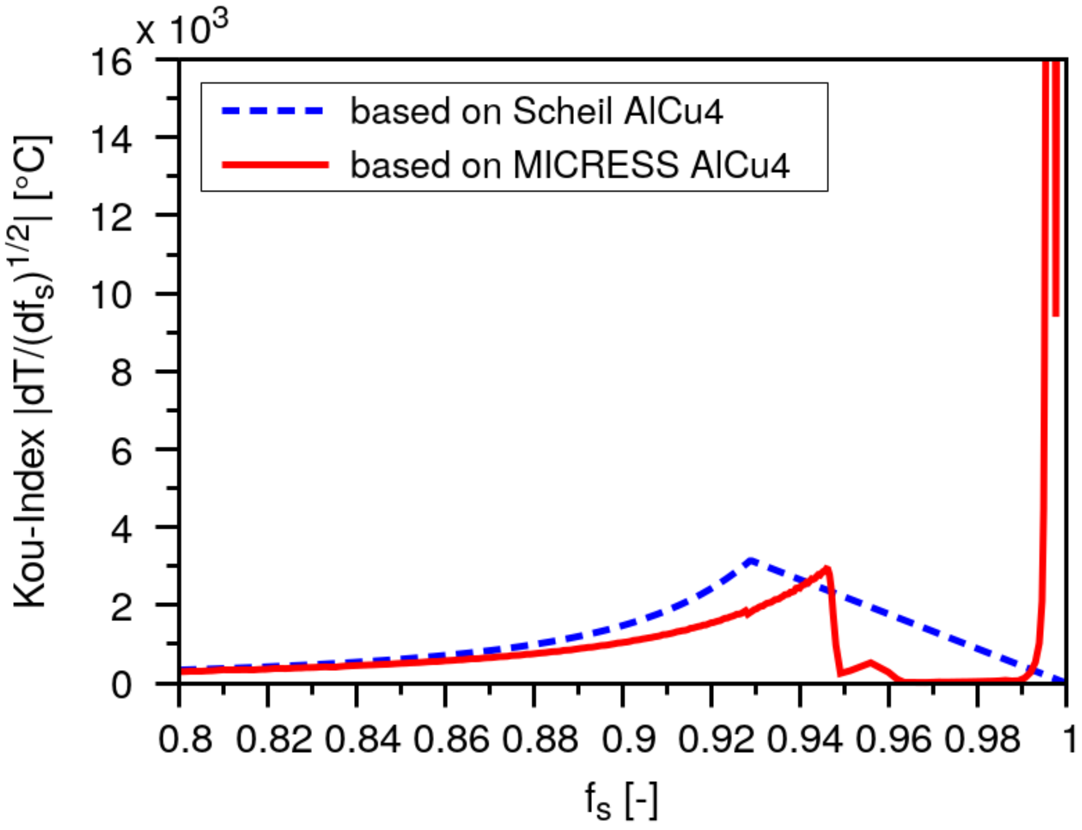
sim. by S.Gor (GI, RWTH Aachen)



Kou-criteria for hot cracking

Kou-index based on f_s curve from Scheil → independent from cooling rate or nucleation undercooling





➡ Kou-index from PF-simulations shows a different magnitude and a different critical f_s

S. Kou, Acta Mater., vol. 88, pp. 366–374, 2015

access

- **CALPHAD informed phase field simulations can provide useful microstructure information, e.g.:**
  - input data for process simulations → solidification path beyond Scheil, H(T), mushy zone permeability, …
  - element distribution / microsegregation → input for heat treatment simulations
  - nature and distribution of phases → quantitative information

Simulations done with: micress® www.micress.de www.thermocalc.se

Financial support from the Deutsche Forschungsgemeinschaft (DFG) in the framework of SFB1120 is highly acknowledged