Modelling of microstructures during in-situ alloying in additive manufacturing for efficient material qualification processes

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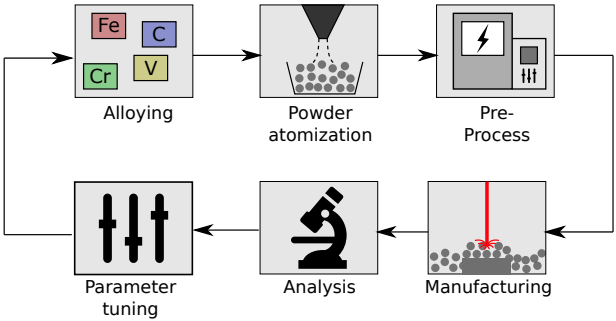
15th September 2021

Outline

Introduction

Material qualification in metal-additive manufacturing

- Empirical material qualification is usually costly and tedious



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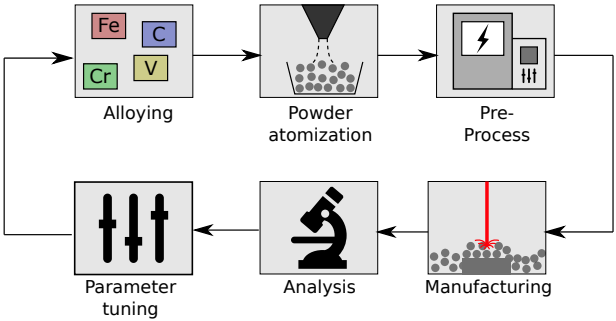

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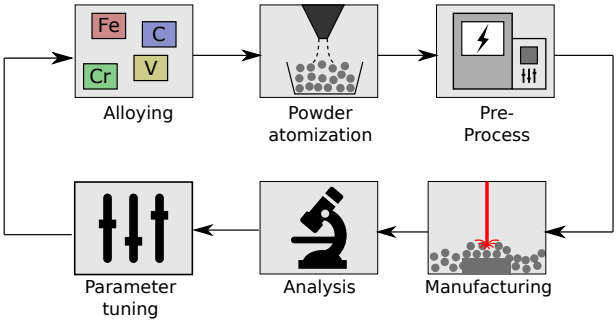

Material qualification in metal-additive manufacturing

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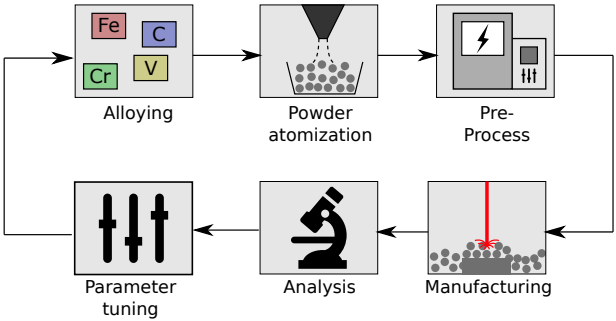
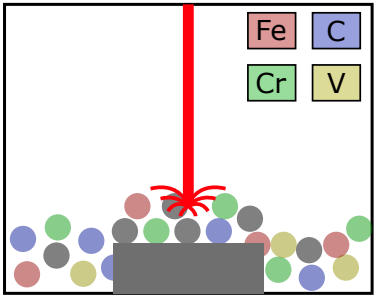
- Though still the way of preference due to lack of viable alternatives
- Final morphology of microstructure is essential for mechanical performance
- Simulation can help, but requires careful attention and tuning



In-situ alloying

- Process of fusing and mixing elemental powder feedstock during melting



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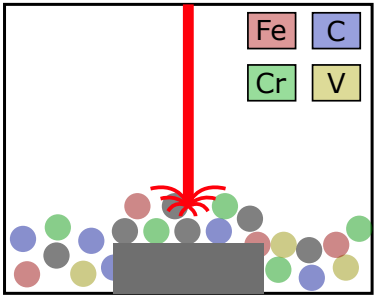

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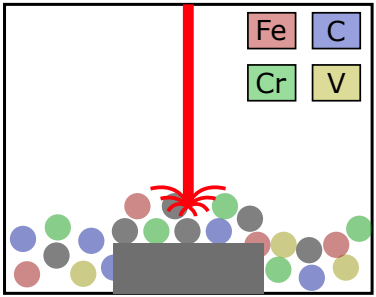

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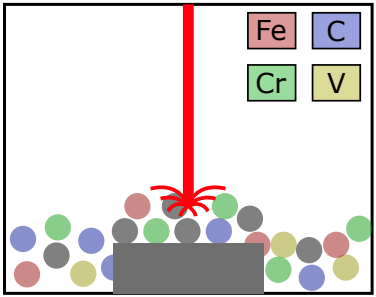

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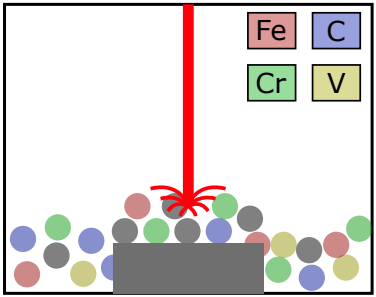

How can this favorable process be modelled, considering the additional model complexity?

Theory and Methods

The Phase Field Method

Basic thermodynamic description of the system: Helmholtz functional $\mathcal{F}$:

$$\mathcal{F} = \iiint_{\Omega} \{\underbrace{f(\phi, C_j, \mu_j, T)}_{\text{energy density}} + \underbrace{\frac{\alpha^2}{2}\Gamma(|\nabla\phi|, \theta - \psi)}_{\text{Dendritic anisotropy}} + \underbrace{sg(\phi)|\nabla\theta|}_{\text{grain growth}} + \underbrace{\frac{\epsilon^2}{2}h(\phi)|\nabla\theta|^2}_{\text{grain boundary motion}} \quad dV \quad (1)$$

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Substitute a thermochemical sub-model for $f(\phi, C_j, \mu_j, T)$:

$$f(\phi, C_j, T) = \sum_{j=1}^{N} C_j[\mu_j(\phi, T) + RT\ln(\frac{C_j}{\rho})] \quad (2)$$

The Phase Field Method

- By taking the variational derivative, we obtain conservation equations for the model variables, e.g. for orientation:

$$\frac{\delta \mathcal{F}}{\delta \theta} = P(\epsilon|\nabla\theta|)\tau_\theta \phi^2 \frac{\partial \theta}{\partial t} - \nabla \cdot \left[\phi^2 \left(\frac{s}{|\nabla\theta|} + \epsilon^2 \right) \nabla\theta \right] \tag{3}$$

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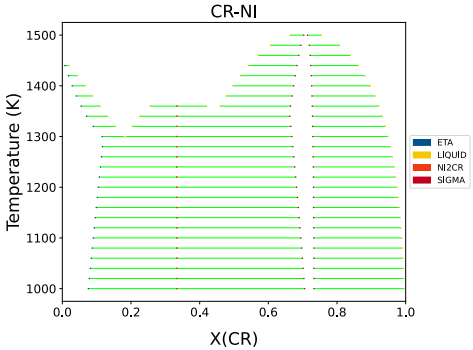
- Another established method to solve this problem is the multiphase field method. However, we would end up with at least 11 coupled equations to be solved.
- Since we now track concentrations additionally, we need the respective chemical potentials $\mu_j(\phi, T)$ as input. How can we obtain those?

The CALPHAD Method

- CALPHAD (**Cal**culation of **Pha**se **D**iagrams) is a method to obtain thermodynamic information based on experimental data



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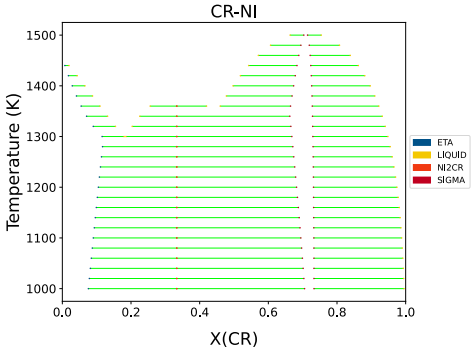

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The CALPHAD Method

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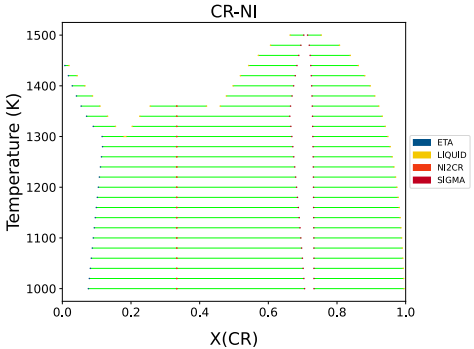
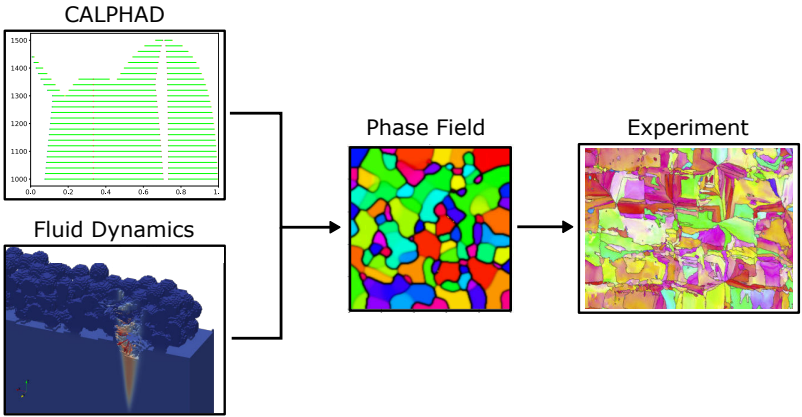
- Analytical assembly of mixture properties and configuration spaces, e.g. for Gibbs energy from two phases A and B:



$$G_m = x_A G_A + x_B G_B + x_A x_B L_{AB} + RT(x_A \ln x_A + x_B \ln x_B) \tag{4}$$

The Overall ICME Workflow



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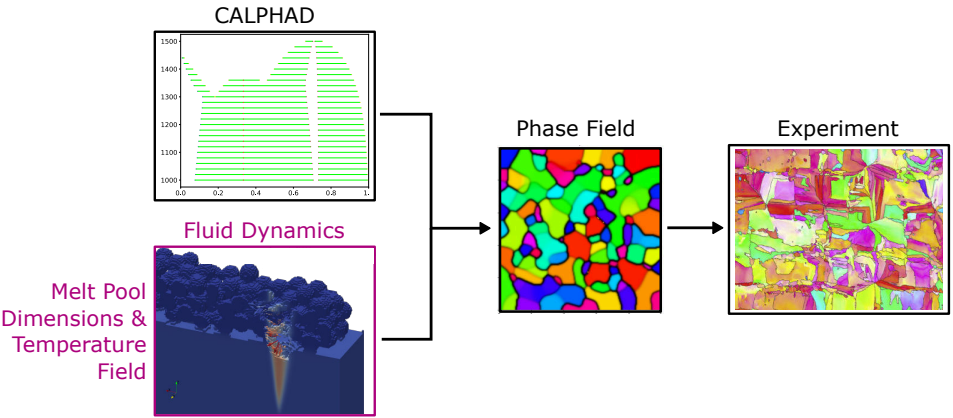

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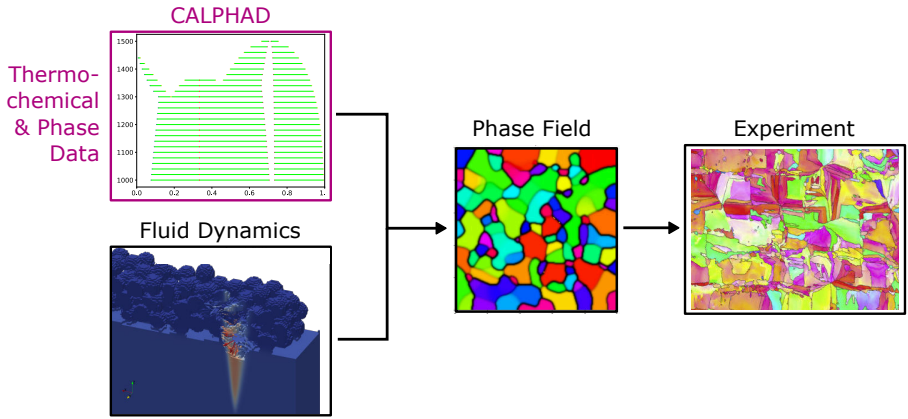

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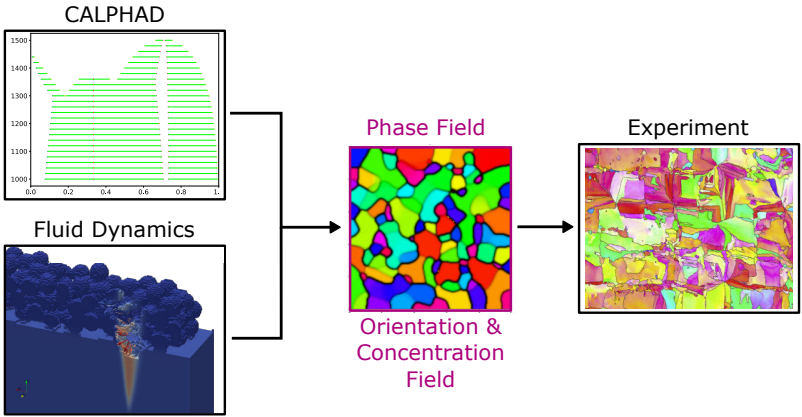

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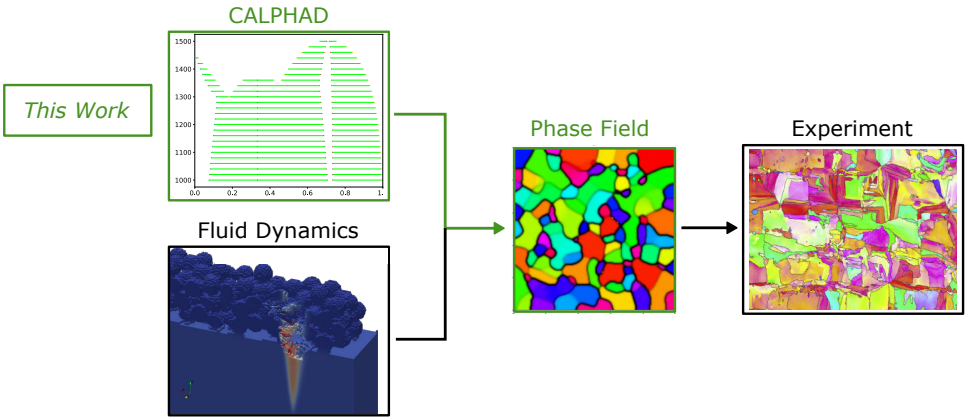
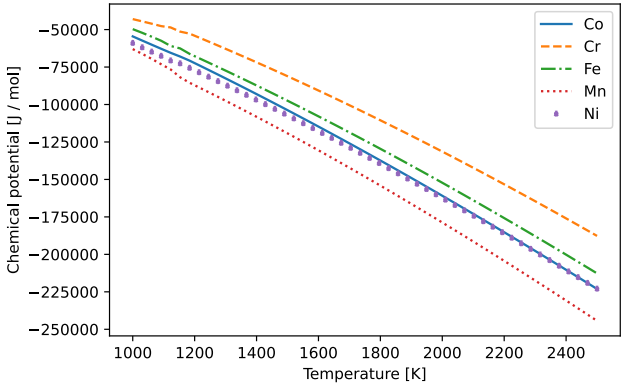


Results

CALPHAD simulation of the CoCrFeMnNi system

- We sample the configuration space of the equiatomic system with 6 possible phases in total



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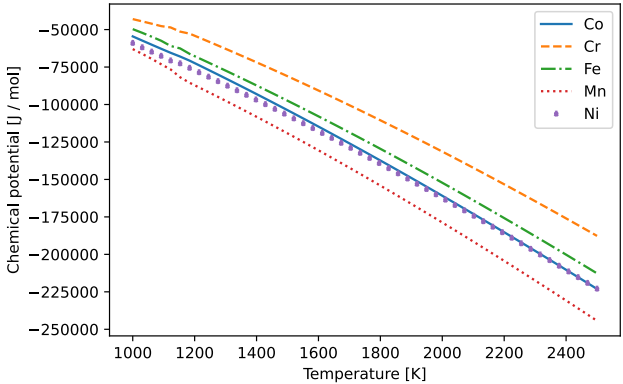

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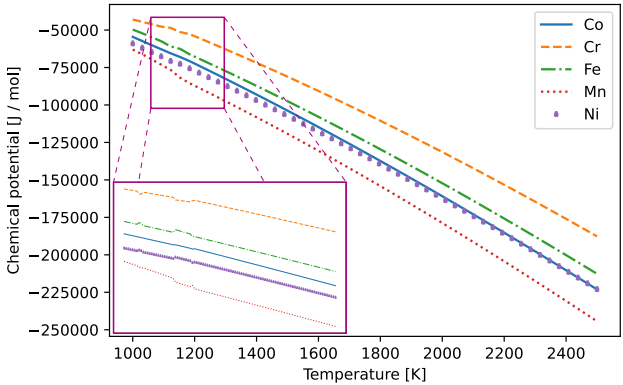
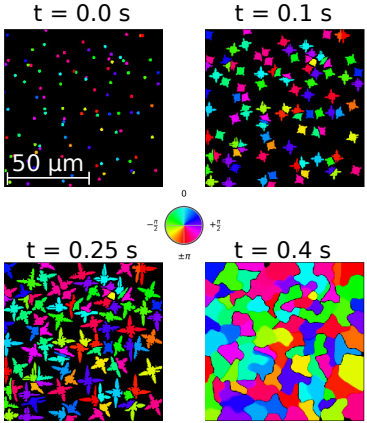


Transient phase field simulation

- We use the Finite Volume Method on a 100 x $100\,\mu\mathrm{m}$ grid with $\Delta x = 0{,}25\,\mu\mathrm{m}$, $\Delta t = 0{,}5\,\mathrm{ms}$ and $\Delta T = 100\,\mathrm{K}$



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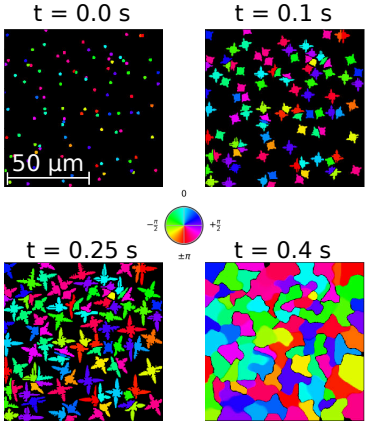

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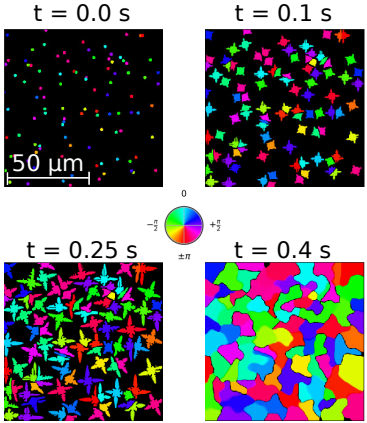

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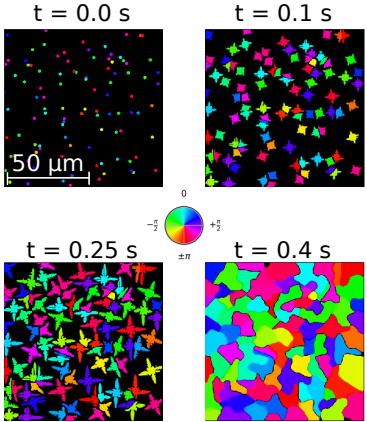
- Grains impinge and form irregular structures
- Final structure further evolves through grain coarsening and rotation



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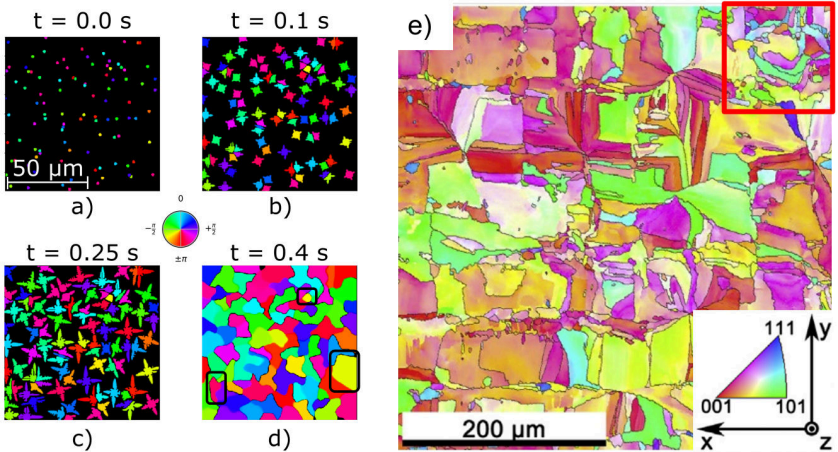
Outlook

- Improve on computing performance - There are better numerical methods than Finite Volume with regards to parallelizability
- Work on coupling with thermo-fluid-dynamic submodel for temperature input, i.e. field transfer from existing self-developed OpenFOAM solver

Thank you!

Questions?

pzimbrod.github.io


t = 0.0 s
t = 0.1 s
50 µm
a)
b)
0
$-\frac{\pi}{2}$
$+\frac{\pi}{2}$
$\pm\pi$
t = 0.25 s
t = 0.4 s
c)
d)
e)
111
y
001
101
x
z
200 µm

Computational effort

Hardware Setup

- Intel Xeon W-2295: 18C/36T @ 3.00 GHz
- 128 GB RAM

Resource Consumption

	CALPHAD	Phase Field
Parallelization	None	OpenMPI
Solution time	10 s	200 min
Memory usage	30 MB	2.5 GB